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Foreword

Dear Reader,

it is with great honor that we present this collection of papers from the XXII B-MRS Meeting, held for the first time in Santos, SP, Brazil. Since its inception in 2002, this event has become one of the most significant scientific meetings in Brazil and is increasingly gaining prominence in the global materials science community.

During five intense days of conferences, relevant topics were discussed, courses and technical lectures were offered, and recent research results carried out collaboratively in research institutions around the globe were presented. We had the opportunity to share experiences, knowledge, and our passion for science, stimulating new studies and discoveries in this vibrant and stimulating area. The event was attended by researchers from 36 countries across four continents, and 24 of the 26 Brazilian states.

Materials science plays a fundamental role in all sectors of society, characterized by its plurality, interdisciplinarity, and multidisciplinarity, impacting the lives of billions of people globally. The topics studied range from nanoscale structures to mechanical, electrical, optical, and magnetic properties of materials, as well as interactions with biological systems, supramolecular properties, and computational simulations.

We recognize that materials science is constantly evolving, rapidly facing new challenges as well as changes occurring in our society and the environment, including sustainability and climate change issues. Our responsibility extends to presenting innovative solutions and proposing new paradigms in this context. The event also promoted the construction of scientific leadership, connections, and collaborations, in addition to valuing the participation of students, who are the future generation of scientists More than that, we took the opportunity to discuss technological innovation, entrepreneurship, scientific communication, and gender diversity in our research area.

We hope that this collection will inspire and contribute to the advancement of materials science, promoting a more sustainable and innovative future. We would like to thank all the participants for their presence, especially our collaborators, volunteers, symposium organizers, and sponsors.

Thank you, and we look forward to seeing you at the next edition of B-MRS.

Laura Péres and Lucas Fugikawa-Santos

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Summary

Nanomaterials Mimicking Cell Membranes

Memorial Lecture

Here comes the Sunlight

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My scientific activity has been mostly focused on semiconductor physics, particularly on "defects" - impurities and/or misplaced atoms that alter the behavior of the original crystal, negatively or positively. In my presentation, I will briefly review our first published results of inorganic crystals, followed by our studies of organic polymers (where "defects" are inherently present), and finally, organic-inorganic composite systems. These studies explore the electronic and optical properties of such materials. The ever-present discussions in our community, which I find truly enjoyable, have led me to focus on light-matter interaction, specifically studying materials that capture sunlight and can transfer energy in a controlled manner, that is, the photovoltaic path to clean energy.
Acknowledgements: IF-USP, IFGW-UNICAMP; Computational access CINECA-HPC Europe, CENAPAD Brazil, LCCA-USP, CCE-USP; Main research support INCT-INEO, CAPES, CNPq, FAPESP.

Plenary Lectures

Control of Self-Assembly of Solution Processable Semiconductors for Electronic Applications

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The self-organization of solution processable semiconductors plays a critical role in determining the charge transport properties of these materials. This is because the morphology and molecular order of the semiconductor film, which is formed during the solution deposition process, directly influences the efficiency of charge transport within the material. In particular, the self-assembly of semiconducting molecules or polymers into ordered structures, such as crystalline domains or nanofibers, can significantly enhance the charge carrier mobility and reduce the likelihood of charge trapping. The ordered structure provides a continuous pathway for charge transport, while also minimizing the number of defects and disorder within the material. The self-assembly of solution processable semiconductors can be controlled by the processing conditions. Thereby, it is a challenge to control the organization locally at the scale of few Å as well as macroscopically over several µm in the semiconductor thin film to favor the charge carrier transport between the electrodes in the device. Overall, the role of self-organization in determining the charge transport properties of solution processable semiconductors is a crucial factor in the development of high-performance electronic devices. By understanding and controlling the self-assembly of these materials, it is possible to optimize their performance and enable the development of new and advanced electronic technologies.

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Emerging materials for next generation energy technologies

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Our research aims to address Sustainable Development Goals n.7 (clean and affordable energy) and n.12 (responsible consumption and production). We study structure property/relationships in emerging materials, enabling the design and synthesis of systems that exhibit multiple functionalities. Such systems are then used as building blocks for the fabrication of next generation energy devices. We focus in particular on recent developments in solar technologies that aim to address the energy challenge, aiming to replace and/or recycle critical and toxic elements towards sustainable technologies. [1-21].

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Ionic liquids as versatile compounds for polymeric materials and nanocomposites

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Ionic liquids are considered versatile compounds that find promising applications in several fields of material science due to their unique properties such as low pressure vapor, low melting point, non-flammability and good ionic conductivity. This presentation will focus on the use of these compounds as additive in conducting polymeric nanocomposites. The ability of ionic liquids as dispersing agents for CNT and graphene nanoplatelets contributes for achieving higher electrical conductivity for applications as microwave absorbing materials and epoxy-based anti-corrosion coatings. For the first topic, polymer composites loaded with dielectric (nanocarbon materials, conducting polymers) were preferred due to their easy processability, flexibility, cost effective production, corrosion resistance and low weight. The efficiency of ionic liquids combined with other materials on the corrosion resistance of epoxy coatings will be also discussed. Additionally, ionic liquids are also employed on the synthesis of nanoparticles involving silica, organic modified silica and titania. Due to the ionic characteristic, ionic liquids are able to improve the polarizability of these nanoparticles, enlarging their application as electrorheological fluids.

Fundings: CNPq; FAPERJ.

Lithium-ion Batteries in the Future Energy Transition

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Since their first commercialisation in Japan in 1991 lithium-ion batteries (LIB) have gained an impressive market growth to reach above $100B in sales in 2023. The LIB' commercial success comes along with outstanding performances in terms of energy density (smaller, lighter), power density (fast charge and discharge), lifespan (5 to 10 years), safety (lower risks of thermal events), costs ($120-$200/kWh), environmental friendliness and recyclability. Continuous improvements over the years of the LIB performances resulted from a tremendous academic and industry research effort to conceive new materials for anode, cathode and electrolyte together with cells engineering and design. There are three major market applications of LIB: mobile electronics (cell phones, cordless tools...), energy storage (renewable energy, homes, buildings...) and electric mobility (cars, buses, 2-wheelers, boats, drones...). Electric mobility is the fastest growing market since most of worldwide vehicle's manufacturers are moving toward electric traction vs. conventional thermic systems. For the next decades the demand for Li-ion batteries is anticipated to increase dramatically, with a GWh requirement that will rise from over 880 GWh in 2023 to around 4.7 TWh by 2030, 4.3 TWh of which is expected to go to the electric mobility sector.
Such a market trend requires more and more natural resources to be used in the LIB industry such as lithium, graphite, cobalt, nickel, manganese, iron, phosphate and fluorine. In fact, Brazil ranks among the top five largest world natural reserves in iron, graphite, manganese, aluminum and lithium. No wonder announcement of Brazil hosting the first LIB GigaFactory in Latin America has been made. Brazil is expected to lead the LIB industry locally. This presentation will review the LIB status and future perspectives with a special emphasis on the ultra-fast charging technologies for electric vehicles such as non-linear voltammetry will be presented and discussed.

Paper as a sustainable material to develop smart electrochemical (bio)sensors with unprecedented features

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As reported in my review entitled “Electrochemical paper-based devices: When the simple replacement of the support to print ecodesigned electrodes radically improves the features of the electrochemical devices” published in Current Opinion in Electrochemistry SI: Emerging Opinions (2022) [F. Arduini. Curr. Opin. Electrochem. 2022, 101090]: “Paper-based electrochemical (bio)sensors have emerged as highly attractive analytical devices for their superior sustainable features, such as avoiding the use of polyester as support and the reduction of waste, being incinerated after use. However, paper-based electrochemical (bio)sensors have recently demonstrated further advantages, including the simple combination with vertical microfluidics and their use as a reservoir to deliver smart electrochemical (bio)sensors able to i) contain the reagents, ii) preconcentrate the target analyte, and iii) synthe the nanomaterials inside the paper network. Furthermore, these devices have demonstrated their ability to overcome the limitations of the other printed electrochemical sensors in the measurement of entirely liquid samples by detecting the target analyte in the aerosol phase or solid sample, without the additional sampling system. These achievements highlight their valuable and varied advantages in the sensing sector”.
In this plenary lecture, I will report on the roadmap research activity carried out in the last 8 years related to the development of paper-based electrochemical (bio)sensors for delivering smart lab-on-a-chip-on-paper with unprecedented features, overcoming also the limitation of polyester-ceramic-based printed (bio)sensors.

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Horizon Europe Reliance Project grant agreement N. 101058570, Horizon Europe EIC 2023 Pathfinder Open Phoenix-OoC grant agreement N. 101130395, PRIN 2022 Smartmask4CF

Photonic and Magnetic Nanostructures for Applications in Energy and Biomedicine

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This presentation will describe the fabrication and characterization of a variety of photonic and magnetic nanostructures and their emerging applications. Examples will include various photonic nanostructures (e.g., nanostars and nanospheres with and without core-shell architectures) having near-infrared extinctions for photothermal enhancement of materials performance. The presentation will also describe biocompatible iron oxide nanoparticles (e.g., nanocubes and nanospheres with and without core-shell architectures) having tunable particle and crystallite grain es with magnetic tunability between single-domain and multi-domain regimes, allowing precise manipulation from the ferrimagnetic to the superparamagnetic state. Details of the synthesis of these materials will be discussed along with details of their structural characterization, properties characterization, and stimuli-driven materials performance. The exploration and development of these nanoparticle systems will not only expand our fundamental understanding of the relationships between nanoparticle structure/composition and their response to external stimuli, but will also lead to advances in nanoparticle-based applications in energy and biomedicine.

AC01-In situ/operando nanomaterial characterization: from a better control of the functional matter synthesis to its optimized device integration

In situ liquid phase transmission electron microscopy: from biomaterials to electrocatalysts

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Direct probing of dynamical processes at the nanoscale is key to move forward in the comprehension of formation, degradation and catalytic mechanisms of biological and synthetic materials. Furthermore, a deepened understanding of such processes in realistic synthesis or functioning conditions is crucial to improve their production and implementation methods in functional devices. Thereby, the development of *in situ* and *operando* characterization techniques arises as a logical step in the advancement of material sciences. *In situ* liquid phase transmission electron microscopy (LP-TEM) is part of the thriving characterization techniques allowing real time monitoring with nanometric resolution of processes taking place in liquid environments. Herein, we will show some examples of how *in situ* LP TEM have brought light to new aspects of the behavior of materials in their formation and working environment. In a first instance, we show the formation kinetics of gold NPs affects their and density on Tobacco Mosaic Virus (TMV). Then, we have investigated whether MoS2 nanosheets pose a potential hazard to the lung environment and how it can be related to the fate and biotransformations of these nanomaterials over 1 month. To do so, we traced the mechanisms of nanotransformation of MoS2 patches in intracellular biomimetic media using *in situ* LP-TEM. As a last example, we will discuss some preliminary results of our current research regarding the study of electrocatalysts for electrolyzers and fuel cells. In this study we have implemented a complementary methodology to track the precipitation of Ni(OH)2 on top of Pt nano-assemblies using electrochemical LP-TEM, which allowed to verify the growth of a layer around the Pt nano-assemblies during cyclic voltammetry and have correlated to other microscopy techniques such as interferometric optical microscopy and scanning transmission x-ray microscopy allowing to paint a multi-scale picture of the reaction.

Magnetic Fluorescent Nanofluids Obtained By A Colloidal Approach

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Magneto-photoluminescent nanomaterials have emerged as highly appealing systems and have usually been elaborated based on single nanoparticle strategies. Here, we propose a novel method involving the colloidal assembly of carbon dots and magnetic nanoparticles, achieved by adjusting the surface charge of individual components, to produce fluorescent magnetic liquids [1, 2]. Investigating interactions in aqueous dispersions of nitrogen-rich carbon nanodots and ferrofluids based on core@shell nanoparticles through zeta potential experiments, we achieve colloidal stability by fine-tuning pH and ionic strength. The nanofluids are characterized by multiscale analysis using optical microscopy and SAXS experiments, demonstrating their long-term colloidal stability, even under external magnetic field. The magnetic and optical properties were investigated by SQUID magnetometry and fluorescence spectroscopy. Additionally, we assessed the capability of the nanofluids for magneto hyperthermia. The saturation magnetization and the magnetic interactions between magnetic particles are not altered by the presence of the carbon dots. Although we observe fluorescence quenching due to the presence of the magnetic nanoparticles, fluorescence tunability is preserved at the same wavelength as the carbon dots dispersions. The systems also maintain their heat generation efficiency, showing possible use in magneto hyperthermia-based therapy.

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Exploring the impact of Zeolitic Imidazolate Frameworks (ZIF) on Membrane Performance

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Composite membranes, formed by combining multiple materials to leverage the unique properties of each component, offer enhanced performance and versatility in water purification and separation processes. They could potentially provide several advantages over traditional membranes, including higher flux rates, improved selectivity, and greater resistance to fouling and degradation. An emerging advancement in composite membrane technology involves the integration of Zeolitic Imidazolate Frameworks (ZIF), aimed at enhancing water permeability. In this study, ZIF-8 was synthed and incorporated into polyethersulfone (PES) membranes at concentrations of 0.5% and 1%. The objective was to investigate the dispersion of ZIF-8 into the casting solution, evaluate membrane morphology, and determine water permeability. Dynamic Light Scattering (DLS) analysis revealed that ZIF-8 nanoparticles could be better suspended in the casting solution with the addition of PVP 1%. Specifically, the water permeability of the membranes varied with the concentration of ZIF-8, with values of 9±3.3, 11.4±7.7, and 7.4±3.7 L/m^2.h.bar for the pure membrane, membrane with 0.5% ZIF-8, and membrane with 1% ZIF-8, respectively. These results indicate that the water permeability can be modulated even in the presence of ZIF-8, highlighting the potential for tailored membrane performance in water treatment applications. Further research is necessary to optimize the synthesis and integration processes to maximize the benefits of ZIF-based composite membranes.

In-situ Synchrotron Light Studies of Cobalt Ferrite and Cobalt(II) Oxide Synthesis via the Polyol Method: Uncovering Mechanistic Complications and Pre-nucleation Cluster Presence through Continuous XRD and SAXS Monitoring

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The fabrication of cobalt ferrite (CFO) and cobalt (II) oxide (CO) nanoparticles (NPs) via the polyol approach has attracted significant attention due to their promising utility across various domains including catalysis, electronics, biomedical engineering, and magnetic materials science. A thorough understanding of the synthesis dynamics is imperative for fine-tuning the synthesis parameters accurately. In this study, we utilized synchrotron radiation X-ray diffraction (XRD) and small-angle X-ray scattering (SAXS) techniques at the Elettra synchrotron radiation facility to monitor the real-time formation of CFO and CO during polyol synthesis. By analyzing time-resolved XRD and SAXS patterns, we gained insights into the evolving crystallographic structure and morphological transformations throughout the synthesis process. Our observations unveil intriguing details about the evolution of reactants, including the presence of intermediates such as layered hydroxide salts (LHS) and the emergence of sub-nanometer-scale precursor phases likely serving as pre-nucleation clusters for NP-CFO/CO phases. The results were also treated by means of fine elaboration techniques, such as the Principal Component Analysis (PCA). Tracking these intermediates in real-time enabled us to comprehend their dynamic evolution, providing valuable insights into their formation pathways and growth kinetics. The identification of these intermediates elucidates the complex mechanisms governing the synthesis and represents a pivotal stride toward optimizing polyol synthesis for enhancing the purity and crystallinity of the products. Additionally, these findings offer pertinent details for a more accurate interpretation of the magnetic properties of these antiferromagnetic materials, crucial for mitigating ambiguities, particularly considering the relatively subdued magnetic signal of CO.

Probing Nanoscale Heterogeneity in HER Activity of Mo2C Catalysts via Scanning Electrochemical Cell Microscopy: Insights into Native Oxide Effects

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Molybdenum carbides (Mo2C) have emerged as promising catalysts for hydrogen generation due to their distinctive physicochemical properties.1,2 While numerous studies have investigated the synthesis methods, structural properties, and catalytic mechanisms of Mo2C in electrochemical hydrogen generation, a comprehensive understanding of their behavior at the nanoscale remains elusive. Nanomaterial properties are known to be -dependent; moreover, electrocatalytic activity differs with respect to the structure, e.g.: basal plane vs edge. In this work, we address this gap by a comprehensive investigation of the hydrogen evolution reaction (HER) activity of α-Mo2C crystals with well-defined morphologies, grown via chemical vapor deposition (CVD). Herein, scanning electrochemical cell microscopy (SECCM) was employed to provide nanoscale mapping of HER activity in acidic media. SECCM was previously used to characterize the electrochemical activity of catalysts, solving heterogeneities within individual particles.3 High-resolution HER current maps of single Mo2C particles, ranging from 1 to 40 μm in , were obtained using nanoscale SECCM probes with ~150 nm diameter. Our findings reveal significant variability in HER activity at the sub-particle level, which does not straightforwardly correlate with basal plane vs. edges structures. Specifically, particles smaller than 5 μm exhibit a homogeneous high HER activity at the basal plane, surpassing activity at the edges, whereas larger particles (>5 μm) display lower and heterogeneous HER activity at the basal plane. We attributed this behavior to native oxide formation on lager particles during the CVD growth, as indicated by X-ray diffraction. This study underscores the importance of local characterization of individual Mo2C particles, shedding light on the impact of -dependent native oxide formation and providing insights to guide the optimization of carbide CVD growth methods.

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Role of the Second Metal on Cu Species Evolution and Its Effect on CO2 Hydrogenation Activity

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Thermocatalysis plays a major role in CO2 valorization, notably via methanol hydrogenation, often using Cu/ZnO/Al2O3 catalysts. It has been shown that the interfacial region between Cu nanoparticles and ZnO is the main catalytic site[1,2]. However, recent studies indicate isolated Cu+ sites significantly enhance methanol selectivity and catalyst stability, hinting at a completely new catalytic site for CO2 hydrogenation that has been overlooked[3,4]. We propose a new synthesis method employing molecularly defined bimetallic precursors to provide CuZn and CuZr pairs simultaneously, ensuring spatial proximity from impregnation, increasing the probability of the pairs sticking together after the catalysts' activation protocol. Also, we use 1 wt.% loadings to improve atomic efficiency, promoting isolated Cu, Zn, and Zr sites. We have showed that the second metal influences Cu's electronic properties, fine-tuning catalytic outcomes. Efficient Cu (I) formation from the precursors yields two Cu+ species: one favoring methanol, the other methane, attributed to the stabilization of key reactional intermediates. In this sense, stabilization of monodentate formates promote methanol hydrogenation, while strong CO binding favors methane. We also showed that, H2O and CO byproducts significantly influence Cu speciation, favoring methanol and methane Cu species, respectively. The catalysts are at an advanced stage of characterization, including quasi-in situ XPS, in situ XAFS, in situ DR-UV-Vis, in situ CO-DRIFTS, and operando DRIFTS (250 ºC, 20 bar).

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Shedding light on oxygen vacancy-induced phase transformations of Ti-FeOx using total X-ray scattering

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Oxygen vacancies are the most common defects on reducible metal oxides, which can be associated with both intrinsic and extrinsic point defects. These oxygen vacancies, and their intrinsic oxygen mobility, play a key role in diverse research fields, such as catalysis, sensors, and energy conversion and storage. The addition of dopants into the metal oxide structure can lead to drastic changes in their redox properties by introducing strain and distortions, increasing the oxygen vacancy concentration, and/or enhancing their thermal stability. In this work, we explore the hydrothermal synthesis of $Ti_{1-x}Fe_xO_{2-0.5x}$ nanostructures with different Ti:Fe ratios, aiming for the generation of oxygen vacancies upon the incorporation of Fe atoms into the TiO_2 lattice. XRD and Raman analyses revealed that undoped TiO_2 led to the formation of anatase phase, with crystalline domains of c.a. 7 nm. Fe loadings greater than 10 at.% triggered an anatase-to-rutile phase transition, while Fe loadings greater than 30 at.% induced the formation of particles with the rutile structure. Total X-ray scattering and PDF analysis suggest that the rutile structure contains defects, which we associate with Magnéli-like structures (e.g. Ti_5O_9). Structural defects evidenced by the lattice fringes of the particles, observed by TEM, corroborate these findings. EPR measurements at 5 K and room temperature were employed to correlate the structural changes upon Fe addition to the generation of oxygen vacancies. Moreover, *in situ* hydrothermal total X-ray scattering measurements provided valuable insights into how Fe incorporation impacted the nucleation and growth mechanism of the particles. Our findings present, from an atomistic point of view, the impact of Fe incorporation into the TiO_2 structure, with insights into the material formation, crystallization process, and the relation between Fe loading and oxygen vacancy-induced phase transformations.

Cold H_2-Ar plasma interaction with nickel α-hydroxide as a versatile nanofabrication tool of Ni@C_{gr} nanoparticles

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Fabrication of tailored functional nanomaterials is at the heart of modern nanoscience and technologies. Various solids are required and different fabrication methods are developed for such a purpose. Among these numerous methods, common gas (H2, CH4, N2, NH3, O2, Ar) assisted plasma interaction with given nano (in thickness) substrates has attracted more and more research interest. So, tacking advantageous from their open structure and then their high reactivity, turbostratic disordered single layered nickel hydroxyacetate were produced by forced hydrolysis in polyol and exposed to a cold H_2-Ar (90:10) microwave plasma for different times (from 0 to 10 hours), to study their reactivity toward such reductive conditions. X-ray diffraction and transmission electron microscopy evidenced a quite complex phase transformation kinetics, with the simultaneous production of rhombohedral Ni_3C and cubic NiC_y ($y < 0.25$), the former disappearing in favor of the latter accompanied with a progressive carbon demixing from the cubic nanocrystals, leading to Ni@C_{gr} core-shell nanoparticles. The reaction kineticks was thus followed thanks to a systematic characterization of the as-produced powders after each exposition time.

The obtained results are discussed hereafter, highlighting the role of the organic content of the hydroxide phase, mainly the intercalated acetate ions, which decomposed providing carbon source for carbon implantation in the in situ formed metal nanoparticles.

Enhancing e-tongue Performance through Controlled Metallic Nanoparticle Deposition

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The integration of metallic nanoparticles (MNPs) into (bio)sensors offers a several advantages, including increased surface area, enhanced electron transfer, and improved electric double-layer effects, depending on the sensor architecture, thereby augmenting overall performance. However, achieving reproducible sensing units with consistent MNP incorporation remains a challenge. In this study, we address this challenge by tracking the deposition of MNPs, synthed in the gas phase, onto interdigitated electrodes (IDEs) utilizing a custom-built impedance meter. Our setup enables real-time monitoring of MNP deposition from its very initial stages to the percolation limit. In proof-of-principle experiments, IDEs coated with poly(allylamine hydrochloride) (PAH) and poly(sodium 4-styrenesulfonate) (PSS) films were employed in an impedimetric electronic tongue, successfully discerning human palate flavors and umami-based enhancers. Furthermore, we extend this methodology to tailor IDEs' electrical performance for immunosensors. Despite the inherent challenges in achieving consistent electrical responses, our apparatus demonstrates promising potential for (bio)sensor development, laying the groundwork for enhanced practical applications.

Enhancing Photodegradation of Rhodamine-B with ZnO Nanoparticles: Investigating the Influence of Thermal Annealing Atmosphere on Photocatalytic Activity

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In this study, our primary goal is to evaluate the effectiveness of zinc oxide nanoparticles sourced from two distinct samples in catalyzing photodegradation reactions. Specifically, we aim to understand how the photocatalyst evolves during experimentation. Initially, we synthed zinc oxide nanoparticles using polymeric precursor methods at 400°C for 6 hours. To examine any changes in defects, we subjected the synthed nanoparticles to two different post-thermal annealing processes: one in air and the other in a high vacuum atmosphere at 500°C for 6 hours. X-ray diffraction (XRD) measurements confirmed the presence of the ZnO phase and confirmed the nanoscale of our samples. Further characterization through Fourier transform infrared spectroscopy (FTIR), Raman spectroscopy, and electron paramagnetic resonance (EPR) analysis allowed us to quantify the differences in vacancies and defects between the ZnO sample synthed in a vacuum and conventionally. We then conducted photocatalysis assessments using a Rhodamine B solution at neutral pH, under near-UV lamp irradiation, with a mass ratio of nanoparticles to dye volume set at 1 mg/ml. Impressively, we achieved over 70% degradation of Rhodamine-B within one hour. To investigate potential photo corrosion, we utilized inductively coupled plasma mass spectrometry (ICP-MS) to analyze the solution post-photodegradation for traces of zinc (Zn). This recent fact has been reported in the literature. [1]

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Ferrofluids based on Co-Zn-Cu Mixed Ferrites Nanoparticles for Hyperthermia

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Spinel ferrite nanoparticles are versatile materials that can be used in a wide range of areas. Aiming magnetohyperthermia applications, we present here the study of ferrofluids based on nanoparticles of mixed ferrite of cobalt, zinc, and copper, elaborated to finely tune magnetization and magnetic anisotropy of ferrite magnetic nanoparticles by varying the chemical composition. Indeed, such mixed ferrite nanoparticles could present enhanced magnetic properties for this purpose [1]. These NPs are obtained by hydrothermal coprecipitation in alkaline medium followed by a surface treatment that creates an iron-rich surface layer allowing their dispersions in acid medium [2]. The nanoparticle chemical composition has been determined by chemical analysis using ICP-OES and EDX. This crossed analysis allows us to precisely determine the proportions of core and shell volumes and the stoichiometry of the core materials in all samples investigated here. The crystalline structure and the nanoparticle s were studied by using the XRD. The TEM pictures show their morphology and allow a mean determination, which well matches the one deduced from XRD analysis. An extensive magnetic characterization was carried out using a SQUID magnetometer. The first results show that magnetization and anisotropy can be tuned by the core composition and the core/shell architecture. Additionally, the SAR has been initially measured in few samples showing rather high values when compared to the literature and the value increases with the addition of Zn and Co in the core composition.

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FMR study of the Exchange-Bias effect’s dependence on the Ru layer thickness in Si/Ru/IrMn/Co/Ru(x)/Py/IrMn/Ru multilayer films

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Magnetic thin films are two-dimensional materials with magnetic properties that differ greatly from their bulk counterparts. Their primary investigation motivation lies in their potential application in data storage technology, particularly magnetic recording [1]. This study employs Si/Ru/IrMn/Co/Ru(x)/Py/IrMn/Ru multilayer films, made by two ferromagnetic layers (Co and Py) and two antiferromagnetic IrMn layers. The magnetic interaction between those layers is expected to manifest itself in the exchange-bias effect, which is characterized by an asymmetric displacement in the hysteresis MxH loop [1]. The ferromagnetic resonance spectroscopy (FMR) technique is well established for determining the main parameters of magnetic systems and facilitates the investigation of coupled layers [2]. In that sense, this study aimed to examine the effect of the Ru(x) central layer’s thickness on the exchange-bias effect of the previously mentioned films. By probing the angular dependence of the in-plane resonance fields we found evidence of an in-plane magnetic anisotropy and the corresponding anisotropy constants [3].

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Graphite coated with copper selenide as modifier in carbon paste

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It was insvetigated the possibility of synthesizing graphite covered by copper selenide to be applied as a modifier in a graphite paste electrode. Studies have shown that through electrodeposition it is possible to obtain graphite covered by electrodeposited metals (silver and gold) [1]. Copper electrodeposition on graphite occurs using an aqueous grafite paste containing CuCl2 + NaCl + Glycerol, which is inserted into the tip of a electrode made in a syringe. After electrodeposition, the copper-coated graphite is removed and washed, and reacted with sodium selenosulfate to obtain graphite coated with copper selenide. The electrodeposition process was made by cyclic voltammetry. Factorial planning methods are used to identify which electrodeposition parameters influence the graphite coated with copper. The copper selenide produced will be analyzed using techniques such as X-ray fluorescence spectroscopy, scanning electron microscopy and electrochemical measurements with modified graphite paste (cyclic voltammetry measurements in a solution containing potassium ferrocyanide). Therefore, the search for new and improved materials is an essential part of this line of research, enabling new applications, whether in the development of electrochemical methods or other applications.

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Influence of carbon nanotubes aspect ratio on the preparation and properties of buckypapers

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Multi-walled carbon nanotubes (MWCNTs) have received special attention for the preparation of buckypaper (BP). BP is a thin surface formed by carbon nanomaterials, which can be produced by randomly entangled carbon nanotubes using the vacuum filtration method. The BP presents a highly porous structure, with pores of the order of 10-15 mm, low density, and high electrical conductivity [1]. In this way, the unique properties of the nanostructured film allow good applications as a construction material for aerospace vehicles, body armor, as well as new generation devices and displays. In this work, two MWCNTs with different aspect ratios (S-MWCNT with an aspect ratio of 158 and L-MWCNT with an aspect ratio of 600) were used to prepare BPs. The MWCNTs were characterized by X-ray diffraction (XRD) and Raman spectra. Both MWCNTs showed similar standards in XRD patterns. The main observable difference between the XRD patterns was for L-MWCNT. This sample has a slightly narrower and more intense peak at 25.8°, indicating more walls and a larger diameter, as expected. For both samples, the Raman spectra showed the D and G bands typical of carbon materials. The BPs were prepared using the vacuum filtration method. Obtaining BP consists of dispersing 0.050 g of MWCNT in 100 mL of Milli-Q water and 1 g of Triton–X100® surfactant, with the aid of high-power sonication and using an electrospun blanket of polyacrylonitrile (PAN) as sacrificial material for the formation of the BPs. The buckypapers were characterized by XRD, Raman, and SEM-FEG. The preparation of BPs with L-MWCNT presented greater difficulty, requiring sacrificial material, without which it hinders or prevents the formation of BP. On the other hand, S-MWCNTs facilitate the formation of BPs.

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Influence of the synthesis method for $SrTiO_3$ particles on their adsorption capacity for Cd(II) ions

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Strontium titanate ($SrTiO_3$) has attracted scientific interest due to its physical properties, such as piezoelectricity, high dielectric constant, and high chemical and thermal stability [1]. The synthesis method employed in producing $SrTiO_3$ (ST) plays a crucial role in its adsorptive properties, as it influences the crystallinity, morphology, and particle . Based on this, this study aims to synthe ST and evaluate its adsorption potential towards Cd(II) ions. ST was obtained through various synthesis methods, such as polymeric precursors (MPP), hydrothermal (HT), and microwave-assisted hydrothermal (HTMW) methods. X-ray diffraction indicated that all synthesis methods were effective in obtaining the crystalline phase of ST. Characterization by FESEM showed that particles obtained by MPP exhibited the most distinct morphology, with observed blocks of rigid appearance. BET analyses demonstrated that the formed particles are mesoporous. Adsorption studies revealed that, after 30 minutes of contact, all materials were capable of removing over 70% of Cd(II) ions from an aqueous solution at pH = 7 and an initial adsorbate concentration of 1.5 mg L^{-1}. Therefore, it can be concluded that ST is a promising adsorbent.

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Selective Bioelectrooxidation of Seawater using Artificial Apo-reconstituted Copper Proteins

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Seawater is widely considered an abundant renewable resource for to produce molecular hydrogen and oxygen. However, its practical application is hampered due to chlorine-related competing reactions at the anode. Their significance lies in their improved selectivity and stability, as we reported here for copper(II) porphyrins when conjugate with the cavity of the apo-protein myoglobin shell [1,2]. Our strategy showed significant advances for bioelectrooxidation of seawater (pH 7.6), with the artificial Cu(II) protein having onset potential for OER ~10 mV lower compared to copper(II) porphyrins. The data was also supported by the monitoring of the electronic structure of the redox states Cu+2/Cu+1 by in situ XANES absorption spectroscopy as well as the monitoring of the products of reaction by online differential electrochemical mass spectrometry (DEMS). Our approach also demonstrates the capability of abiological reconstituted copper proteins to be designed for the seawater bioelectrooxidation reaction [3].

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Synthesis of aqueous magnetic fluids via One-Pot approach combining Polyol and Massart's method

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Magnetic fluids (MFs) have been extensively studied in recent decades, and their intriguing physicochemical properties have directed attention towards various applications in science and engineering, such as diodes, cosmetics, and drug carriers[1]. Due to their interesting magnetic properties, magnetic nanoparticles can be used for tumor treatment. It is noted that the use of nanotechnology in healthcare is increasing the need to produce more precise, biocompatible, and low-cost materials. Thus, this work aims to contribute to the understanding of the physicochemical phenomena involving magnetic nanoparticles. By combining two highly relevant methods to understand the morphology, composition, and properties, magnetic core/shell type nanoferrites ($CoFe2O4$) were obtained were obtained through the combination of two well-known methodologies: polyol and hydrothermal co-precipitation[2-3]. The nanoparticles were characterized by X-ray Diffraction, Transmission Electronic Microscopy, Atomic Absorption Spectroscopy, and SQUID to analyze their morphology, composition, specific properties, and magnetization respectively.

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Two Sample Environments for Catalysis Studies at the QUATI Beamline

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QUATI (QUick x-ray Absorption spectroscopy for TIme and space resolved experiments) beamline is designed for perform high-quality X-ray Absorption Spectroscopy (XAS) experiments 1. Employing in-situ/operando techniques to identify the structure of heterogeneous catalysis under operational conditions enables exploration of the often complex structure-property relationships. In this work, we present 2 designs of sample environments to be used at QUATI beamline, which include i) a versatile capillary plug-flow microreactor which mainly aims to reproduce industrial conditions of chemical processes (temperature and pressure up to 1273 K and 20 bar, respectively) to explore: phase transition, reaction kinetics of gas-solid interaction, and heterogeneous catalysis 2 and ii) a spectroelectrochemical cell (SEC) devoted to the study of intermediate temperature solid oxide fuel cell (ITSOFC).

Understanding the Interactions of ZIF-8 with Solvents: Implications for Stability

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Zeolitic Imidazolate Frameworks (ZIFs) have emerged as new materials with numerous applications. Specifically, ZIF-8 has been investigated for applications in adsorption processes, membrane technology, gas separation, catalysis, drug delivery, and sensors due to its microporous structure. Additionally, ZIF-8 nanoparticles have been applied in membrane technology; however, fewer studies have considered the stability of ZIF-8 nanoparticles in the presence of organic solvents used to dissolve polymers for membrane production. In this study, both synthed (ZIF-8S) and commercially obtained samples (ZIF-8C) were characterized through Dynamic Light Scattering (DLS), Zeta Potential (ZP), X-ray diffraction (XRD), Brunauer-Emmett-Teller (BET) analysis, and Scanning Electron Microscopy (SEM) measurements. Although many studies have reported on the chemical stability of ZIF-8, we aim to investigate the impact of water and the organic solvent NMP on the structure of ZIF-8 over time. DLS revealed that the particle of ZIF-8S in water was 183 nm, with a corresponding ZP of -13.2. ZIF-8C exhibited a particle in water of 877 nm, with a ZP of 9.1. XRD analysis confirmed the successful synthesis of ZIF-8S, as evidenced by the presence of similar peaks to those observed in ZIF-8C. However, after 24 hours of stirring in water, the crystallinity of both samples was reduced. Subsequent stirring of ZIF-8S and ZIF-8C in NMP for one hour resulted in observable changes in the crystalline structure, with further alterations becoming more pronounced after 24 hours of stirring. These findings underscore the importance of considering solvent effects on the stability and performance of ZIF-8 nanoparticles, especially in membrane applications.

Voltammetric behavior of a hybrid Cu(II)octa(aminopropyl)silsesquioxane (SCuH) nanomaterial and its interaction with nitrite

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A new compound of silsesquioxane and copper hexaferrocyanide was prepared from octa(aminopropyl)silsesquioxane, resulting in a nanocomposite (SCuH), which was then characterized by different spectroscopic techniques. The cyclic voltammograms of the graphite paste electrode modified by SCuH indicated a redox couple with formal potential (Eθ′)=0.54 V, attributed to Fe2+(CN)6/Fe3+(CN)6, in the presence of Cu (redox couple) . The graphite paste electrode modified with SCuH was sensitive to nitrite concentrations, showing a linear response in the concentration range of 2.0 x 10-4 to 1.0 x 10-3 mol L-1, with a detection limit at and 2.65 x 10-5 mol L-1.

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AC02-Combining characterization techniques to understand and restore Cultural Heritage objects and sites

MA-XRF and MA-XRPD imaging of 15th-20th century painted works of art

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Macroscopic X-ray fluorescence (MA-XRF) and powder diffraction (MA-XRPD) are forms of non-invasive hyperspectral imaging that allow to obtain information on painted works of art, often in the form of elemental or chemical images. By means of these methods the following can be done:

- revisualization of overpainted representations, revealing early stages of the creative process or intentional alterations of the composition done during the lifetime of the artwork;
- (highly specific) identification of the pigment types used and the pigment subtypes present, providing opportunities to study the provenance and authenticity of works of art; and
- identification of the nature and distribution of secondary products, formed on the paint surface by degradation of the original painting materials.

In the past decade we have imaged a variety of (renowned) paintings, mainly in European museums. In a number of cases, macro-scale information was combined with (X-ray based) micro-analysis of paint samples,

After describing the principles of MA-XRF and MA-XRPD and an outlining their strong and weak points, several case studies will be discussed, including (a) imaging the panels of the 15th c. Ghent Altarpiece (~1432) by J. & H. Van Eyck [1], (b) scanning highlights of 17th c. Dutch art such as Rembrandt’s Nightwatch (1643) [2,3] and (c) analyzing the degradation of pigments in Munch’s The Scream (1910?) [4,5].

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A synchrotron radiation study of a 200 year-old Gaylussite ($Na_2Ca(CO_3)2{\cdot}5H_2O$) specimen from Mérida, Venezuela. A historic perspective of its discovery.

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Gaylussite, $Na_2Ca(CO_3)2{\cdot}5H_2O$, was first identified from samples obtained in 1823 by the French chemist Jean-Baptiste Boussingault and the Peruvian mining engineer and chemist Mariano de Rivero. The samples were collected from Laguna de Urao, a salt lake in Lagunillas, Mérida, Venezuela. The new mineral was named gaylussite by Boussingault, in honor of the eminent French chemist. The complex thermal and hydration/dehydration behavior of gaylussite has been the subject of different studies, carried out on synthetic gaylussite.

The specimen ENSMP 37496 (collected in 1823 by Boussingault) was an irregular cylinder-like grey fragment of 1.5x0.5 mm approximately. A small piece was gently ground in an agate mortar and used to fill a 1.0 mm borosilicate capillary. High resolution XPD patterns were collected at the ID22 beamline of ESRF. A Search/Match analysis using the PDF-5+ database and a subsequent Rietveld analysis with TOPAS-Academic indicated the presence of aragonite (29.2%), calcite (2.6%) and, surprisingly, sodium acetate trihydrate (67.9%). The examination of an inner section of the specimen indicated the presence of 46.5% of aragonite, 42.3% of Na(CH3COO)·3H2O, 0.3% of quartz, and 10.9% of gaylussite. Calcium acetate efflorescence has been extensively reported in calcareous museum objects stored for long periods due to the emission of acetic and formic acid from wood (particularly oak) cabinets. Na(CH3COO)·3H2O efflorescence has been reported mainly for glass objects. For comparison, a study of specimen ENSMP 53763 from Lake Magadi (Kenya) indicated that this sample is almost pure gaylussite. The thermal behavior of both samples was studied.

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Heritage Science: Use of multi-techniques and instrumental innovations

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Studies using multi-techniques and new instruments have grown in recent years for characterization of historical-cultural heritage objects. At the Laboratory of Archaeometry and Sciences Applied to Cultural Heritage (LACAPC), mobile instruments have been used routinely, since 2012, to analyze and study objects from museums and collections “in situ”.

The intention of using various analytical techniques is to better understand the materials of cultural heritage objects and the creative processes of artists and thus contribute to the preservation and conservation of these objects. The growing demand for new research in this area leads to the creation of the new Heritage Science Center that is being built at the Museum of Contemporary Art. This center will have multiple analytical facilities and will be the first heritage science laboratory within a Brazilian museum.

The team involved in this project is made up of different professionals from different areas such as Physics, Engineering, History, Art History, Museology, Conservators and Restorers, etc.

Various objects with different supports could be analyzed using imaging and spectroscopic techniques that could provide important information both about the artists' creative process and the existing materials.

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Hydrogels from citrus pectin for cleaning Cultural Heritage objects

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Gels are identified as substances that have great potential for cleaning objects that belong to Cultural Heritage. In this context, this research includes the development of hydrogels based on citrus pectin, with the purpose of application in Conservation and Restoration procedures for cultural assets. The use of citrus pectin to the hydrogels is justified since it is a sustainable and innovative alternative, from an economic and scientific point of view, in addition to being a completely new project in Brazil. The objectives of this work were to prepare, characterize and to evaluate the performance of new hydrogels based on agar agar and citrus pectin as a cleaning material. The hydrogels were applied on different supports, such as paper and metal and characterized using FTIR Spectroscopy, Raman Spectroscopy and Scanning electron microscopy (SEM). The optimal mass proportion was AGAG1 2 wt%, Pc 2 wt % and AC 10% wt%. The results demonstrated the good performance of the hydrogels in removing adhesives from brushed aluminum as well as the preservation of the mechanical properties of them.

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The Influence of Provenance and Material History Studies on Decision-Making for Conservation Treatments: Preserving a Non-Original Coat of Arms on a Frans Hals painting

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In 2022, an interdisciplinary project, led by the São Paulo Museum of Art (MASP) in collaboration with the Frans Hals Museum and two Brazilian universities, the Federal Institute of Rio de Janeiro and the Institute of Physics of the University of São Paulo, focused on studying and treating three Frans Hals paintings from MASP's collection: portraits of Captain Andries van der Horn (1638), Maria Pietersdochter Olycan (1638), and Seated Officer (1631). The project aimed to conduct a comprehensive analysis of the paintings' historical, technical and aesthetic aspects through archival research, scientific analyses, and close examination. Understanding the paintings' history and condition was crucial for accurate diagnoses and treatment proposals.

The portraits of Andries and Maria were created as pendants for their wedding. A 2007 external research identified the coat of arms in Andries' portrait as non-original, a later addition containing Prussian blue, a pigment not available in 1638. The subsequent study in 2022 further explored the paintings' provenance, revealing that the coat of arms was overpainted in the past, later unveiled in 1939 by Kurt Erasmus. At the time, this discovery enabled the identification of the van der Horn family and consequently identified the portrait’s companion piece as that of Andries’ wife.

Although the added coat of arms altered the composition from Hals' original intention, it has historical significance, aiding in character identification in the past and reflecting Dutch heritage. Ethical debates on non-original coats of arms in Hals' portraits are observed in other museums globally and were considered. The options for treatment were to cover it, tone it down, or leave it as it is. Removing it was deemed irreversible, erasing a part of the painting's history. Considering its past and present circumstances, it was decided to preserve the coat of arms, acknowledging its historical significance and the specific Brazilian context it is in.

All that glitters is not gold: Curbing Illicit Activities in the Historical and Contemporary Gold Trade

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The traceability of gold for forensic purposes, from its mineral deposits through the stages of processing and beneficiation, emerges as an urgent necessity in combating illicit activities involving illegal extraction and trade of the metal, which result in environmental damage, human health issues, among other economic, social, and historical impacts.

In the historical-cultural context, the gold produced in Minas Gerais at the beginning of the 17th century significantly influenced the global economy and capitalism, with direct impacts on the Industrial Revolution. Part of the brazilian gold, which left the mines in Brazil in a pre-processed form, returned as jewelry and especially as gold leaves used in sculptures and altarpieces in eighteenth-century churches in Minas, Bahia, Pernambuco, and various other cities of the colony. In contemporary times, these sacred art pieces are constant targets of theft and illegal trade.

In the current context, the rise in global gold prices poses challenging effects for production and trade controls, affecting national economies and indirectly sparking increased interest from criminal groups who violently exploit nearly all stages of production and commercialization.

This study aims at using lead (Pb) isotopic signatures and the elemental compositions related to the source, particularly copper, silver, and trace elements, to determine the provenance of the mineral raw materials. It seeks to integrate mineral and isotopic geochemistry methods to curb crimes related to the production chain of gold and pieces of Brazilian cultural heritage, tracing its entire contemporary and historical commercial chain.

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A microstructural study of a natural chrysoberyl encapsulated in beryl

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Microstructural analysis combining chemical and crystallographic analysis is an important aspect in the study of heterogeneous samples. The study of naturally occurring minerals is important in clarifying questions such as the genesis of the region where the mineral is found, or provenance studies both for cultural heritage and forensics, or in mineral liberation analysis for mining purposes.

Emeralds belong to a beryl group of minerals with a general formula (Be3Al2Si6O18), containing chromium or vanadium responsible for the green color. They are quite rare, but present in several countries, in between them Brazil, mainly found in the southeast, northeast, and central regions of the country. Chrysoberyl (BeAl2O4) can occur together with emerald deposits. Several studies [1,2] have been performed on hundreds of samples aimed on the classification of the minerals based on trace elements which could explain their probable geological formation.

Seven Chrysoberyl embedded in emerald crystals were prepared for microanalysis and its microstructure is being studied using scanning electron microscopy with energy dispersive spectrometer and microprobe analysis. Trace elements were identified in both minerals and a co-existence with other mineral phases as several micas. A comparison with beryl data from the literature will be presented and preliminary results on the chrysoberyl mineral which presents a distinct variation in chromium content not found in the literature. The additional co-existing mineral phases will also be presented.

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Effects of Tea Tree Oil vapor on twentieth century photographs

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Studies on antimicrobial activity of essential oils (EO’s) are not new.[1] Though it seems that the issue has been more addressed lately with more studies dedicated to analyze different oils and their possible application on cultural heritage field. [2] This research analyzes possible effects of EO’s vaporization on contemporary photographs. Tea tree oil has been chosen as the EO to be tested because of reports of its use by some professional in the field. Twentieth century photographs were chosen as the object to be analyzed, because there are fewer studies on these objects specially on chromogenic processes and due to their complex composition, they could indicate reactions in other materials such as plastic, metals and paper. They were selected in order to represent different decades and brands in a total of six samples: three chromogenic and three gelatin silver. Each photograph was divided in 5 stripes: one submitted to no procedure, one submitted only to degradation by temperature and humidity and three submitted each one to different concentrations of tea tree oil vapor and degradation thereafter. For monitoring and evaluation of the pieces, different types of analysis were chosen: FTIR, XRF, Raman, espectrophotometry and microscopy. Three points on each stripe were selected to be monitored and evaluated before the evaporation, after it and after degradation. The results of this experiment will be presented on this presentation.

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Use of voltammetry of microparticles for the identification of metallic elements in inorganic pigments

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Voltammetry of microparticles (VMP), a solid-state electrochemical technique of analysis first introduced by Scholz et al. in 1989 [1], is a valuable option for the study of cultural heritage objects due to it being considered non-invasive (or microinvasive) and low cost, having portable equipment and its results being easy to interpret. The present work uses VMP to analyse inorganic pigments containing metallic ions, comparing the results to a database previously created through the analysis of standard metallic samples. Eight pigments were used, which were divided in commercially available pigments (by Sennelier) and pigments belonging to the collection of German artist Eleonore Koch, which is currently under the care of Pinacoteca de São Paulo. As references, standard samples of copper, iron, tin and tungsten were used to confirm the voltammetric results. Initially, all samples were characterized by SEM-EDX, and the pigments were also characterized by Raman spectroscopy. A three-electrode electrochemical cell was used for the measurements, with an Ag|AgCl|KCl (sat) reference electrode, a platinum auxiliary electrode and a paraffin-impregnated graphite electrode (PIGE) for immobilization of the different samples, which was achieved by means of an abrasive method. After parameters optimization, cyclic voltammetry and square wave voltammetry were performed in HAc/NaAc buffer (pH 4.75). The results showed that sampling small amounts of powder allowed the identification of oxidation peaks associated with the metallic elements present in the different compounds.

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AC03-Synchrotron Radiation Nanoscopy of Heterogeneous and Hierarchical Materials

Microplastic pollution in northeastern Brazil: a large-scale spatio-temporal investigative effort using FTIR and Raman spectroscopy.

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Plastics have become an integral part of human life due to their numerous benefits. However, they have also emerged as one of the most complex and forceful pollutants produced by humans, owing to their diverse uses and the intensity with which they are used. Once plastic waste enters the environment, it undergoes various forms of weathering resulting in continuous fragmentation, making it an invisible form of pollution. Microplastics, one such fraction of this fragmentation, is a major concern in this context. In Brazil, the research on microplastic pollution in the marine environment is still relatively new but has been intensifying since the early 2000s. The MicroplastiX Consortium (MicroplastiX.org) was an initiative that brought together European and Brazilian partners to investigate microplastic pollution on a large scale in the western Atlantic Ocean, particularly in the Northeast region of Brazil. Using advanced infrared spectroscopy and Raman techniques in unprecedented partnerships with other countries, the consortium has revealed the composition, abundance, distribution, trajectories, and possible sources of microplastic pollution in the Western South Atlantic. The research also shed light on the impacts of microplastic consumption by planktonic organisms. The results produced by the consortium represent one of the most comprehensive productions of referential knowledge on microplastic pollution in the Northeast of Brazil, owing to the large spatio-temporal scale of the research.

Multimodal synchrotron analyses of soil microaggregates to connect physical, chemical, and biological processes affecting nutrients and carbon

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Soils are hierarchical porous media comprising multiple minerals, organic matter, biomass, and residues in heterogeneous spatial arrangements. Interactions between physical, chemical, and biological processes regulate nutrient and contaminant behavior in these complex matrices. Our objective was to characterize the nanostructure and biogeochemical properties of soil microaggregates to gain insights on their potential role in immobilizing nutrients and stabilizing carbon. Aggregates of 10 - 50 microns were isolated from a highly weathered soil in a tropical forest, reacted with aqueous orthophosphate or deionized water, lyophilized, and analyzed at several complementary beamlines at the Sirius synchrotron [1]. Fungal hyphae were prevalent in the microaggregates. X-ray diffraction showed primarily quartz, kaolinite, hematite, and gibbsite. X-ray coherent diffraction imaging (CDI), scanning transmission X-ray microscopy (STXM), X-ray fluorescence tomography (XFT), nano-XANES, and FTIR hyperspectral imaging revealed physical, chemical, and biological spatial structures. Spatially isolated areas of high electron density were enriched in iron of varying mineralogy, along with titanium and manganese. Results led to a model of microaggregate formation and associated processes that likely influence retention of nutrients and carbon.

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Structural Evolution of Nanocatalysts in the Light of In Situ Bragg Coherent Diffraction Imaging

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The advent of the new 4th generation x-ray light sources represents an unprecedented opportunity to conduct in situ and operando studies on the structure of nanoparticles in reactive liquid or gas environments. In this talk, I will illustrate how Bragg coherent x-ray imaging [1] allows to image in three dimensions (3D) and at the nanoscale the strain and defect dynamics inside nanoparticles as well as their refaceting during catalytic reactions [2–4]. As an example, we have successfully mapped the lattice displacement and strain of a Pt nanoparticle in electrochemical environment [5] and under CO reaction [3,4]. I will also discuss the possibility to measure particles as small as 20 nm [6] and to enable high-resolution and high-energy imaging with Bragg coherent x-ray diffraction at 4th generation x-ray light sources [7]. Finally, I will highlight the potential of machine learning to predict characteristic structural features in nanocrystals just from their 3D Bragg coherent diffraction patterns [7].

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X-ray microscopy characterization of metal halide perovskites at CARNAÚBA/SIRIUS

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Metal halide perovskite (MHP) emerged in the last two decades and received attention due to its optoelectronic properties appropriated to use in several applications, such as X-ray detectors, LEDs, and solar cells. Besides the high efficiency obtained in the last years, several aspects need to be better understood to lead this technology to maturity. In this context, X-ray microscopy plays an important role in allowing the characterization of the MHP in films or complete devices ex-situ, in situ, or operando conditions.[1] CARNAÚBA beamline at the Brazilian Synchrotron Light Laboratory (LNLS) is a nanoprobe multi-technique beamline that offers great opportunities for MHP characterization.[2] Here, the first scientific results on MHP obtained at CARNAÚBA will be presented. First, the damage caused by the high photon flux of the beamline was investigated. With a multi-technique approach using nano-X-ray fluorescence (nano-XRF), micro-FTIR, AFM, and micro-PL, we revealed the effect of the X-ray beam in the chemical, optical, and morphological properties of the $CsFAMAPb(Br,I)_3$ and proposed strategies to mitigate the damage. In safety conditions, nano-XRF maps reveal a homogenization of the halide distribution on the perovskite film using methylammonium as an additive.[3] The combination of the nano-XRF with X-ray excited optical luminescence (XEOL) also reveals the chemical heterogeneities in perovskites with wrinkles. Besides that, we also developed a special photovoltaic setup for the operando characterization of perovskite solar cells. The setup allows precise control of the device temperature, atmosphere, illumination, and photovoltaic characterization simultaneously with X-ray characterization.

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Deciphering the impact of silica nanoparticle concentration on intracellular localization via nanotomography

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Silica nanoparticles (SiNPs) have been recognized as promising nanoplatforms for diagnosing and treating diseases [1]. To advance the field of nanomedicine, a comprehensive understanding of the interaction between these nanoparticles and cells is crucial. Several factors significantly influence the cellular uptake of SiNPs. One such factor is the protein corona (a protein layer formed spontaneously on nanoparticles when injected into the bloodstream) that drastically modifies the nanoparticle-cell interaction [2]. Here, we consider the effects of protein corona on SiNPs, considering previous research that has presented a meaningful cytotoxicity reduction [3]. In this study, we demonstrate that the spatial distribution of SiNPs within cells can change due to the concentration and doubling time of cells. This phenomenon was investigated in 3D imaging acquired through cryo-soft X-ray tomography (cryo-SXT) and super-resolution fluorescence structured illumination microscopy (cryo-SIM) advanced techniques at B24 beamline at Diamond Light Source. The evidence in the images shows that nanoparticles enter cells via vesicles across all concentrations and localize in the cytosol. An interesting and intriguing aspect is that, at higher concentrations, SiNPs are present within the cell nucleus, a phenomenon not observed at lower concentrations. Furthermore, the nanoparticles aggregated predominantly in the perinuclear region after two doubling times of cells. These findings have significant implications for the field of nanomedicine, as they offer three-dimensional characterization and high-resolution ultrastructural imaging of cells with nanoparticles using an innovative technique.

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Mastering the Use of Nanoprobes Beamlines for Electrochemistry: The Importance of Radiation Damage and Material Heterogeneity

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The integration of synchrotron radiation (SR) into nanoscale electrochemistry has opened new avenues for understanding the intricate behaviors of electrocatalytic materials under various conditions. This advancement is pivotal for the development of efficient energy conversion and storage systems. However, the application of SR, particularly through nanoprobe beamlines, introduces complex challenges that can significantly impact the interpretation of experimental data and the overall conclusions drawn about material properties and behaviors.

One of the primary concerns in utilizing SR for electrochemical studies is radiation damage. High photon flux, essential for achieving the desired spatial resolution and sensitivity, can alter the chemical and physical state of the materials under investigation, leading to misleading conclusions about their intrinsic properties and behaviors. Strategies to mitigate radiation damage, such as adjusting photon flux, employing different absorption edges, and conducting preliminary damage assessments, are critical for ensuring the integrity of the results.

Another significant challenge is the interpretation of material heterogeneity. Nanoprobe beamlines enable the detailed examination of material variations at the nanoscale, revealing heterogeneities that are obscured in bulk analysis. This capability is essential for identifying active sites and understanding the mechanisms driving electrochemical reactions. However, it also complicates the analysis, as variations in local composition, structure, and electronic state must be carefully correlated with electrochemical performance. The development of multiscale characterization techniques and the integration of complementary analytical methods are vital for constructing a comprehensive picture of material behaviors. Thus, in this work, we will present proof-of-concept experiments where these challenges are observed and will highlight best scientific practices for the field.

Mogno Beamline, the micro and nanotomography beamline at Sirius: early scientific outcomes and future installations

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Mogno, the micro and nanotomography X-ray beamline at Sirius, was designed to operate in zoom tomography mode, high-throughput, and for in situ experiments. With a nano-focus source, Mogno promises unprecedented resolution for nanostructural analysis at a high-energy beamline, reaching up to 150 nm with energy levels of 22, 39, and 67 keV. Currently partially open to users, the nano-station is attracting researchers from around the world, while the micro-station installation is underway. Mogno's scientific potential spans diverse fields, including groundwater studies, soil characterization, biomaterial research, and fossil examination. As a forthcoming installation, a HPHT (high pressure, high temperature) environmental cell will be available for studying rocks under Brazilian reservoir conditions, a capacity unprecedented in any other beamline and which has the ability to collaborate on very important topics, such as CO2 storage in depleted reservoirs.

Shedding Light on the Biological World: Infrared Insights from IMBUIA Beamline at Sirius

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The IMBUIA Beamline (Microspectroscopy and Infrared Imaging) is an advanced facility dedicated to studying materials at the molecular and nanoscale levels. With its high brightness, this facility offers synchrotron-based infrared spectroscopy and imaging techniques, enabling researchers to explore the molecular and vibrational properties of samples with exceptional sensitivity and spatial resolution. Infrared radiation (IR) has become a valuable tool in the investigation of biological systems, allowing for the analysis of molecular composition, structure, and dynamics without the need for chemical markers. For example, IR can detect DNA damage in fungi exposed to volatile organic compounds by leveraging the natural molecular vibrations of the samples. IR spectral microscopy provides chemically specific information with spatial resolution, enabling researchers to map the distribution of specific biomolecules within tissues and cells. Infrared imaging is particularly useful in cellular research, as it facilitates the characterization of local chemical variations and the identification of specific components within complex systems. By integrating spatial and spectral information, researchers can reveal the composition and distribution of materials in biological, geological, and materials science research. The versatility of the IMBUIA Beamline, with its synchrotron-based infrared microspectroscopy and imaging capabilities, offers powerful opportunities to delve into the molecular world and gain a deeper understanding of material properties. The application of IR in the study of biological systems offers benefits such as the characterization of biomolecules, spatial imaging, probing interactions and changes, and dynamic analysis without relying on chemical markers. These applications will significantly advance our understanding of the biological world and drive technological progress in infrared spectroscopy.

Synchrotron infrared nanospectroscopy at the brazilian 4th generation storage ring Sirius

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Fourth-generation synchrotron storage rings represent a remarkable leap forward in synchrotron technology, offering intensely bright and finely focused X-ray beams crucial for a wide array of scientific inquiries. However, their tightly configured magnetic lattices historically posed challenges for accessing lower-energy radiation, such as infrared (IR) and THz. Here, we introduce the inaugural IR beamline successfully integrated and operational within a fourth-generation synchrotron storage ring [1]. Our endeavors encompass numerous pivotal advancements, including an exhaustive analysis of the new IR source at Sirius, a comprehensive elucidation of the radiation extraction method, and a thorough validation of our optical framework through meticulous measurements and simulations. This refined optical setup has enabled an impressively broad spectrum for our nanospectroscopy pursuits. Through the application of synchrotron IR nanospectroscopy on samples spanning biological and hard matter, we effectively demonstrate the practicality and efficacy of this beamline. We highlight the advantages of fourth-generation synchrotron IR sources, now capable of operating with unparalleled stability, thanks to stringent standards ensuring the production of low-emittance X-rays.

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Using synchrotron nanoprobe techniques to investigate lamellar minerals

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This work is particularly motivated by recent research that demonstrated interesting properties of phyllosilicate minerals in their few-layer form [1-3]. Phyllosilicates have a lamellar structure that allows them to be exfoliated down to monolayer, making them naturally hierarchical materials. They are large band gap insulators, with the common presence of impurities and hydrated phases. Understanding how impurities and hydration can be manipulated in these minerals is crucial, as it could lead to the optimization of their properties for applications in future hybrid nanoelectronics based on lamellar materials. This can be a key for reducing effective costs while increasing chip functionality, since they are abundant on Earth and easy to extract.

In this sense, we first need to probe impurities and retrieve mineralogical information at the few-layer limit with nanometric resolution. Here, we will demonstrate X-ray fluorescence and X-ray absorption near edge structure techniques using synchrotron radiation as powerful tools for identifying and mapping impurities in ultrathin phyllosilicates with nanometric resolution and sensitivity to number of layers. Moreover, we will show that synchrotron infrared nanospectroscopy technique based on near-field interactions can provide broadband infrared spectra of ultrathin phyllosilicates, enabling the analysis of their vibrational modes, hydration and retrieving of mineralogical phases. We will emphazise that the use of synchrotron nanoprobe techniques can be useful not only for the investigation of lamellar minerals, but of any 2D material.

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Visualising Hierarchical Zeolites with Coherent X-ray Diffractive Imaging

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Zeolites are microporous aluminosilicate materials extensively used as catalysts. The unique properties of zeolites arise from their microporous structure, their small-scale pores and the chemical nature of their aluminosilicate framework [1]. The intracrystalline diffusion of adsorbed molecules in the crystals plays a crucial role in the use of zeolites. Controlling simultaneously zeolite selectivity and adsorption properties is of paramount importance and can be achieved by tuning its porosity. Indeed, hierarchical zeolites with micro- meso- and macropores have an enhanced performance compared to their conventional analogues.

Bioethanol has gained increased attention as a possible source of renewable energy and an alternative to produce high value chemicals due to the present depletion of fossil fuels and global warming concerns. However, reactions involving ethanol induce the formation of carbonaceous compounds (also called coke) that can poison active sites and block zeolite pore network.

Hierarchical zeolites were prepared by the desilication methods. They were imaged three-dimensionally by employing plane-wave coherent X-ray diffraction (pwCDI) at the Cateretê beamline [2] at the Brazilian synchrotron light source. The pore network, the pore distribution and interconnectivity of zeolite crystals of ~ 10 micron were revealed by pwCDI. After ethanol dehydration zeolite crystals were also imaged revealing how the coke spreads through the structure, fills the pores and blocks access to the pore network harming the diffusion of reagents and products.

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X-ray Dose Effects and Strategies to Mitigate Beam Damage in Metal Halide Perovskites under High Brilliance X-ray Photon Sources

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Metal halide perovskites (MHP) suffer from photo-structural-chemical instabilities whose intricacy requires state-of-the-art tools to investigate their properties under various conditions.[1] This study addresses the damage caused by focused X-ray beams on MHP through a correlative multi-technique approach: chemical variations of the metallic part and halides were monitored via nano x-ray fluorescence maps at CARNAÚBA beamline [2] while the organic part was tracked by µ-Fourier transform infrared spectroscopy at IMBUIA beamline, both at LNLS synchrotron. The damage after high-dose irradiation is noticeable in many ways: the yank out of iodine and organic components, whose relative amount is reduced; the formation of an excavated area modifying the sample morphology; and an altered optical reflectivity indicating an optically inactive layer. The damage mechanism combines radiolysis and sputtering processes. Interestingly, the bulk underneath the excavated area keeps the initial halide proportion demonstrated by a stable photoluminescence emission energy. We also show that controlling the beam dose and environment is an excellent strategy to mitigate the dose harm. Hence, we combined a controlled X-ray dose with an inert N_2 atmosphere to certify the conditions to probe MHP properties while mitigating damage efficiently. Finally, we applied optimized conditions in an X-ray ptychography experiment, reaching a 15-nm spatial resolution, an outcome that has never been attained in this class of materials. These findings allowed the development of new methodologies that make it feasible to use of techniques such as x-ray nanodiffraction and x-ray excited optical luminescence in MHP.[2]

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X-ray excited optical luminescence of Eu-doped YAG nanophosphors produced via complexing agent in modified sol-gel route

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Phosphor materials based on the garnet structure are promising candidates for scintillator hosts. Among the scintillator materials, yttrium aluminum garnet (YAG) shows great luminescent properties when doped with rare-earth elements. Several chemical methods have been used for YAG nanophosphor synthesis. Among these preparation methods, the sol–gel process provides some advantages for YAG nanophosphor synthesis. Moreover, sol gel-based methods which use alternative chelating agents have been recently presented as a promising modern trend in the preparation of nanocrystalline YAG phosphors. Recently, glucose has been successfully used as a chelating agent to synthe magnetic oxides. In this work, we report the investigation of the effect of YAG/glucose molar ratio on the structural and optical properties of Eu-doped YAG nanophosphors using XRD and XAS techniques. The effect of YAG/glucose molar ratio on the crystalline structure and X-ray excited optical luminescence (XEOL) of YAG were investigated. The results indicated that the average crystallite and XEOL emission intensity change with the YAG/glucose molar ratio. X-ray absorption near edge structure (XANES) and total XEOL yield were measured simultaneously around the Eu L_{III}-edge and indicated that the Eu valence does not change with the YAG/glucose ratio. However, luminescence increases as an energy function. XEOL emission spectra revealed that samples produced with YAG/glucose = 1:1 molar ratio presented the highest light yield. (This work was partially supproted by CAPES, CNPq and FINEP)

A setup for photovoltaic X-ray microscopy characterization at CARNAÚBA/SIRIUS

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Global warming has posed a new challenge: the move from fossil fuel-based to renewable energy sources in the called energy transition. In this context, solar cells, especially perovskite solar cells (PSCs), have gained attention due to attractive characteristics such as versatile fabrication, high performance, and tunable optical properties through composition adjustment. Besides the impressive advances in performance and stability of PSCs in the last few years, the nanoscale properties still need to be understood better, where the X-ray-based techniques offer a crucial advantage for operando characterization.1 The X-ray penetration on materials allows the study to complete devices with minimal sample preparation. Here, we report the development of a custom-made holder for perovskite solar cells for the TARUMA, CARNAUBA's first experimental station at Sirius-LNLS.2 The core of the setup is a homemade substrate heating chip that offers precise control of the temperature in the device. The chip is prepared in the transparent conductive oxide substrate used in the preparation of solar cells and includes a heater and a temperature sensor made of platinum. Infrared imaging of the 3x3 mm2 target area showed a temperature relative standard deviation of 0.48%, revealing a homogeneous temperature distribution. The setup also includes illumination with white light achieving around 1 sun, environmental control (nitrogen flow), and electric solar cell characterization. The setup allows X-ray-based characterizations under different conditions, which is essential for fundamental investigations that boost device optimization and scaling PSC technology. The setup is compatible with X-ray fluorescence (XRF), X-ray diffraction (XRD) in reflection mode, and X-ray absorption spectroscopy (XAS).

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CNPEM-Embrapa collective effort to study the genesis of cohesive soils: A multi-scale and multi-spectral approach to understand the cohesion mechanism in Brazilian Coastal Tableland soils

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Decades of scientific research have aimed to understand the cohesive nature of Brazilian Coastal Tablelands soils, yet conclusive results remain elusive. The CNPEM-Embrapa Cohesive Soils Program seeks to determine the mechanisms behind soil cohesion in this ~100,000km^2 region, with the goal of developing agricultural management strategies to mitigate issues and enhance crop productivity.[1] This study aims to develop experiments utilizing a multispectral approach at Sirius to test hypotheses regarding micro to nanoscale mechanisms of cohesion.

Samples characterized by standard techniques from different soil profiles and horizons will be taken to micro-tomography at MOGNO beamline for detailed 3D imaging of soil microstructure, revealing insights into pore distribution and connectivity. Nano-computed tomography at CATERETÊ beamline will then push to a higher resolution imaging, enabling examination of finer pore network details with unprecedented clarity. Powder X-ray diffraction at PAINEIRA beamline will be employed to quantitatively analyse soil mineralogy.

Nano X-ray fluorescence mapping will be performed in the clay+silt fraction of the soil at CARNAÚBA beamline delineates elemental spatial distribution at the nanoscale, shedding light on elemental associations with mineral and organic components tracked with µ-Fourier transform infrared spectroscopy at IMBUIA beamline which examines spatial distribution of specific organic functional groups. Nanodiffraction will show mineralogical phase distribution associating it with chemical distribution and organic matter interfaces, providing insights into structural integrity and describing the role each part in shaping soil properties.

Correlating this information aims to elucidate the cohesion mechanism and its influences on morphological, physical, and hydraulic properties of the soil.

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Far Infrared Synchrotron Near-Field Nanoimaging of Low-dimensional Materials

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Polaritons, emerging from the coupling of electromagnetic waves with collective lattice vibrations, offer promising avenues for controlling and manipulating light-matter interactions. They enable subwavelength imaging due to their ability to confine light to dimensions smaller than the diffraction limit. Polaritons also support guided modes and confined electromagnetic fields, making them promising candidates for on-chip photonic devices and integrated circuits. These applications demonstrate the versatility of polaritons in controlling and manipulating light-matter interactions across various fields, from nanophotonics and quantum optics to sensing and spectroscopy, paving the way for advanced technologies with enhanced performance and functionality. Polaritonic phenomena play a pivotal role, especially in the far-infrared spectral range, yet their nanoscale characterization remains challenging. Through the application of Synchrotron Infrared Nanospectroscopy (SINS)[1], high-resolution mapping of polaritonic resonances could be obtained, offering insights into their spatial distribution and spectral characteristics with unprecedented detail. Nanoscale imaging capabilities allow for the direct visualization and manipulation of polaritonic modes. For this reason, we uncover novel phenomena associated with far-infrared polaritons, including their dispersion, confinement, and interaction with nanostructured materials[2,3]. Here, we present a comprehensive study on far-infrared polaritons utilizing advanced spectroscopic techniques in low-dimensional materials. Our findings deepen our understanding of polaritonic physics in the far-infrared regime and hold immense potential for developing advanced nanophotonic devices and applications.

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Inducing molecular orientation in solution processed thin films of fluorene-bithiophene-based copolymer: photoemission and photoabsorption studies

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Fluorene-based copolymers are highly attractive organic semiconducting materials thanks to their well-known synthetic route, and chemical and thermal stability. Moreover, many optoelectronic properties of devices based on conjugated copolymers depend on the final morphology reached after thin film fabrication. To understand the factors that influence the morphology of thin films based on conjugated polymers, we investigated the electronic structure and morphology of thin films of the poly(9,9-dioctyl-fluorenyl-co-bithiophene) (F8T2) copolymer in its pristine form, as well as samples processed with the solvent additive 1,8-diiodooctane (DIO) and thermally annealed. Measurements carried out using angle-resolved S K-edge NEXAFS in total electron yield (TEY) and fluorescence yield (FY) detection modes showed two main transitions at the S1s NEXAFS spectra, S 1s → π* and S 1s → σ* (S-C), respectively at 2471.7 eV and 2472.6 eV. Additionally, the observed dichroism pointed to a face-on orientation of the conjugated backbone, which is significantly increased for F8T2 films processed with DIO. We analyzed Resonant Auger decay spectra via the Core-Hole Clock method, an elementally-sensitive synchrotron-based approach that utilizes the core-hole lifetime of core levels as an internal reference clock. Enhancement in the charge transfer process was observed for thermally annealed films and samples processed with DIO, indicating an increase in film ordering. We also attested the presence of the thiophene unit in the samples through X-ray photoelectron spectroscopy, where some of its sulfur atoms were shown to have been positively polarized for the F8T2 films.

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Influence of co-solvent and methylammonium chloride additive on low-dimensional perovskites for solar cells

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Low-dimensional perovskite has received great attention due to its higher stability, compared to conventional 3D perovskite, and easy tuning of its optical properties. This type of material is composed of n inorganic octahedra layers separated by two layers of large organic cations. Varying the number of layers (n) between the large cations changes the perovskite optoelectronic properties. However, there is competition between 2D and 3D perovskite crystallization. Hence, the control of phase purity is quite challenging and not entirely understood yet.[1, 2] Here, we investigated the formation and properties of $(PEA)_2FA_{n-1}Pb_n(Br_{1/3}I_{2/3})_{3n-1}$ ($PEA=C_6H_5(CH_2)_2NH_3^+$ and $FA=CH(NH_2)_2^+$) (n=1, 5, 10) using co-solvent DMSO ($(CH_3)_2SO$) or NMP ($OC_4H_6NCH_3$) together with MACl ($MA=CH_3NH_3^+$). In situ grazing-incidence wide-angle X-ray scattering measurements, performed at Microdiffraction/Advanced Light Source (Berkeley-CA) beamline, showed that the co-solvent and MACl strongly alter the formation mechanism. DMSO leads to the formation of more crystalline and oriented perovskite. MACl alters the crystal orientation even when NMP is used. Photoluminescence spectra showed that the lateral heterogeneity in the distribution of n-phases is reduced when MACl is used. The characterization of the horizontal distribution of halides through nano-X-ray fluorescence carried out at CARNBAÚBA/Sirius beamline exhibited that perovskite films prepared with MACl are relatively more heterogeneous than those without the additive. Our data indicated that orientation is the major factor for obtaining efficient quasi-2D perovskites solar cells and that this parameter is dependent on the co-solvent and the presence of MACl. These results allow a greater understanding and facilitate the obtaining of low-dimensional perovskites with improved crystallinity, phase purity, and optical properties.

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Influence of temperature and solvent on the morphology of organic semiconductor films

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The study of organic semiconductors has witnessed significant growth in recent decades, driven by their diverse applications in solar cells, light-emitting devices, photodetectors, and transistors, due to appealing characteristics, including lightweight nature, cost-effectiveness compared to inorganic counterparts, semitransparency, flexibility, and compatibility with various processing techniques[1]. In the realm of organic photovoltaic devices, film morphology plays a crucial role in determining the efficiency of charge transport processes for energy conversion[1,2]. This study investigates three acceptor-type semiconductors: a fullerene derivative, PC71BM, and two non-fullerene small molecules, ITIC and o-IDTBR, in both pristine and blended with the polymer donor, PBDB-T, deposited using the spin-coating technique. Angle-resolved NEXAFS measurements were conducted at the IPÊ beamline at SIRIUS (LNLS-National Synchrotron Light Laboratory in Campinas, Brazil) and the PIRX beamline at SOLARIS (National Synchrotron Radiation Centre in Kraków, Poland). These findings, combined with AFM and XPS measurements, were utilized to explore the relationship between film ordering, surface roughness, composition, thermal treatment, and solvent choice. The study revealed that pristine films of the small molecules and the polymer exhibit clear preferential ordering, whereas blend films indicate possible disorder in the crystalline phases on the surface but maintain preferential order in the bulk. Thermal treatment notably affects surface roughness and composition, while solvent changes do not significantly impact the analyzed characteristics.

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Investigation of Site-Selective Luminescence on Core-Shell Persistent Phosphors using Synchrotron Radiation

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With the growing interest in the development of multifunctional luminescent nanomaterials for applications in energy conversion and storage, several new methods have been studied for the fabrication of efficient core-shell persistent phosphors with long-lasting persistent luminescence in the visible and near-infrared range. Such materials often exhibit particular optical properties that may be precisely tuned via the modification of structural parameters and surface functionalization. [1-3] Hence, in this work, site-selective luminescence of core-shell green-emitting rare-earth-doped strontium aluminate persistent phosphors functionalized with europium β-diketonate (tta, dbm) complexes were investigated utilizing a combination of synchrotron-based techniques at the CARNAÚBA beamline of Sirius, such as X-ray absorption near edge structure (XANES), X-ray Excited Optical Luminescence (XEOL), and X-ray fluorescence (XRF). X-ray excited luminescence spectroscopy revealed that single-shell materials exhibit distinct emission profiles associated with energy-transfer mechanisms via the “antenna effect” for the different β-diketonate ligands, while double-shell materials showed that the ratio between Eu^{2+} (green) and Eu^{3+} (red) emission is intrinsically different for the edge and the bulk of the studied particles. Promising results also revealed the influence of shell thickness and distance in potential energy-transfer processes, outlining an important framework for the development of multifunctional persistent phosphors utilizing rare-earth complexes as luminescent sensitizers.

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In situ XAS investigation of shape-controlled catalysts dynamics in hydride transformations

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Often composed of metallic nanoparticles, heterogeneous catalysts are essential in industry, enhancing the efficiency of chemical processes. The structure and morphology of nanomaterials strongly influence their properties [1]. Palladium-based materials exhibit peculiar characteristics in the presence of hydrogen, making palladium nanoparticles interesting for various hydrogenation reactions. Indeed, they have a high affinity for hydrogen molecules, enabling the effortless adsorption and dissociation of H_2 [2]. To comprehend the impact of the dynamic process under hydrogen on morphology-controlled catalysts, we conducted an *in situ* time-resolved X-ray Absorption Spectroscopy (XAS) study on ROCK at SOLEIL [3]. We tracked the evolution of shape-controlled palladium nanoparticles (PdNP) of different sizes, hydration states, supports, and structures by analyzing both monometallic palladium and gold-palladium core-shell nanoparticles. Under H_2, XANES analysis reveals modifications in the average Pd atomic environment, while EXAFS confirms the reversible formation of hydride species across all samples. This work will discuss the differences in the dynamics of phase transformations observed in our time-resolved study, with the initial parameters of the synthesized nanoparticles.

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Microporosity of deep marine reservoir rocks: multiscale analysis using X-ray zoom microtomography of synchrotron source

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The pre-salt is a geological formation composed by sedimentary rocks with organic content, formed more than 100 million years ago by the accumulation of organic matter on the south-eastern coast of Brazil, during the separation of the American and African continents. The subsequent formation of the Atlantic Ocean led to the deposition of a salt layer, which nowadays reaches 2 km in thickness. This salt layer was responsible for trapping the organic content of the subjacent layer (the pre-salt layer), enabling thermochemical processes that generated oil and natural gas. The salt layer is currently located 5 km deep below sea level.

The goal is to study the microporosity of the reservoir pre-salt rocks in multiple scales using hard X-ray (39 keV) zoom microtomography, at the MOGNO beamline at the Brazilian Synchrotron Light Laboratory. MOGNO's conic beam allows image acquisitions with different pixel s by varying the sample position relative to the source and the detector, also enabling the user to image relatively large samples.

Pre-salt rock plugs of 2 mm diameter were used for testing. The sample was positioned along the beamline for the acquisition of images at four resolutions – 2 µm (full sample image), 800 nm, 500 nm and 300nm – without reducing the sample . The reconstruction aims maximizing the recovery of information, particularly in the zoomed images, as we are interested in part of the sample despite having the whole sample in front of the beam. Segmentation focuses on supervised and unsupervised machine learning algorithms based on image texture, to allow identifying zones of interest, i.e., of microporosity, for enhancing the decision process for zoom tomography during the experiments.

We expect to be able to correlate micropores and pores throughout the different scales and, by future analysis of other pre-salt reservoir rocks with zoom XR-µCT, to shed light into petrophysical models for a more efficient oil exploitation.

Multiscale tomography applied to topics in soil and plant sciences: first commissioning experiments at the MOGNO beamline

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X-ray tomography at the MOGNO beamline, from the 4th generation Brazilian Synchrotron Light Source – Sirius, offer unique capabilities of zoom imaging for investigations in soil and plant sciences, spanning spatial resolutions from dozens of micrometers to hundreds of nanometers in centimetric d samples [1]. The objective of this work is to present examples of experiments in the context of agriculture led at MOGNO beamline during its commissioning. One recent study, which is ongoing, aims at investigating the physical blockages in the xylem vessels of grape berry pedicels. The zoom images in such study revealed secondary wall thickening cells and improved the differentiation between blockages and cell delimitations. Another ongoing study involves the characterization of the combined effects of biochar (applied to the soil) and ZnO nanoparticles (applied on the seeds of beans) on root architecture. In general, the radiation dose deposited in the roots can be a concern. To gauge its impact and help design future experiments, we simulated Monte Carlo dose rates on wheat roots growing in soil across a range of energies and zoom imaging configurations [2].

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NMR and High-Resolution imaging on the MOGNO Beamline for dynamic system analysis on Porous Media

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Time-domain NMR stands out for being a non-intrusive technique, that allows the measurement of information regarding the molecular dynamics of fluids. Its application in porous media is noteworthy as it also enables the measurement of properties strongly correlated with the material morphology [1]. This technique has been extensively utilized in the oil industry for fluid characterization and porous media analysis. MOGNO is a micro and nano X-ray imaging beamline dedicated to time-resolved experiments (4D tomography) through in-situ experiments, where a material can be observed under specific conditions [2]. Integrating NMR and X-ray imaging is a perfect combination for studies of porous media, mainly under dynamic conditions. It is in this context that the LEAR group at the University of São Paulo, in partnership with the Brazilian Center for Research in Energy and Materials, is developing an NMR system to be installed at MOGNO for simultaneous acquisitions of high-resolution images and NMR data. Data from both techniques will be crucial for understanding the material's evolution and will also complement computational data processing models. Areas involving processes like saturation, imbibition, and flow—including CO_2 capture and storage, soil, cement, and aquifers—can be explored. In addition to areas involving chemical reactions such as porous media acidification. This work will present some aspects of the project that is under development, and previously obtained results that will be explored in the future with the combination of both techniques.

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Quati, the XAS beamline dedicated to dynamic studies of functional materials at SIRIUS

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The development of innovative materials requires an in-depth understanding of their structure related to their macroscopic properties. X-ray absorption spectroscopy (XAS) provides chemical, atomic, electronic, and structural information about a selected element. It gives detailed insights into the local geometric structure on the atomic scale, the unoccupied density of states and the valence.

In situ/operando XAS studies became essential for explaining functional materials structure-activity relationships. In particular, time-resolved studies under increasingly complex conditions, in sophisticated ways, are required. At the Brazilian synchrotron light source SIRIUS [1], the new beamline Quati has focused its design on probing the dynamic nature of functional materials under realistic conditions.

Taking advantage of the 4th generation synchrotron SIRIUS, Quati will provide a high photon flux of ~10E11 ph/s from 4.5 to 35 keV with an in-house designed monochromator: HD-DCM-lite [2]. Besides, a moveable experimental table will offer an adaptable spot (~10’s µm to 6 mm), giving flexibility on the beam and flux density, essential for avoiding beam damage of sensitive materials.

In this work, we will present the new beamline, in particular its end station and the first commissioning results. Besides a few selected examples will be discussed to illustrate scientific cases that will be possible to tackle shortly on Quati.

Acknowledgements: The authors acknowledge all the LNLS staff working on this project.

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Sample environments for in situ, in vivo, and operando experiments at the Carnaúba beamline

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In situ, in vivo, and operando experiments at the Carnaúba provide valuable insights at the nanoscale into the behavior of materials and systems under realistic conditions [1]. For this purpose, important setups involving electrochemistry, microfluidic reactors, holders for batteries [2-3], heating, and gas systems have been developed and undergone constant upgrades in the last few years. These fruitful sample environments were developed to take advantage not solely of the small beam (180 x 180 nm2 @10 keV) at the Tarumã station, but also to utilize its coherent flux through ptychography and Bragg coherent diffraction imaging.

In the context of electrocatalysis, we have developed miniaturized (photo) spectroelectrochemistry cells that allow to perform spatially resolved analysis such as two-dimensional fluorescence and absorption mapping, contributing to studies of charge transfer processes in different regions of a heterogeneous catalyst, or battery cathode/anode. For single nanoparticles, the three-dimensional strain and morphology can be accessed using Bragg coherent diffraction imaging. In addition to these cells, we will show preliminary results of ptychography and X-ray excited optical luminescence performed in a polycarbonate microreactor after a biomineralization process and injection of luminescent fluid, respectively. Lastly, will be presented an ongoing project; the setup for temperature, which consists of a glassy carbon-based microheater working in transmission mode reaching up to a predicted temperature of 800 °C.

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Selenium speciation in cow's milk and blood using synchrotron-based micro-spectroscopic techniques

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Selenium (Se) is a nutritionally essential mineral for humans. Within the body, selenium contributes to the formation of selenoproteins, which play a crucial role in thyroid hormone metabolism, DNA synthesis and as an antioxidant, safeguarding cell membranes against oxidative stress caused by free oxygen radicals [1]. On the other hand, cow's milk is also an important source of nutrients for humans and is economically affordable for most of the population. Biofortification of cow's milk is the process of adding Selenium to the diet of lactating cows to provide extra nutrients. However, the toxicity of a chemical element depends on the quantity that is ingested and, mainly, on the chemical species to which this element is associated [2]. In this context, it is necessary to study its speciation to better understand its bioavailability.

The purpose of this work is to identify and quantify the different chemical species of selenium in fortified and biofortified cow's milk, as well as bovine blood, using X-ray Fluorescence (XRF) and X-ray Absorption (XAS) techniques. The measurements were performed at Carnaúba, the Coherence X-ray Nanoprobe beamline of the LNLS-Sirius machine [3]. The results obtained in this study will shed light on the selenium biofortification process in the human food chain, hence deepening our understanding of its bioavailability.

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AC04-Artificial intelligence applied to materials science

Learning from machine learning: discovering new science for materials

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Machine learning (ML) methods are now an integral part of materials research thanks to the increasing availability of curated datasets containing structural and electronic data derived from quantum-mechanical calculations. Also, the accessibility and user-friendliness of ML algorithms and software have extended their utility to a broader scientific community. We can currently observe in the literature many ML works that try to predict a certain property of a material. Here, we will show examples of using ML where we can go beyond prediction. We will show results related to interpretable machine learning to understand the band gap directness in semiconductors and related to natural language processing, where we can retrieve latent knowledge related to CO2 reduction from the literature.

We reached the era of Universal Machine Learning Interatomic Potentials?

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Machine learning interatomic potentials (MLIPs) are one of the main techniques in the materials science toolbox, able to bridge ab initio accuracy with the computational efficiency of classical force fields. This allows simulations ranging from atoms, molecules, and biosystems, to solid and bulk materials, surfaces, nanomaterials, and their interfaces and complex interactions. A recent class of advanced MLIPs, which use equivariant representations and deep graph neural networks, is known as universal models. These models are proposed as foundational models suitable for any system, covering most elements from the periodic table. Current universal MLIPs (UIPs) have been trained with the largest consistent dataset available nowadays. However, these are composed mostly of bulk materials' DFT calculations. In this article, we assess the universality of all openly available UIPs, namely MACE, CHGNet, and M3GNet, in a representative task of generalization: calculation of surface energies. We find that the out-of-the-box foundational models have significant shortcomings in this task, with errors correlated to the total energy of surface simulations, having an out-of-domain distance from the training dataset. Our results show that while UIPs are an efficient starting point for fine-tuning specialized models, we envision the potential of increasing the coverage of the materials space towards universal training datasets for MLIPs.

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Application of regression machine learning algorithms for predicting membrane permeability under different operation conditions

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Membranes are an efficient technology for removing contaminants in water and wastewater treatment processes to ensure high effluent quality. They act as a physical barrier in which contaminants are separated based on their molecular and interaction with the membrane systems. They are efficient for separating colloidal particles (i.e., microfiltration), macromolecules (i.e., ultrafiltration), molecules of medium molecular weight (i.e., nanofiltration), and dissolved salts (i.e., reverse osmosis). In addition, membrane technology is an environmental-friendly approach that requires low energy demand and less complicated operation schemes. However, it is highly dependent on the surrounding operation conditions such as water source, pollutant type, and applied pressure. This emphas the importance of employing data-driven models using machine learning (ML) algorithms to better understand the performance of these membranes under various operation conditions. ML algorithms can model complicated systems in a simple manner by relating input and output variables to identify correlations between them. These models can also describe the cause-result relationship between different process variables. Therefore, the main objective of the current study is to apply different regression ML models (e.g., random forest) on a lab-scale dataset pertaining to membrane performance under multiple filtration scenarios. The operational conditions (e.g., pressure and casting speed) were used as the model input variables while the membrane permeability was the major target variable. The performance of ML models was assessed using different evaluation metrics (e.g., R2 and RMSE), specifying the optimal model for predicting the target variable. The results of the current study can be used to better understand the response of membrane under various operation condition, recommending the optimal operation scheme of membranes for higher productivity with less operation and maintenance costs.

Artificial Neural Network applied on surface integrity prediction regarding special cutting tools

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The geometry of the cutting tool is particularly important inside the machining process, affecting cutting forces, tool life itself and surface integrity of the workpiece [1], which may impose restrictions on mechanical design and impair fatigue strength. In this study, an artificial neural network (ANN) was implemented to predict the effects of tool nose radius (macrogeometry) and cutting edge preparation (microgeometry) over surface roughness after a straight turning operation on 4142 alloy steel using different feed rates. Both training and validation of ANN were done using specially ground K10 cemented carbide tools with PVD TiAlN coating. Results show that ANN demonstrated good capability for the roughness prediction with strong agreement between the experimental and model results, however the variation of neurons applied in the ANN model played some difference in the absolute percentage error.

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Artificial Neural Network-Based Density Functional Approach for transition Metal Complexes

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Even with the efforts of the quantum chemistry community, some electronic properties of materials are challenging to compute even with our best methods. One of those cases is the accurate depiction of the effects of spin-crossover (SCO) on materials like metallic complexes and metal-organic frameworks (MOFs). Ideally, a quicker and easy to automatize electronic structure method to describe the SCO effect is desirable, allowing screening for new SCO materials. This work proposes to delve into the on-growing field of machine learning functional for a possible solution for this problem within Density Functional Theory.[1] A few parameters (about 1.5K) version of the previous physically constrained artificial neural network (ANN) functionals was trained to reproduce a small set of energies and densities using a non-gradient based bio-inspired training method we adapted from Particle Swarm Algorithm. Our results show that a robust meta-GGA functional created in this way can outperform most known density functionals in the prediction of adiabatic energy differences in a large variety of systems, while preserving the generality necessary to predict reasonable energetics and densities.

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Genetic Algorithm integrated with Machine Learning for high toughness High-Entropy Alloy design

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The vast compositional space of high-entropy alloys (HEAs) can be explored with computational methods, which enables the development of innovative materials with tailored properties for a variety of applications [1]. One such method is the genetic algorithm (GA), where optimization is achieved by iteratively creating new generations of alloys through crossover and mutation processes, gradually refining their properties to match the desired specifications [2]. In this study, a new methodology was developed that integrates the GA with machine learning (ML) to reproduce CALPHAD calculations at reduced computational cost. The algorithm's performance was evaluated in predicting single-phase FCC alloys, hardened by grain refinement and solid solution, with potential TRIP/TWIP effect. Classification and regression ML models were employed to predict the single-phase FCC and TRIP/TWIP features, respectively. A robust training dataset, derived from CALPHAD calculations, established correlations among compositions, formed phases, and Gibbs free energy. Additionally, grain refinement was evaluated by the Hall-Petch constant (K), while solid solution hardening was quantified by the critical resolved shear stress (σy), both determined via mathematical equations. The insights gained from this study will contribute to the development of novel methodologies for designing HEAs.

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GlassNet: A Multitask Deep Neural Network for Predicting Diverse Glass Properties

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GlassNet, a novel multitask deep neural network, has been developed for predicting diverse properties of glasses. Trained on a dataset comprising over 200,000 glass compositions, the network capitalizes on the intrinsic correlation between composition and properties in non-crystalline glasses. It covers a wide spectrum of glass chemistries, including oxide, chalcogenide, halide, and others, requiring only the glass composition as input features. Leveraging its multitasking capability, the model efficiently predicts a wide range of physical, thermal, electrical, optical, and mechanical properties simultaneously. Explainable AI (SHAP) offers valuable insights into the underlying relationships between input data and predicted properties. This model, named GlassNet, is freely available and implemented within the GlassPy Python module, thereby empowering researchers to accelerate computer-aided design of novel glasses.

Inverse Project of New Bioactive Glasses

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Bioactive glasses represent a crucial class of materials that interact with biological tissues, showing great potential in various applications in human health, such as dentistry, orthopedics and regenerative medicine[1]. However, traditional research approaches in this field, currently based mostly on trial and error, have significant limitations in terms of efficiency and time. The main objective of this study was to collect data from the literature[2] in order to induce Machine Learning (ML) models capable of classifying glass compositions according to their bioactivity properties[3]. The application of these models aims not only to identify new compositions of interest, but also to more comprehensively meet the demands of patients and health professionals in the area of tissue regeneration and engineering. For this analysis, we used computational tools based on the Python language, including pandas for data management and analysis, NumPy for linear algebra and scikit-learn for machine learning algorithms. The results obtained when applying machine learning algorithms have been promising, both for linear and non-linear classifier models, with some of them showing a ROC-AUC index of just over 0.87 (the maximum being 1, which would indicate that the model predicted 100% correctly); indicating the significant potential of using ML in the area of bioactive glasses. These results will be discussed in detail during the event, highlighting future opportunities to further improve this approach.

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Physics inspired machine learning at the atomic scale

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In industry, the blinding rate of progress in machine learning comes, in large part, thanks to the use of more powerful GPUs and more training data. Indeed, Richard Sutton's famous "bitter lesson" suggests that trying to inject expert knowledge into machine learning models is ultimately counterproductive. And yet, physical systems such as molecules and materials obey well understood laws that we know cannot be violated. In this talk, I will outline how Euclidean symmetry-equivariant Neural Networks (E(3)NNs) provide a powerful counterexample where incorporating the symmetries of 3D space allows us to achieve state-of-the-art performance on a variety of learning tasks focused on predicting properties of atomistic systems. Beyond the exceptional accuracy of these models, they also exhibit excellent data-efficiency as seen for interaction potentials, a particularly important property when labels typically come from time-consuming experiments or quantum-mechanical calculations.

Additionally, symmetry-equivariant models open the door to using tensorial quantities as both inputs and outputs of our models. By way of example of the former, I will show how the occupancies of atomic orbitals around transition-metal ions can be used to predict Hubbard parameters for DFT calculations leading to significantly more accurate predictions (e.g. for bandgaps, energy differences, open-circuit voltages, etc) but 80-100x faster a fully ab-initio scheme. As an example of the latter, I will show that we can predict Raman tensors, Born effective charges, NMR shieldings, all using very little training data. Finally, I will show a glimpse of how such ML models can be easily built using the 'tensorial' python code developed in my group.

Smart Surfactant Discovery with Machine Learning and Molecular Dynamics

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In this study, we combine classical molecular dynamics (MD) and machine learning (ML), to optimize the selection of surfactants for reduced interfacial tensions (IFT). The applications of surfactants are vast, and choosing a suitable surfactant for a desired application is a demanding task, as the number of possible surfactants is broad.
We have employed MD simulations to create an oil model representative of complex hydrocarbon mixtures found in presalt crude oil reservoirs. In addition, ML models were trained using the IFT obtained from the simulations, predicting the IFT values for nonsimulated surfactants, and we used the inferred results to perform new simulations iteratively. We then identified a surfactant with an exceptional IFT reduction. Subsequently, the proposed surfactant was experimentally tested, which confirmed the simulated results.
These findings hold significant promise for a smart process to find the best surfactant, as the number of available surfactants is large, and the combinations of fluid interfaces are as well vast.

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A combined DFT and machine learning study to understand catalyst and solvent effects on the conversion of CO2 into ethanol

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The conversion of CO2 into valuable fuels and chemicals has drawn significant attention due to the possibility of tuning the fuel yield and selectivity by changing the catalyst. In this work, our approach combines machine learning methods and DFT data to screen catalysts and find new candidates to use as a catalyst for CO2 conversion to products of higher commercial interest, such as ethanol. The C-C bond coupling is the determinant step in obtaining C2+ and is usually related to intermediates, such as C*, CH*, CH2*, CO*, CHO*, and COH* [1]. Using DFT at the BEEF-PAW level of theory, we obtained the reactions from gaseous CO2 to the previously mentioned intermediates. To accelerate the screening, we develop a machine learning algorithm that can predict reaction energy with a mean absolute error and a median absolute error close to 0.10 eV, which is very accurate in catalysis. Combining information from your DFT results and machine learning predictions, we obtained a full dataset containing information from your reactions of interest. Two of the best catalysts experimentally described are Fe and Co [2]. Therefore, using these two metals as a reference, we select fifty new potential catalysts between 2035 possibilities of pure metals and alloys. We are studying the energy barrier for C-C bond coupling over these new potential catalysts using the nudged elastic model to sort the best candidates. The side reactions to unfavorable products such as methanol and methane are also being evaluated to improve the selectivity of these new potential catalysts. As the solvent and alkaline metals were previously experimentally demonstrated to play an essential role in these reaction pathways, they will also be considered.

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Artificial neural network for classifying Raman spectra of starch/graphene oxide bio-nanocomposites

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Polymeric nanocomposites have been studied and used in industry since the mid-20th century due to the growing of concerns about the environmental impacts caused by non-biodegradable synthetic polymers. Therefore, motivated by the search for more sustainable alternatives, this study focused on the development of starch reinforced with graphene oxide (GO) bio-nanocomposite films with the aim to improve their mechanical and thermal properties, as well as their barrier properties [1-2].

The computational experiment consisted of the development and performance study of a two-level classificatory neural network multilayer perceptron. At the first level, the network structure was 1024 input neurons, followed by hidden layers with 100 and 50 neurons, respectively. At the second level, the same structure was adopted, however with hidden layers of 200 and 100 neurons. Both levels were trained with a learning rate of 0.01, alpha regularization of 0.0001, and cross-entropy loss functions, as well as the ReLu activation function [3]. For Raman spectroscopy data acquisition, we measured Raman spectra in 20 specimens of 10 different formulations of nanocomposites, which GO contents changed from 0.1 p/p.% to 1 p/p.% of GO, totaling 200 spectra per formulation. The results show high accuracy in the developed neural network in discriminating GO content in starch/GO nanocomposites through Raman spectroscopic data, which could have important implications in the scale-up of these nanocomposites by the industry, allowing the quality control using Raman spectra.

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Artificial Neural Network for predicting nonlinear optical properties of organic molecules

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One of significant interests in Photonics is the development of new technologies and devices for diverse areas, ranging from telecommunications to medicine. However, before these innovations are developed, the appropriate materials must be chosen, in this case, materials that present adequate nonlinear optical properties. Machine Learning (ML), recently, has been growing and gaining attention as a way to accelerate and facilitate the processes of finding new materials that exhibit the desired properties for their particular applications. For example, using deep learning models for compound classification in drug development [1] or using ML for predicting compositions for best glass properties [2]. This work aims to develop an artificial neural network (ANN) model for predicting organic molecules' nonlinear optical properties and understanding the effects of structure and composition in two-photon absorption, by taking advantage of the computational vision provided by ML tools. As a training database, chalcone-based molecules previously thoroughly studied by the Photonics Group in IFSC/USP will be used. The database consists of 33 molecules described by SMILES, with information of optical linear and nonlinear properties that will be trained with multilayer perceptron ANNs with different configurations aiming to find the one that best represents the results seen experimentally. With the ANN giving satisfactory results, we will be able to expand the model to organic molecules from different groups, achieving a computational tool able to assist in choosing molecules that have potential for study and applications in nonlinear optics.

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Development of WebApp for classification of dye-contaminated wastewater and solid surfaces: deep learning and adsorption studies

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The present study aims to develop cell phone software (WebApp) based on a deep learning study (convolutional neural networks – CNNs) to identify the contamination of wastewater and solid surfaces with organic dyes. Thus, several pictures of beakers (100 mL) containing water contaminated with crystal violet dye were used to feed CNN algorithms for image processing and classification [1]. Ethyl alcohol and distilled water were used as blank samples. The parameters of the CNN were: one fixed hidden layer with 128 neurons, batch (2, 4, 8, 16, and 32), and activation functions (rectified linear unit function and hyperbolic tangent function), with softmax activation in the output layer due to the presence of 2 classes as response variables. Dropout and Adaptive Synthetic Sampling (ADASYN) methods were used to prevent overfitting. According to the results, CNN performed best at the conditions: batch = 16, dropout = 0.65 (65 % of neurons turn off to prevent overfitting), and reLU activation function at the hidden layer. The algorithm showed 98% and 79% accuracy for training and test data, with training error = 1.15 and test error = 1.21. The confusion matrix reported 18 true positives and 2 false positives, but 1 true negative and 3 false negatives. Thus, the deep learning model showed high accuracy for the "water contaminated with dye" class, but low for the "water not contaminated with dye" class, suggesting that more images should be used for image classification. Future studies are intended to verify the use of the algorithm in identifying the contamination of dyes on solid surfaces. Therefore, it was possible to verify that CNN algorithms can be successfully used for image classification as a promising preliminary and fast identification of dye contamination in wastewater.

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Experimental Images Analysis Through Computer Vision and Artificial Intelligence: A Case Study of AFM and KPFM Images.

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Atomic Force Microscopy (AFM) and Kelvin Probe Force Microscopy (KPFM) are sophisticated imaging techniques under the umbrella of Scanning Probe Microscopy (SPM)[1], which offer nanoscale insights into material surfaces by detailing their physical and chemical properties. AFM generates a detailed topographical map through a sharp probe that scans the surface, measuring interactions. Conversely, KPFM measures the contact potential difference between the probe and the surface, shedding light on local surface potentials. Despite the advances, the correlation between surface characteristics, local charge densities, and photoluminescence remains a challenging and underexplored domain in research[2]. This study leverages computer vision[3] and artificial intelligence[4] to enhance the analysis of AFM and KPFM images, aiming to deepen our understanding of these complex relationships. We envisage that our study will establish a solid groundwork for the advancement of image analysis techniques. For instance, we can develop correlated images with embedded correlation metrics, enhancing our understanding of intricate relationships within the data. Moreover, exploring the interactions among parameters holds significant promise for the progress of materials science, especially in the realm of nanoimaging.

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Materials Informatics for ultra-wide bandgap design: A study of 1D perovskites of the Jakobssonite family

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In this work, we applied Materials Informatics to design new materials with ultra-wide bandgap for application in ultraviolet light-emitting diode. We conducted a systematic search in Materials Project[1] and in data from materials synthesis routes mined from scientific literature using natural language processing[2]. The intersection of these two databases, aligned with screening filters, identified the Jakobssonite as a potential candidate. Jakobssonite is a volcano mineral with chemical formula $CaAlF_5$[3] that having already been synthed in the laboratory[4]. Its structure is formed by AlF_6 octahedra, which are connected in only one direction, qualifying it as a 1D perovskite. We expanded the search space through atomic substitutions in the original structure using a chemical heuristic: we assume compounds with ABC_5 formula, where A are alkaline earth metals (Be, Mg, Ca, Sr, Ba), B are atoms from the boron group (B, Al, Ga, In, Tl) and C are halogens (F, Cl, Br, I), resulting 100 target materials. Then, high-throughput density functional theory simulations were performed using PBE-GGA and R2SCAN functionals. Structural relaxation were compared with universal machine-learning interatomic potentials based in graph neural networks: ALIGNN-FF[5], M3GNet[6] and CHGNet[7]. To determine synthesizability, we calculated thermodynamic stability by formation enthalpy and convex hull. As result we obtained new phase diagrams, band structures and effective masses of charge carriers of these new compounds.

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Meta-research on removal of emerging contaminants in water treatment process using nano-filtration membranes: Application of a text mining algorithm

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The increasing concerns over water pollution from emerging contaminants (e.g., pesticides) have highlighted the need for effective treatment methods. Nano-filtration membranes offer promising solutions for the removal of these emerging contaminants in water treatment process. Through their selective permeability, they can separate contaminants based on and molecular properties, ensuring high treatment degree and safe effluent for public health. In the literature, some studies examined the applications of nano-filtration technologies in removing emerging contaminants and pesticides in water treatment process. However, these studies were diverse because of the variety of the application scale (e.g., lab-scale) and operational conditions (e.g., pressure). Therefore, meta-research using text mining, a type of artificial intelligence (AI), is an effective technique to quantify the most significant topics related to application of nano-filtration membrane in water treatment. In our study, meta-research was implemented to extract the main trends and knowledge gaps in the field of removal of contaminant emerging using nano-filtration membranes in the literature through quantitative and qualitative analyses. The quantitative analysis was constructed through applying topic modeling and text analysis on the abstracts of these studies while the quantitative analysis was used to determine the most frequently examined topics in the literature. Accordingly, 235 articles related to our topic were gathered to perform meta-research and text mining on their abstracts to determine the most frequent topics covered in the literature. Multiple research gaps were illuminated based on the absence of these topics in the results of topic identification. The insights of the quantitative analysis can be used to define the knowledge gaps that should be investigated in future studies while the qualitative analysis can serve as a reference for the most frequent topics published in this field.

Printability of bioinks: a consolidated definition for future prediction models

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Printability is a term widely used nowadays for research on bioinks for additive manufacturing. Despite of this, it seems to be an absence of a common and universally accepted interpretation of the term, which can be source of misunderstanding among researchers, whereas some of them use printability and shape fidelity or shape accuracy indistinctly, other authors take into account different aspects of the printing process, such as, shape fidelity, extrudability, shape accuracy, including them as factors that, combined, lead to a more complete concept. In any case, and based on works reported in literature, a consensus is still lacking. In the case of bioprinting, cell viability is an extremely important factor to be included. This impacts any study on printability, since a partial view it would be based on a partial view of this property. For instance, studies relating rheological properties and printability and the prediction of this property on the physical properties of the inks will suffer of a generality as poor as the definition of the target property, independently of the methodology (physical modeling, machine learning, etc.). Thus, this scenario avoids any prediction of the complete manufacturing process. In this work a literature review between the years 2011 and 2023 on the concept of printability, following the evolution of the term and how it has been increasingly applied in the area. By using data science and machine learning tools, particularly text mining and text analytics, we can identify some cluster ideas leading to a general definition with greater acceptance in a wide range of different areas of application of additive manufacturing. Based on this we propose more general definition of printability in order to build such consensus.

Raw SMILES as descriptor for surface tension prediction with natural language processing techniques

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This study aimed to predict various properties of hydrocarbons through NLP techniques, utilizing as input features only the SMILES representation (simplified molecular-input line-entry system). For this purpose, we employed a recurrent neural network known as Long Short-Term Memory (LSTM) [1], implemented using PyTorch and Lightning libraries. We chose this network to extract intrinsic chemical bonds and atomic information from the SMILES for predicting the target properties, which were obtained from Yaws tables with physicochemical properties of molecules [2]. Initially, for validation and refinement, we utilized the dataset on surface tension as the target variable. In this process, we explored various approaches for extraction and prediction, including the use of one-hot encoding and embedding layers, as well as complementary techniques such as padding and dropout. The results obtained were promising, with a root mean squared error (RMSE) of 3.14 m/N and a coefficient of determination (R^2) of 0.81. Based on these findings, we have confidence in the neural network's capacity to extract intrinsic information from hydrocarbons, enabling the prediction of additional properties.

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AC05-Computational Design in Materials Science, Methodologies and interplay between Theory and experiment

A New Selectivity Descriptor for Electrosynthesis of H2O2: A Dream Come True?

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Understanding selectivity trends is a crucial hurdle in the developing innovative catalysts for generating hydrogen peroxide (H2O2) through the two-electron oxygen reduction reaction (2e-ORR). The adsorption free energy of O* and OOH* intermediate and the degree of O2's adsorption to the surface and have been suggested as selectivity descriptors for 2e-ORR.1 These approaches have been the main guide for understanding and predicting selectivity for 2e-ORR catalysts over the past decade. Yet, none of them has yielded an appropriate selectivity descriptor capable of quantifying selectivity, thereby serving as a metric for describing trends in selectivity. To resolve this issue, we provide a thermodynamically derived selectivity parameter (ΔΔG) based on computational hydrogen electrode (CHE) model2 which allows to quantify selectivity using predicted adsorption free energies of ORR intermediates (OOH* and O*) and free energy of H2O2.3 We validate the efficacy of this parameter, across a wide spectrum of reported binary alloys4 and demonstrate that only a small number of binary alloys with a single active site that have been reported to have high activity are selective for 2e-ORR.5 These findings highlight the potential of ΔΔG as a selectivity parameter for identifying high-performance 2e-ORR catalysts. It also demonstrates the significance of concurrently considering both selectivity and activity trends. This holistic approach is crucial for obtaining a comprehensive understanding in the identification of high-performance catalyst materials for optimal efficiency in various applications.

From basic research to new materials and technological applications: a journey through inorganic metal semiconductor industry and its sustainability

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This talk aims to provide clarity on the usefulness, diversity, properties, and applications of inorganic metal semiconductors. The joint use of advanced experimental techniques and quantum mechanical simulations allows us to navigate within innovative pathways for the synthesis, characterization, and rationalization of the behavior and underlying mechanisms behind these nano- micro-materials. To illustrate this, three topics are selected to contextualize the framework of this presentation from basic research to new materials and technological application: 1. Morphology, 2. Generation of reactive oxygen species. 3. Antimicrobial tecnologies.

Hydrogen pick-up and embrittlement in Nickel – an (atomistic) multiscale approach

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Hydrogen embrittlement (HE) remains a persistent challenge in metallic materials, posing a significant barrier to the advancement of a sustainable hydrogen economy. Nickel (Ni), with its single-phase microstructure, is a prominent model for HE studies in fcc metals. HE in polycrystalline nickel is characterized by a transition in fracture models from ductile transgranular (TG) to brittle intergranular (IG). Even though the detrimental effect of hydrogen in metals and alloys has been studied for decades, the interaction between hydrogen and the alloy microstructure still needs to be better understood. From a scientific standpoint, hydrogen is difficult to detect by conventional experimental techniques due to its small and high diffusibility. On the other hand, ab initio computer simulations can easily model hydrogen in alloys. However, atomistic studies related to H-embrittlement mechanisms usually focus on a single mechanism and are limited to idealized pseudo-2D setups.

Here we report two important aspects related to H embrittlement. First, we show how hydrogen pick-up may occur via a chemical reaction pathway namely the water conveyer mechanism. We highlight how hydrogen may reach defect-rich alloy microstructures, such as grain boundaries and crack tips. Then, we show a fully 3D atomistic simulations of cracks to study the effect of hydrogen in crack propagation under strain. The setup allows us to systematically vary the crack system, type and orientation of GBs, as well as the character and position of pre-existing dislocations. Interplay of different HE mechanisms and the occurrence of defect phases are also included in this work.

Multi-scale Modeling of Nanomaterials

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Carbon atoms exhibit various hybridizations (e.g., sp, sp2, and sp3), forming a wide array of structures with adjustable mechanical and electronic characteristics. Additionally, these structures can manifest diverse topologies across different electronic dimensions (0 for fullerenes, 1 for nanotubes, 2 for graphene, and 3 for diamond). These topologies have been exploited in developing numerous materials, including bucky papers, carbon nanotube-based artificial muscles, foams, and auxetic crystals [1-2]. However, the complexity of some of these materials' topologies poses challenges in accurately modeling their mechanical and structural properties. In this presentation, I will introduce and explore multi-scale modeling approaches for these materials, from fully atomistic to macroscale. It will include using artificial intelligence techniques, such as bioinspired ANT algorithms. Particularly noteworthy are the emerging molecular dynamics simulation methods based on reactive potentials, which allow the simulation of multi-million atom systems at a significantly reduced computational cost compared to fully quantum methods. These techniques also extend to non-carbon materials like chalcogenides and the newly realized 2D materials from non-van der Waals solids [3].

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Unraveling the advanced properties of magnetic and non-magnetic semiconductors from surface calculations

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In recent years, it has become evident that there is a strong connection between the improvement of available technologies and the development of new ones with the design of functional materials. Hence, materials development has increased in the last decades, standing out as one of the most important research fields. In particular, the interest in semiconductors has increased drastically due to their potential to treat water effluents contaminated with organic pollutants through a photocatalytic process, biocide activity aiming to minimize the dissemination of diseases, or improvement of advanced properties aiming at technological purposes. Among the advanced properties responsible for such interest in solid-state semiconductors, the electronic, optical, ferroelectric, magnetic, photocatalytic, biocide, ferroelectric, charge storage, and other properties are noteworthy.

Initially, computational methods played the traditional role of studying materials well-characterized; over the years, theory level and computational power have increased, enabling the investigation of novel materials with reliable results. In the case of solid-state materials, a large portion of the manuscripts based on computational approaches focus on assessing the bulk properties due to the high complexity related to surface calculations. However, it is well-stated in the literature that the properties of the bulk are different from those observed for exposed surfaces, being mandatory that this kind of model be adopted.

In this investigation, modern computational simulations based on Density Functional Theory were employed to investigate the surfaces of magnetic and non-magnetic semiconductor materials, namely $MnMoO_4$ and $AgNbO_3$, providing exciting results on the structural features, thermodynamic stability, electronic structure, magnetism, photocatalytic and biocide activity, charge carrier density and stability, as well as excited-states features.

Advances in Raman Confocal Spectroscopy Integration and chemometrics for drug analysis: innovative development strategies on sciences and applications in the characterization of medicines with innovative functionalities.

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This work will explore the fundamental principles of Raman confocal spectroscopy, applying them to different types of materials for physical-chemical characterization, aiming to obtain quantitative analysis methods for excipients and active pharmaceutical ingredients, applied in the development of medicines with innovative functionalities in solid pharmaceutical form with a direct impact on the therapeutic performance of the product. At the forefront of analyzing complex samples, chemometrics emerges as an essential discipline. The integration of optical microscopy with Raman spectroscopy, under the umbrella of chemometrics, not only offers a comprehensive and dynamic view of the complexity of samples, but also highlights the crucial importance of a complete and detailed characterization. This approach enables microstructural characterization both physically and

chemistry of the samples, allowing the precise assessment of chemical interactions that can affect the stability of medicines. In this context, an advanced computing methodology will be presented for the development and validation of analytical methods, with a updated approach, focused on solving complex problems related to microstructure of the components, especially relevant for the pharmaceutical sector. This methodology incorporates two key areas of chemometrics: experimental planning (DoE) and multivariate calibration. Furthermore, we will discuss rational strategies for the appropriate treatment of information, considering the order classification of data, as established within the scope of chemometrics. This approach guarantees an accurate analysis and reliable data, allowing deeper interpretation. It will be presented advanced experimental planning techniques, combined with the processing of higher order data, which can be strategically be applied in a synergistic way for accurate determination, making assertive decision and embracing risk analysis .

Condensed-to-atoms Fukui indexes as charge transfer descriptor for NFA-based organic solar cells

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Solar cells are photovoltaic devices that convert the sun's light into electrical energy, being a promising alternative energy source. In particular, organic solar cells (OSC) are well regarded devices as they present some advantages, including, but not limited to, relatively low cost, mechanical flexibility, synthesis versatility, and lightweight [1]. Among the OSCs, the non-fullerene acceptor (NFA) based ones can be highlighted, breaking power conversion efficiency (PCE) records in recent years [2]. Aiming to investigate how these OSCs can reach such high efficiency, in this study we explore some fundamental molecular properties of one of the most relevant NFA, the molecule Y6. The main approach is to use the condensed-to-atoms Fukui indexes (CAFI) [3], a reactivity descriptor, to rationalize some details regarding charge transfer and electron transport processes in these systems. Our results show that an appropriate alignment between nucleophilic and electrophilic reactive sites lead to efficient charge transfer routes in Y6-based systems, offering a reasonable explanation for high efficiency of such systems.

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Control of energetic landscapes in an acousticfluidic resonator made with polymers

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Acoustofluidic resonators employ acoustic radiation forces and microfluidic flows to manipulate cells and micropaticle in a levitated state. These resonators have garnered considerable attention due to their wide-ranging applications, from cellular microculture to biomedical diagnostics[1]. The structure of the resonator typically consists of a piezoelectric actuator at the bottom, a lateral substrate made of hard or soft material, and an upper glass reflector. The acoustic radiation force acting on particles or cells is directly linked to the spatial distribution of acoustic energy density (energy landscape) within the resonator. Therefore, achieving precise control over the energy landscapes becomes crucial for optimizing the performance and functionality of acoustofluidic resonators. In this study, we propose a novel approach utilizing computer-generated holography to achieve refined control over energy distributions within cylindrical resonators. We investigated several polymers (ABS, PMMA, and PE) to find the best outcome. Using the finite element method in the COMSOL Multiphysics software, we simulated the physics of acoustofluidic resonator waves. By defining desired energy distributions through mathematical functions, we employed the Nelder-Mead optimization algorithm to identify holograms that store wavefront information corresponding to the desired energy landscapes. Through this optimization, we achieved a high energy density of 10.6 kJ/m3 for PMMA. This study illustrates the capability of computer-generated holography as a valuable tool for adjusting radiation force in acoustofluidic resonator systems and demonstrates the feasibility of efficient acoustofluidic resonators using polymers as the base material in construction.

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Deciphering intermolecular interactions in natural rubber latex/lignin bio-based systems: a nanoscale and computational simulation approach

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Natural rubber latex (NRL) and lignin present distinct advantages due to their abundant availability and competitiveness compared to petroleum-based materials. Their unique properties, such as NRL's elasticity and lignin's hydrophobicity, make them promising candidates for composites formulations. However, the combination of both components is practically unexplored in the literature. This study aimed to develop innovative bio-based composites by combining NRL and lignin [1], focusing on assessing intermolecular interactions through experimental analyses and computational simulations. The incorporation of NRL with lignins extracted via various pretreatments (organosolv, alkali, and Kraft) was investigated. The nanoscale interaction between NRL and lignin was studied by atomic force microscopy (AFM), unveiling an intrinsic interaction with NRL according to the lignin extraction method. Computational models based on density functional theory (DFT) elucidated the energetically favorable interactions between NRL and lignin. Mechanical properties of NRL@lignin films replicate nanoscale and molecular interactions, indicating the optimal route for lignin addition in NRL. This synergy between experimental insights and computational simulations highlights the potential of NRL@lignin composites for various applications, such as adhesives, emphasizing the role of intermolecular interactions in optimizing mechanical and adhesion performance.

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Description of Excitonic Absorption in Metal Tri-Halide Pervoskites using Dispersion Models, a Hydrogen-Polaron Model and First Principles.

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Studies of excitonic absorption of metal tri-halide perovskites have depicted several attention for the high efficiency rates reaching up to 25%. Correct descriptions of excitons in these systems can lead to improvements to solar cell devices based on them. In this work, we present an optical study that covers modeling of the spectral curves, an effective model and first principles. First, the modeling of the excitonic absorption is studied in terms of a recently proposed model based on the Elliott equation and the band-fluctuations approach. This model is used to fit the absorption of metal tri-halide perovskites with different concentrations $FAPbI_{3-x}Br_x$, $MAPbI_{3-x}Br_x$, $CsPbI_{3-x}Br_x$ and $MAPbBr_{3-x}Cl_x$. Thus, retrieving information such as bandgap, exciton binding energy and Urbach energy. Secondly, the polar nature of this semiconductors can be modeled in terms of a hydrogen effective model with a potential that mimics the electron-phonon interaction. As a consequence, the exciton-polaron binding energy depends on five parameters. These are the low and high frequency dielectric constant, e_0 and e_∞, the effective masses of electron and hole, m_e and m_h, and the LO phonon energy $h\omega_{LO}$. These parameters can be estimated from first principle calculations using the independent particle approximation (IPA) for dielectric response, and the finite differences approach for phonon calculations. Thirdly, we perform an study of excitonic absorption based on first principles by solving the Bethe-Salpeter (BS) equation. Here, we use an approach that solves the BS equation using maximal localized Wannier functions and an analytical screened potential. The advantage of this approach is that it saves computational time up to two order of magnitude so that exciton properties of large systems becomes feasible. The comparison of binding energies and bandgaps retrieved by the different methodologies show a good agreement with other literature reports.

Electronic and mechanical properties of doped two-dimensional diamond

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Graphene is the leading two-dimensional material due to its unique properties as a zero-gap semimetal with a hexagonal carbon structure and sp2 hybridization. Moreover, It is the building block for various nanomaterials like fullerenes, nanotubes, graphite, and single-layer diamond (2D diamond). Doping or functionalizing carbon-based materials with different atoms and integrating them with diverse 2D systems could change their properties [1, 2]. Recent advancements in synthesizing and characterizing 2D materials have sparked considerable interest in 2D diamond, showing promise across multiple domains, including batteries, quantum computing, nano-optics, and nanoelectronics. This study investigated the structural, thermodynamic, dynamic, elastic, and electronic characteristics of C_4X_2 (X = B or N) systems. These structures comprise three graphene sheets with four covalently bonded C atoms per unit cell, resembling a 2D diamond. The outer layers are 50% doped with X atoms, with each X atom bonded to three C atoms. Our findings reveal that C_4X_2 systems exhibit stiffness comparable to diamond, with C_4N_2 nanosheets featuring wider indirect bandgaps and C_4B_2 systems showing narrower direct bandgaps in contrast to pristine 2D diamond. These results offer avenues for modifying the electronic properties of 2D diamonds through doping for specific applications, notably in nano-optoelectronics [2].

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Exploring the potential of Ag-based semiconductors for biocidal applications using high-throughput calculations with Density Functional Theory

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The ongoing SARS-CoV2 pandemic has posed a significant challenge to global health, leading researchers to search for effective materials that can combat its spread [1]. Ag-based semiconductor oxides have been identified as a promising solution due to their ability to generate Reactive Oxygen Species (ROS) that can kill microorganisms and prevent their transmission [2].

This research aims to further explore the potential of Ag-based semiconductors in combating the SARS-CoV2 virus and other microorganisms by applying a high-throughput computational approach using Density Functional Theory to analyze the surface stabilities and reactivities of these Ag-based materials [3]. The ultimate goal of this research is to improve public health outcomes by providing insights into the most effective Ag-based materials for ROS formation and the inhibition of microorganism transmission.

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Film thickness dependence of the optoelectronic properties of tin-doped indium oxide films studied experimentally and by DFT calculations

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Nowadays, the fabrication of thin films of transparent oxide-based semiconductors, such as metal-doped indium oxide, is of great interest to improve optoelectronic properties. In this work, we present the effect of the film thickness on the optoelectronic properties of tin-doped indium oxide films. Tin-doped indium oxide films with different thickness (235 to 513 nm) were grown by a DC sputtering technique. Subsequently, the as-grown films were subjected to thermal annealing at 500°C in vacuum atmosphere, for 2 h. X-ray diffraction analyzes confirmed the formation of the bixbyite-type cubic phase without no secondary phase. A subtle preferential orientation along the [400] direction was evidenced for the thinner films that was assigned to the presence of oxygen vacancies [1], whose density increases with the reduction of the film thickness, in agreement with the increase of the n-type charge carrier density as evidenced by Hall effect measurements. Besides, that carried density increase could be responsible for the enlargement of the band gap energy in accordance to the Moss-Burstein model. These experimental results are in agreement with theoretical calculations using density functional theory (DFT) where the oxygen vacancies generated in the ITO structure caused changes in the band structure, showing an augment in the energy gap values and in the n-type charge carrier density after including oxygen vacancies in the calculations. Resistivity measurements as a function of temperature carried out in the range of 80K to 300K reveal a metal-insulator transition, which transition temperature shows a direct dependence on the film thickness, achieving a minimum value of T~109 K and a high charge carriers (~1.1×10^{21} cm^{-3}) for the 235 nm film. Those values are found to be optimal for optoelectronic applications.

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Free radical generation process of novel quinoline photoinitiators in the photopolymerization of acrylic resins: a computational modeling study

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Acrylic resins have several applications mainly due to their great chemical versatility, and are widely used as biomaterials, especially in the field of dentistry. However, the typical photoinitiator (PI) materials present some toxicity, especially in cases when the photopolymerization process is not effective, highlighting the importance of a search for new PI with improved properties [1]. In this context, quinoline derivatives have been proposed as PI for acrylic resins, mainly due their excellent biocompatibility, low toxicity and appropriate optoelectronic properties. However, the mechanism involved in the radical generation process in these materials still deserves more studies [2]. Here we present a set of experimental and theoretical analysis of quinoline derivatives photopolymerization aiming to identify mechanisms and relevant interactions in such systems. Experimental data suggest that nitroquinolines with hydroxyl and methacrylate side groups (QNOH and QNMA) can act as type II PI in the polymerization of commercial resin monomers. Computational studies based on density functional theory (DFT) suggest an effective role of nitro groups on the PI activity, as well as the relevance of intermediate quinoline structures for the activation of reactive sites for resin formation.

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Induced magnetic moments and spin textures in synthetic ferrimagnetic Pt/Co/Gd heterolayers

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Interface-induced properties in thin films and multilayers are crucial in modifying the electronic structure, including inducing magnetism at materials interfaces. Recent interest in induced magnetic moments (IMM) in ferrimagnetic systems highlights their potential in processes like all-optical switching and the development of ultrafast spintronics devices, challenging the traditional focus on ferromagnetic/non-magnetic interfaces. This work analyzes the IMM in Pt/Co/Gd heterostructures, utilizing experimental techniques, such as scanning transmission X-ray microscopy and X-ray magnetic circular dichroism, and a multiscale theoretical approach. Key findings include the observation of zero-field ferrimagnetically coupled spin spiral textures, and the IMM transferred by Co across the Gd paramagnetic thickness, both at room-temperature. Density functional theory, atomistic spin dynamics and micromagnetic simulations uncover the microscopic origins of those observations, also revealing the existence of a flipped spin state within the Gd layers. In Pt/Co and Gd/Pt interfaces, IMM aligns with Co's magnetic moment, with negligible effect in Gd/Pt.

Magnetic nanostructures on intermetallic multilayers by ab-initio calculations

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Magnetic nanostructures have gained new importance in recent years due to the possible new applications in spintronics. Despite a huge amount of investigation in this field, many important challenges still need to be overcome.

Here we perform ab initio electronic structure calculations in the framework of the Density Functional Theory (DFT)[1] to investigate transition metal nanostructures on transition metals multilayers. We explore the versatility of the Real Space Linear Muffin-Tin Orbital in the Atomic Sphere Approximation (RS-LMTO-ASA) method [2], which allows a description of magnetic interactions in non-periodic systems in a natural way, due to its development in the real space. Particular attention is given to the formation of Skyrmions and conditions that may prevent Skyrmions annihilation at a film edge and stabilize zero-field skyrmions. We also discuss the proposal of J.Stephman et al. [3] where a suggestion is made that by decorating the film edge of Pd/Fe/Ir(111) multilayers with Co/Fe patches Skyrmions annihilation at the film edge can be prevented and zero-field skyrmions stabilized.

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Mechanical and Electronic Properties of a Zigzag Carbon nanotube with Pza-C10 sheet in a superlattice structure

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Carbon nanotubes (CNTs) are sheets of graphene rolled into a tube shape, that have garnered increasing interest due to their potential applications in nanoelectronic devices [1]. However the graphene is not the only 2D carbon material with which nanotubes can be formed; there are also 2D carbon allotropes, which can have various carbon rings, differing from the hexagonal (C6) rings present in graphene. A clear example is the Pza-C10 sheet, which consists of C5, C7, and C6 carbon rings, and exhibits semiconducting properties [2]. This study investigates the mechanical and electronic properties of a hybrid nanotube formed by a zigzag carbon nanotube (6,0) with metallic character and a nanotube (3,0) formed from a Pza-C10 sheet which is a semiconductor. Results through Density functional theory (DFT) and atomistic molecular dynamics (MD), implemented in the SIESTA and LAMMPS software, demonstrate the thermal stability of the new ZCNT-Pza hybrid NT model, while stress-strain calculations indicate minimal change in the Young's modulus and a reduction in tensile strength. Furthermore, band structure calculations reveal a transition from a metallic state to a semiconducting state depending on the number of Pza-C10 sheet atoms present in the NT. Additionally, ab initio stress-strain calculations show the presence of weakly dispersed bands for a strain value of 4% [3]. These findings indicate the potential for investigating novel hybrid nanotube structures formed from diverse 2D carbon allotropes.

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MOFs Learning : a data-based platform to accelerate functional MOF discovery

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Metal-organic frameworks (MOFs) are highly porous crystalline solids researched for applications in gas storage, separations, catalysis, sensing, and biomedicine. Their synthesis and the vast array of building blocks (metal precursors and organic linkers) allow for structural tuning to specific needs. The systematic cataloging in the Cambridge Structure Database (CSD) and other databases facilitates property characterization using molecular simulations, covering adsorption, thermal, mechanical, and electronic properties. However, synthed materials often exhibit more complexity than 0K crystal structures resolved by X-ray diffraction, and synthesis conditions are challenging to extract from literature due to lack of metadata and standardized data formats.

The "MOFs Learning" project, part of a national French consortium, sets best practices for managing and digitizing data in materials research. Collaborating with synthesis (IMAP), molecular modeling (IRCP), and materials testing laboratories (CEA), the project utilizes a broad range of measurements (volumetric and gravimetric adsorption, TGA calorimetry, XRD, FTIR, column adsorption, simulations, ...) to characterize materials. This work presents our management strategy and the tools developed to create a library of functional porous materials. We replicate materials like MIL-53, MIL-160, and CAU-20, ensuring accurate identification and property comparison with existing databases (NIST, synthesis mining). We design computational workflows to compute in-silico properties using FAIR practices, including containers (Apptainer) and workflow environments (AiiDA). A workflow for calculating the thermodynamics of adsorption is highlighted. The final project architecture will be presented as a database of standardized Sample Identity Cards (SID) integrating synthesis, characterization and simulation data and will eventually be available hosted on a web platform.

New insights into the catalytic behavior of α-MoO_3 catalysts for biofuel production: A jointed DFT and experimental approach

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α-MoO_3 micro- and nanoparticles were synthed by a modified-Pechini method, and the impact of crystal structure and crystal growth orientation on the formation of ionic defects and, therefore, on the catalytic performance for biodiesel production was investigated. Structural XRD refinements and Raman spectra revealed the formation of α-MoO_3 in a *Pbnm* orthorhombic phase [1], with ribbonlike morphology and with an anisotropic orientation growth along the (0*k*0) planes with the increase of the calcination temperature. We empha the dependence of the orientation change with the elimination of ionic-type defects (oxygen vacancies – V_O, and reduced Mo^{5+} centers) by the temperature using complementary techniques such as XPS and EPR spectroscopy. The catalytic activity of the samples depends on the orientation and the presence of defects that act as acid-active sites in the biodiesel production. This effect was confirmed by surface stability and reactivity simulated by DFT calculations using CRYSTAL17 software [2], suggesting that the Mo and O surface terminals greatly impacted the interface catalytic reaction. The highest catalytic performance toward the biodiesel conversion (89% of conversion at 150 °C for 2 h) was achieved for the polycrystalline catalyst calcined at 500 °C, which was correlated with random crystal orientation and the presence of reduced Mo^{5+} and V_O centers on the different facets exposed on the surface. The biodiesel production was confirmed by ^{1}H and ^{13}C NMR and by gas chromatography (GS) analysis.

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Probing $Ca_3Ti_2O_7$ crystal structure at the atomic level: Insights from PAC spectroscopy and ab-initio studies

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In 2011, Benedek and Fennie identified the Ruddlesden-Popper (RP) compound $Ca_3Ti_2O_7$ as a prototypical hybrid improper ferroelectric system. The sequence of structural phase transitions that $Ca_3Ti_2O_7$ undergoes to achieve polar symmetry as temperature decreases remains a topic of debate. To clarify this transition pathway from the low-temperature polar structure to the high-temperature phase, we have used Perturbed Angular Correlation Spectroscopy combined with Ab-initio electronic structure calculations [1]. This approach monitors the evolution of the electric field gradient tensor at calcium sites, effectively capturing the local environmental changes. Our findings indicate that above 1057 K, the local environments suggest a shift from the $A2_1am$ symmetry to an orthorhombic *Acaa* symmetry in the $Ca_3Ti_2O_7$ crystal lattice. This observation challenges the widely reported abrupt transition from the polar $A2_1am$ phase to the aristotype *I4/mmm* phase [2]. Furthermore, we noted that the temperature dependency of the electric field gradient within the stability range of the $A2_1am$ phase is sensitive to the previously suggested decrease in ferroelectric polarization of $Ca_3Ti_2O_7$ between 500-800 K, before the actual transition to the paraelectric phase takes place [1,3].

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Reversible Actuation of α-Borophene Nanoscrolls

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The discovery of graphene has led to increased interest in low-dimensional materials, including carbon nanoscrolls and boron-based materials, due to their unique properties and potential applications. Carbon nanoscrolls, tubular structures formed from spirally wrapped graphene sheets, have been synthed using various methods and exhibit unique structural, mechanical, and electronic properties. The exploration of graphene-like structures of other elements has also been realized, with borophenes, composed of boron atom monolayers, being of particular interest due to their structural stability and diverse configurations. Based on this, we proposed and explored for the first time, the structural and electronic properties of boron-based nanoscrolls (both armchair and zigzag configurations) using the DFTB+ method. It was investigated the electroactuation process involving charge injection and removal, in which, notably, we observed significant electroactuation, but there are distinct differences between borophene and carbon nanoscrolls. Molecular dynamics simulations revealed that these scrolls remain thermally and structurally stable across a wide temperature range (up to 600K), and the electroactuation process can be precisely tuned and even fully reversible for certain configurations.

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Structural, electronic and mechanical properties of double core carbon nanothreads

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Double core carbon nanothreads (NTHs) have been recently synthesized [1, 2] by compressing aromatic molecules that contain two rings connected by short chains featuring either double or triple bonds (such as azobenzene, diphenylacetylene and stilbene). These structures feature two conventional 1D NTH cores that are interconnected by covalent bonds arranged in various ways. In this work [3], we present a thorough examination of potential atomic structures for isomers of double-core NTHs, assessing their relative stability, and computing some electronic and mechanical properties through Density Functional Theory calculations. These 1D materials can exist in numerous isomeric configurations, distinguished by the core's intrinsic structure and the covalent crosslinking bond nature. The NTHs exhibit mechanical behavior akin to conventional single core materials, but are strengthened when continuous chains inter-link the cores. Their electronic behavior varies from metallic to insulating based on the arrangement of bonds connecting the cores, and the narrowest band gap materials exhibit electron delocalization along the interlinking chains. The variations in properties linked to the presence of bonds connecting the cores present fresh prospects for electronic and optical device design utilizing this class of materials.

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Theoretical investigation of $AgNbO_3$ as an effective electrocatalyst for hydrogen production

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There is great concern in the international community about studying alternative energy sources that can meet current and future demands. Hydrogen (H_2) appears as a good option, as it has a large amount of energy per unit mass. However, it must be obtained sustainably, and then the heterogeneous photocatalysis stands out. Focusing on the development of visible-light active materials, this project aims to study the catalytic properties of niobium-based semiconductors through computer simulations since Brazil holds 87% of the world's reserves of this metal.[1,2] The work was developed using theoretical-computational methods based on Density Functional Theory and WC1LYP hybrid functional to simulate structural and electronic properties of the $AgNbO_3$ bulk and surface models using CRYSTAL17.[3] Theoretical analysis of the electronic structure of (010), (100), (101), (110), (011), and (114) surfaces helps us to identify the most important facets of hydrogen production through water splitting mechanisms. Indeed, the bulk and (010), (100), (101), (011), and (114) surfaces are active in oxygen and hydrogen evolution reactions (OER and HER). These findings were analyzed based on the electronic descriptors of electrocatalysis, suggesting the potential for future applications in this field.

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TopIso3D Viewer: a topological analysis tool

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We present TopIso3D Viewer1, a software that generates 3D maps to analyze descriptors based on the Quantum Theory of Atoms in Molecules (QTAIM). It uses a software (Topond) already established in topological assessment, especially for users of the Crystal package, from the simple concept of creating 3D maps from a sequence of 2D maps. This concept greatly facilitates the topological analysis of periodic structures, by allowing any plane to be chosen and growing from the axis perpendicular to this plane. TopIso3D takes care of automating the launch of the Topond calculations, organizing their results in folders that can be easily accessed. The 3D maps are rendered in the user's standard browser, allowing an HTML file to be saved for later viewing, without the need for a new calculation launch. In addition, TopIso3D allows the issuance of a report, with the main properties of atoms and critical points calculated for the structure under study. Furthermore the manipulation of 3D maps is easy and intuitive. TopIso3D also presents the possibility of creating two-dimensional graphs that help in the classification of chemical interactions,based on two established methodologies2, For validation of the software, the classic system of molecule and Crystal urea was revisited. Acknowledgement:

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Understanding Multistability in Water Adsorption on Graphene and Graphene Oxide Membranes

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The interaction of water molecules with multi-layer graphene and graphene oxide membranes offers unique insights into adsorption dynamics, challenging conventional expectations. While graphene's properties has been extensively investigated, including its electronic, mechanic and impermeability properties [1,2], the behavior of water as an adsorbate has not been completely understood due to its divergence from other substances' behavior. Particularly in structures composed of multiple graphene layers, the expected behavior in gas adsorption following the increase of porosity, a reduction in uptake, is not observed when the adsorbate is water, thus classifying it in a different class of systems, that see an increase in molecule uptake upon the interlayer increase $-$ this is largely due to the formation of hydrogen bond networks. This deviation in behavior cannot be fully explained by typical models such as the BDDT. We employ a combination of molecular dynamics simulations via LAMMPS and the Grand Canonical Monte Carlo method to simulate physical adsorption of water in graphene structures for different interlayers and temperatures. We show that while increasing the interlayer leads to enhanced water uptake, increasing the temperature reduces the number of molecules that are adsorbed. To further investigate and explain this behavior, we make use of a mean-field approach based on the Ono-Kondo model [3], so the effects of Hydrogen bonding are represented through the addition of lateral interactions. Via the combination of both approaches, we find a great agreement between the mean-field predictions and the computational simulations, thus finding a reliable explanation for the condensation curves, in the isotherms, for the cases studied.

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Ab initio theoretical studies on the use of $CuMoO_4$ as a catalyst for CO_2 reduction

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The increase in the world's population, economy, and industry has brought with it an intense demand for energy, much of which is provided by the burning of fossil fuels, such as oil and coal, for example. This, in turn, has brought significant impacts on the planet's climate and ecosystem due to greenhouse gases, with carbon dioxide (CO_2) being one of the major contributors. A viable solution to address this problem is the process of reducing this molecule, in which it can be converted into chemicals and liquid fuels, such as carbon monoxide, formic acid, methanol, and ethanol. Thus, CO_2 can be used as a fuel while reducing the amount of carbon in the atmosphere [1].

One approach to CO_2 reduction is the use of transition metal-based molybdates ($AMoO_4$, where A = Cu, Ni, Co, Fe, or Zn, for example), as these substances have shown good electronic, magnetic, and catalytic properties. Therefore, copper molybdate ($CuMoO_4$) has emerged as a good option for this purpose. There are approximately six different polymorphs of $CuMoO_4$, which can vary according to temperature [2].

In this work, based on Density Functional Theory (DFT) calculations, we report the most accessible crystal morphologies of this material and discuss the main geometrical and electronic features that control the catalytic activity for CO_2 reduction.

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A computational modeling study on stability optimization of hybrid perovskite solar cells

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Hybrid organic-inorganic AMX3 perovskite structures are considered promising systems for solar cell applications, mainly due to their high efficiency and synthesis versatility. However, despite the exceptional performance noticed for perovskite-based solar cells (PSCs) over the past few years, the typical low stability of these devices is still a barrier for large-scale production and industrial application. The main challenges are the exposure to moisture, oxygen and UV light, as well as the structural instability, ion movement into the active layers, and interfaces between perovskite and charge transport layers [1, 2]. Recent studies indicate the potential of chelating agents to minimize the degradation rate of these compounds, however systematic studies are still necessary to clarify the associated processes and obtain improved materials [3]. In this study, density functional theory-based calculations are employed to evaluate the selectivity and effectiveness of the interaction between PSC constituents and typical chelating organic structures, aiming to identify optimal compounds for capture/retention of PSC ions. Condensed-to-atoms Fukui indexes, local softness analysis and adsorption studies were conducted to select the most promising systems. The results show the potential of non-hydrogenated carboxyl-based groups as relevant chelating groups for stabilizers of Pb 2+ and I-1 ions.

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Application of FEM for modal analysis and frequency response of a conductive ABS bipolar plate printed by the fused filament fabrication method.

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The 3D printing technology has been widely explored in various fields, including the manufacturing of electronic components. This study investigates the structural properties of a bipolar plate of a PEMFC (Proton Exchange Membrane Fuel Cell) printed in 3D with an electrically conductive filament based on ABS (acrylonitrile butadiene styrene). Using the FEM (finite elements method) on MSC PATRAN NASTRAN software, modal and frequency response analyses are conducted with the aim of understanding the dynamic and structural characteristics of this plate, especially regarding its natural frequencies and behavior under resonance.

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Characterization of Fe nanoparticles on $SrTiO_3$ (001) using X-ray photoelectron diffraction (XPD) and low energy electron diffraction (LEED)

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The perovskite ceramic strontium titanate (SrTiO3 or STO) possesses remarkable properties that make it highly promising for catalytic, photocatalytic, electronic, magnetic, spintronic, and biomedical applications. The bulk SrTiO3 crystal is composed of alternating TiO2 and SrO layers along the (001) direction, and its ideal (001) surface can be terminated by either of these two layers [1]. Deposition of Fe onto SrTiO3 (001) can yield Fe nanoparticles with various applications, whether in magnetic and electrical applications, biomedical applications, or for use as contrast agents in magnetic resonance imaging, among others [2]. X-ray photoelectron diffraction (XPD) and low energy electron diffraction (LEED) have been successful in determining various SrTiO3 (001) surface structures. This study focuses on investigating the formation and structural characterization of Fe nanoparticles deposited on a Nb-doped SrTiO3 (001) surface using these techniques. Comparison of experimental diffraction patterns with simulated theoretical patterns using the "Multiple Scattering Calculation of Diffraction" software suggests the formation of Face-Centered Cubic (FCC) iron nanoparticles.

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Characterization of Si segregation in AISI9254 steel and FEM modeling of microstructural effects on the mechanical behavior of railway fastening systems

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The study involved the evaluation and quantification of the volumetric fraction of Si segregation present in AISI9254 steels obtained from railway fastening clips. A brief investigation is presented to analyze the sensitivity and effectiveness of commonly used etching reagents for revealing Si segregation bands in the martensitic microstructure of the specimens. Specific transverse and longitudinal sections of the Fastclip model clamp were analyzed. The most effective etching reagent for this purpose was Teepol, which enabled to assess the volumetric fraction of segregation present in the clamp samples. Additionally, optical micrographic images and high-resolution scanning electron micrographs were employed for FEM microstructure modeling. Object-oriented finite elements (OOF2) and Abaqus software were used to evaluate the mechanical elastic and elastoplastic behavior of Si segregation in microstructure assuming plane stress conditions. Nanoindentation measurements were employed for characterizing the mechanical properties of Si segregation bands at the nano-/microscale. The measured material properties were used in the numerical models, allowing for a more detailed analysis of the structural (defects) and mechanical behavior of the railway fastening system under different operational conditions such as tension and compression loads. The influence of Si segregation on the mechanical properties was evidenced from the experimental results and also from the FEM models, which showed that stress field changes due to the presence of silicon segregation. It was found that an increase in the volumetric fraction of Si segregation in the microstructures introduces strain accumulation, with is maximum at the interfaces of segregation and steel.

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Computational evaluation of experimental models for exciton diffusion parameters

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Understanding the energetic efficiency problem in organic photovoltaics (OPV) relies on investigating exciton's transport mechanisms. The transport properties of excitons in OPV systems are influenced by a myriad of factors, such as morphology, temperature, absorption coefficient α and excitation conditions. Experimentally, the typically determined parameter is the diffusion length Ld, which characterizes exciton dynamics. To measure Ld , experimentalists rely on spectroscopic techniques, such as photoluminescence quenching methods [1]. These measurements are limited by assumptions about exciton behavior, which can result in inaccurate estimations of Ld. In this work, we conducted computational tests to evaluate the assumptions typically incorporated into experimental setups for estimating Ld, specifically focusing on: homogeneous excitation, annihilation effects and normal diffusion. This was done by employing Kinetic Monte Carlo (KMC) algorithms combined with Förster Resonance Energy Transfer (FRET) theory to simulate exciton dynamics [2]. Our methodology included electronic structure calculations using Density Functional Theory and its time-dependent extension to evaluate absorption and emission spectra of selected compounds. Here, we accounted for vibronic effects by employing the nuclear ensemble method [3]. Our results demonstrate that assuming the homogeneous generation of excitons can significantly impact the estimation of Ld. Additionally, annihilation effects were considered. This work aims to examine the common methodologies for estimating diffusion parameters in optoelectronic devices.

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Computational Investigation of the covalent functionalization of Group 14 layered materials

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Computational Investigation of the Covalent functionalization of Group 14 layered materials

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We have employed density functional theory to investigate the covalent functionalization of group 14 layered materials: graphene, silicone, germanene, stanene, and plumbene. Eighteen functional groups were considered: H, F, Cl, Br, O, S, Se, OH, SH, CH3, CF3, NH, NH2, C6H5, C6H4, CCl2, CBr2, and the azomethine ylide. The results indicate that in all cases, oxygen the most reactive reagent, followed by fluorine. However, the reactivity experiences notable and unexpected changes as we move down in the periodic table. For example, germanene and stanene are less prone to oxidation than silicene. The five materials studied present a rich organic chemistry, and functionalization with azomethine ylides, benzynes, and carbenes can be easily accomplished, as indicated by the exergonicity of the processes. The reaction energies become lower as the number of functional groups increases, thus favouring the agglomeration of functional groups attached unless the steric effect alters this pattern. The electronic properties of the functionalized monolayers are discussed. In all cases it is possible to fine the band gap up to 2 eV by adjusting the type and number of functional groups utilized. Nevertheless, caution must be taken because the layers may decompose at high levels of functionalization. We expect that this work can motivate new experimental investigations that pursue the synthesis of new layered materials based on the functionalization of group 14 monolayers.

Computational studies of metallic ions incorporation in melanin for biomedical applications

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Melanin-like dopamine compounds are widely used for the design of biomaterials, presenting a huge potential for biomedical applications [1]. It is mainly due its biocompatibility and presence of active functional groups which allows effective interactions with molecules, enzymes and/or ions. A relevant aspect is the melanin capacity of ion chelation, which allows the formation of a variety of bioactive complexes. In particular, it has been reported the use of melanin+Zn+2 complexes as an effective antibacterial agent [2]. Despite the number of works in the literature, there is still a notable gap regarding the role of ion-melanin interactions for biological applications, mainly due to the difficulty of experimentally analyzing such systems [3]. In this report, we use density functional theory (DFT) based calculations to evaluate melanin+Zn+2 (oligomeric) complexes and lipopolysaccharide molecular models, to better understand the influence of metal ion on the electronic properties of such materials, and underline possible relevant mechanisms that rule their biological activity. The results show that the presence of the metal center on the oligomers affects the structural properties and the local reactivity of the melanin-based systems, leading to an intense electric polarization, and activation of the metal (increase of its local reactivity), which play a relevant role in their interaction with typical lipopolysaccharides present in gram-negative bacterias. Our data are also compatible with other experimental spectroscopic results associated with such systems, allowing us to interpret additional effects of ion chelation on the electronic structure of the complexes.

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Correlations of mechanical properties by SPT and conventional tensile test for stainless steel 316L

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The Small Punch Test (SPT) method is an "almost non-destructive"[1] method by uses miniaturized samples to obtain mechanical properties of materials. It was development by nuclear industry to analyses mechanical behavior of irradiated materials principally by small volume of the samples, which facilitates their storage and handling. Its applications are spreading across several areas of materials engineering, for use in situations where conventional methods do not apply. SPT consists of pressing a sphere, with a diameter equal to 2.5 mm, in a miniaturized sample of circular geometry (diameter d = 8 mm and thickness about 0.5 mm)[2], which has fixed edges, tested in conventional mechanical testing machines with the aid of a device developed for their achievement.

In this work, mechanical properties of stainless steel (316 L) were abstained by two different methods: conventional tensile test and the small punch test (SPT), for comparing the results and allow the evaluation of the method. The SPT results depends on graph interpretations and discussions take place at now. Correlations of results guide us in choosing the most appropriated method for interpreting the force x displacement graph from SPT.

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Describing heat dissipation in the resistive state of three-dimensional superconductors

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In this work we study the role of the heat diffusion equation in simulating the resistive state of superconducting films. By analyzing the current-voltage and current-resistance characteristic curves for temperatures close to T_c and various heat removal scenarios, we demonstrate that heat diffusion notably influences the behavior of the resistive state, specially near the transition to the normal state, where heat significantly changes the critical current and the calculated resistance. Furthermore, we show how the efficiency of the substrate has important effects in the dynamics of the system, particularly for lower temperatures. Finally, we investigate the hysteresis loops, the role of the film thickness and of the Ginzburg-Landau parameter, the findings reassuring the significance of accounting for heat diffusion in accurately modeling the resistive state of superconducting films and provide valuable insights into its complex dynamics. To accomplish these findings, we have used the 3D generalized Ginzburg-Landau equation coupled with the heat diffusion equation.

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Development of Empirical Potentials for Fe-Si Alloys

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Steel, a key iron-based alloy, changes its mechanical properties from alloying, introducing elements like silicon (Si) that modify its microstructure and enhance mechanical properties through solid solution strengthening. Si improves steel's strength, hardness, and ductility. Molecular dynamics (MD) simulations, simplifying Schrödinger's Equation to solve atom dynamics using Newton's Motion Equations, are restricted by a lack of Embedded Atom Method (EAM) [1] interatomic potentials for Fe-Si systems, particularly at low Si concentrations. This work uses an optimization program to refine EAM potential parameters using Density Functional Theory derived data, focusing on defects' interaction energies, lattice distortions, and Si-vacancy interactions in bcc-iron supercells through a Simulated Annealing algorithm [2]. It integrates Ackland's [3] state-of-art iron potential functions and optimal fitting values for silicon and iron-silicon functions, improving MD simulation accuracy for specific alloys. The work aims to compare reference and test data, not used in optimization, to assess the potential's transferability. The resulting potentials align well with both datasets, proving the potential's effectiveness and it can generate new potentials for other binary ferrous systems with low concentrations of alloying element.

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DFT Analysis of volatile organic compounds sensing on the Ag-decorated BPN

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Efficient, miniaturized and highly sensitive sensors to detect volatile organic compounds (VOCs) have become vital tools to minimize pulmonary diseases and other sicknesses [1,2]. In this work, the adsorption capabilities of methanol and ethanol were investigated on the recently synthed biphenylene (BPN) monolayer [3] using the Ag decoration strategy. Although the pristine BPN has suitable VOCs adsorption, the lower adsorption strength and the small charge transfer affect the sensor performance. On the other hand, the Ag decoration increases the gas sensitivity, with moderate chemisorption values of –0.67 eV and –0.83 eV for methanol and ethanol, respectively, and presenting transitory chemical bond character (neither ionic nor covalent) between Ag atoms and the –OH radical. In addition, significative work function changes ($\Delta\phi > 0.23$eV), great charge transfer and rapid recovery times at room temperature (0.18s and 87.9s for methanol and ethanol, respectively) indicate a great VOCs sensitivity. The feasibility of the Ag-BPN and Ag-BPN + VOCs systems by ab-initio molecular dynamics (AIMDs) was analyzed, which confirms that both systems are stable at 500K. Therefore, the DFT calculations employed here can guide experimentalists in exploring new miniaturized sensor devices based on BPN.

Disclosing the stability, electronic structure, and band alignment of $AgNbO_3$ surfaces for ROS production

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$AgNbO_3$ represents a notable perovskite material that synergistically combines the benefits of both Ag- and Nb-based materials. In particular, the silver niobate exhibits ferroelectric properties, which can effectively promote the migration of photo-generated carriers responsible for the piezo-photocatalytic process to lead to efficient redox reactions on the catalyst surface for the degradation of different pollutants through the generation of reactive oxygen species (ROS).[1,2] In this work, DFT calculations have been employed to delve into the structural, electronic, and optical properties of (010), (100), (101), (110), and (011) low index, and (114) surfaces of $AgNbO_3$ were analyzed in detail by DFT calculations carried out using CRYSTAL17.[3] Wulff constructions were used to predict the available morphologies and their transformations, which were matched with the experimental images obtained by electron microscopy. Additionally, theoretical results show that the co-adsorption process of both H_2O and O_2 molecules opens a thermodynamically favorable pathway for the initial stages of the formation of reactive oxygen species: hydroxyl (·OH) and superoxide ($\cdot O_2^-$) radicals, thereby revealing a previously unreported chemical mechanism for the generation of these high reactive species. Our results present clues into utilizing these $AgNbO_3$ surfaces on technological applications based on ROS generation.

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Disclosing the structure and electronic properties of copper-doped lead apatite

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A superconductor is a material that, when cooled below a specific critical temperature, loses its electrical resistance, allowing the conduction of electric current without dissipation.[1] Additionally, superconductors also exhibit the Meissner effect, characterized by the expulsion of a magnetic field from their interior during cooling. This property is crucial for applications in electrical transmission, where minimizing energy losses is essential. However, the need for extremely low temperatures to achieve superconductivity limits its practical viability due to the complexities and costs associated with cooling. Recently, a material called LK-99[2] was proposed as the first room-temperature superconductor, although its synthesis has yielded controversial results. Consequently, an investigation was initiated to explore lead apatite through the hydrothermal method as a possible alternative to facilitate synthesis and evaluate its superconducting properties. However, the data obtained revealed a distinct phase from that of LK-99. Using theoretical simulations based on Density Functional Theory (DFT) implemented in the CRYSTAL17[3] program, mechanical calculations were performed, including material volume optimization, to analyze its morphology, surfaces, and superconducting characteristics. This integrated approach between experimental and theoretical data will not only enable facilitated synthesis but also comprehensive characterization of the electronic and morphological properties of this potential superconductor.

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Effect of oxygen vacancies on the structural and magnetic properties of Fe-doped ITO studied by first-principles DFT calculations

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Nowadays, the manufacture of thin films based on *Transparent Conductive Oxides* (TCOs) doped with transition metals, such as Fe-doped I*ndium Tin Oxide* (ITO), is of great interest in order to improve optoelectronic and spintronic technology. In this work, the effects of oxygen vacancies on the structural and magnetic properties of Fe doped ITO compound were studied using D*ensity Functional Theory* (DFT). The spin polarized DOS results reveal that Fe impurities provide magnetic properties to the Fe-doped ITO. In addition, the incorporation of oxygen vacancies produces changes in the DOS, inducing the appearance of new electronic states, and causing a decrease in the magnetic moment which suggests an antiferromagnetic order [1].

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Electronic and structural properties of 2D biphenylene network deposited on different metallic surfaces

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Different carbon allotropes arouse significant interest due to their distinctive characteristics and potential applications in diverse fields, especially those in their 2D form. Recently, a nonbenzenoid carbon allotrope named biphenylene network was successfully experimentally fabricated [1]; however, although it has been predicted that biphenylene may possess some key properties for technological applications such as spintronics [2], some of its electronic, mechanical, and structural properties on different surfaces are not yet completely understood. In this work, we investigated the structure and electronic properties of the biphenylene network on different surfaces as Cu3Au(001), Cu/Cu3Au(001) and Au/Cu3Au(001), using Density Functional Theory (DFT). After we optimized the geometries of the biphenylene on the different substrates, some of its electronic and structural properties was extracted. We found that the biphenylene network can be stabilized on the surface of Cu3Au(001) and prefers a richer Au surface such as Au/Cu3Au(001). Furthermore, biphenylene presents a metallic band structure without Dirac cones as expected in graphene structures.

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Electronic structure of non-fullerene acceptors for solar cells: influence of constituent blocks and side groups

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High-efficiency acceptor materials have been obtained using acceptor-donor-acceptor block structures. Such non-fullerene acceptors (NFA) have been successfully employed in bulk heterojunction organic solar cells (BHJOSC), presenting an intense optical absorption into the visible/near-infrared range, as well as electron mobility, short-circuit current density and power conversion efficiencies higher than fullerene-based devices [1]. However, despite the promising results obtained for NFA-based devices, there is still a relative lack of information regarding the influence of the distinct fused and non-fused rings in their basic structures [2]. Preliminary results from our group have suggested the possibility of identifying relevant patterns linking the properties of small building units (fused rings) and NFAs [3]. In this study, electronic structure calculations based on density functional theory (DFT) were carried out for typical NFAs building blocks, aiming to understand the influence of non fused units on the electronic structure of such compounds as well as their resulting properties. The results allow for identifying relevant patterns for the construction of optimized systems, enabling the proposal of which sites are associated with charge transfer processes in these systems.

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Estimating annihilation coefficients and radii in organic molecules: a methodological study

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Energy transport in organic optoelectronic devices is significantly influenced by bimolecular effects, particularly the interaction between two excited molecules. This interaction can result in the annihilation of energy carriers, representing the predominant non-radiative loss mechanism at high exciton densities [1]. In this process, the annihilation coefficient (κ) and annihilation radius (R_A) are two relevant quantities. The former estimates how significant the annihilation process is in the system, while the latter represents the distance at which the annihilation process predominantly occurs [2]. However, determining these for singlet states in organics is challenging [3]. This study addresses this challenge by proposing a methodology to estimate the κ and its associated R_A for singlet states in organic molecules. We employed density functional theory (DFT) and its time-dependent extension (TD-DFT) to compute the electronic properties of the ground and singlet first excited states of typical organic systems. The photophysical properties of the ground and singlet first excited states were determined using the nuclear ensemble method, enabling the calculation of energy transfer rates via the Förster mechanism. By utilizing the dipole-dipole interaction between singlet excited states to estimate R_A and a Förster-type expression to model the annihilation rate, we conducted Kinetic Monte Carlo simulations to estimate κ of organic materials. A linear relationship between κ and organic system diffusion parameters is found, indicating a similar relationship with exciton diffusion coefficient. This sheds light on energy transport mechanisms and enhances our understanding of non-radiative loss processes.

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Evaluation of cathodic protection effectiveness in offshore flexible pipes: a 3D model of species permeation and corrosion phenomena

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Flexible pipes are offshore structures that connect subsea production wells to floating units. These materials are subjected to dynamic stresses during operation, which can lead to failure, and metallic corrosion, particularly in the annular region, is a common cause of structural damage. Annulus corrosion can be enhanced by permeation of aggressive species (such as O_2 and chloride ions) present in marine electrolyte [1,2]. One of the forms of protection against corrosion is achieved by cathodic protection and the use of sacrificial anodes. In this work, a computational model was proposed for monitoring corrosion phenomena in the annular region exposed to aggressive species, as well as their impact on the effectiveness of cathodic protection along the structure. Simulations were performed using Comsol Multiphysics® software. Part of the permeation phenomena involving species mass transport through the polymer layer was simulated in a 2D model. The behaviour obtained was fitted to a 3D model of a flexible pipe section with polymer and metallic layers. A bracelet-shaped sacrificial anode concentric with the layers was placed in the outer region. Stationary and dynamic simulations were carried out. The oxygen concentration and other species from the marine environment were correlated with the corrosive processes in the annular region and the effectiveness of cathodic protection along the flexible pipe. It was also possible to evaluate the effect of the cathodic protection range and to estimate the anode life in a structure like real operating conditions, considering the influence of transport phenomena.

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Exciton transport efficient OPVs: a Monte Carlo Algorithm study of the cascade architecture

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Organic solar cells have emerged as a promising and environmentally friendly alternative to traditional silicon-based ones. The morphology of these cells plays a crucial role in optimizing their efficiency. Central to their operation is the diffusion of excitons, quasi-particles, within a donor layer containing organic molecules arranged in different configurations. This study explores various cascade-oriented architectures within the donor layer to maximize exciton flow towards donor-acceptor interface[1]. This involves segmenting the donor layer into sublayers, each consisting of different organic materials, strategically arranged to facilitate energy transport towards the interface[2]. Using Density Functional Theory, electronic structure calculations were conducted for four organic molecules, previously used in experiments, and exciton diffusion was simulated using a Kinetic Monte Carlo algorithm. Our results demonstrate that the organization of materials within the donor layer and the thickness of the sublayers significantly impact the overall efficiency of the solar cell. This research contributes valuable insights to the field of organic photovoltaics, aiming to advance its development and eventual widespread adoption.

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Exploring local reactivity of functionalized carbon quantum dots for efficient nitric oxide delivery systems

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Carbon Dots (CD) are nanomaterials that have been receiving increasing attention due to their optical and electronic properties. One of the key advantages of CD is their high solubility in water, making them very attractive for biomedical applications, including for drug delivery systems, alongside facilitating processes such as cellular apoptosis through the liberation of radicals like NO. However, the efficiency of compound release can be affected by various factors, such as the reactivity of CD with other compounds present in the system. In this context, the present study aims to explore the reactivity of CD model systems functionalized with triphenylphosphine (TPP) and cysteine-based ligands for NO release, a radical with applications in drug delivery for inducing apoptosis in cancer cells via Density Functional Theory (DFT) based calculations. The investigation also seeks to understand the formation and bonding process of functionalized CD. The results show that the CD with different terminations exhibits very similar local reactivity and frontier molecular orbitals; however, the very dissimilar optical properties are evidenced in functionalized systems. The findings also highlight the crucial significance of considering the structural changes induced by ligands in CD when assessing their reactivity and optical properties.

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Exploring the halide exchange engineering on lead-free $Cs2AgSbCl_{6-\delta}Br_{\delta}$ mixed-halide double perovskite: A DFT study

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Halide perovskites, commonly studied in optoelectronics, have an ABX3 structure, where A+ is a monovalent cation, B2+ is a divalent cation and X- is a halide ion. The use of Pb2+ ions in the B site poses toxicity problems and can create instability in solar cells. To address this, replacing Pb2+ with heterovalent elements is explored to obtain double halide perovskites, denoted as A2B'B''X6, where B' and B'' are trivalent and monovalent cations, respectively [1]. Anion exchange reactions can tailor the optical and electronic properties of these structures by the band gap energy control. This study seeks to reveal the strong correlation between the structure composition of Cs2AgSbCl6-δBrδ mixed-halide double perovskites by means of modeling and computational simulation methods. The Cs2AgSbCl6 structure belongs to the $Fm\bar{3}m$ space group, but anion substitutions break down the symmetry. This structure consists of a 3D lattice of [SbCl6-δBrδ] and [AgCl6-δBrδ] distorted octahedral clusters. For different δ values, the compounds exhibit different space groups: I4mm (C4v) for δ = 2 and 4, remaining I4mm (C4v) for δ = 1 and 5 and showing R3m (C3v) symmetry for δ = 3. Incorporating Br- significantly reduces structural organization in short and long ranges. All Cs2AgSbCl6-δBrδ compounds exhibit indirect band gap energy at X → L point, reducing from 2.72 eV to 1.77 eV with the increased Br content.

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High Entropy Alloy Nanoparticle Catalysts for Hydrogen Evolution Reaction: A First-Principles Perspective

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Hydrogen (H_2) is recognized for its clean energy potential and high energy density, presenting itself as a promising alternative to fossil fuels[1]. The electrolytic production of hydrogen in water, through the hydrogen evolution reaction, emerges as a mature and widely used approach. However, the efficiency of H_2 production through it has been hampered by low efficiency and significant overpotential. Therefore, the development of catalysts for HER becomes crucial, requiring materials with high efficiency, stability, and durability. Given this, the objective of the work was to investigate a large set of high-entropy alloy nanoparticles formed by 55 atoms with a random composition of Ag, Au, Cu, Pd, and Pt and their physical and chemical properties based on first principles calculations to create a database and apply machine learning for the catalytic investigation of these nanoparticles. First-principles simulations based on DFT were carried out, implemented by SIESTA software based on localized atomic functions. Decision tree-based machine learning models like gradient boosting were used. 1000 simulations were carried out, and the exploratory analysis showed that in most cases, hydrogen atoms end up bonded to two or three metallic elements. When the adsorbed hydrogen has a coordination number $CN(55) = 3$, the best results were obtained for ΔG_H. It is verified that the case in which the initial adsorption site is composed of Au presents the highest frequencies around the thermoneutrality of the Gibbs free energy, which is indicative of an improvement in the catalysis of the hydrogen evolution reaction.

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Influence of Morphological Variations on the Exciton Annihilation in Organic Materials

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Organic optoelectronic devices have witnessed remarkable advancements in recent decades. These advancements are closely tied to the understanding of device photophysical processes. One of the key processes is exciton transport, predominantly described by the Förster mechanism [1], which determines the rate of excitation transfer between neighboring molecules. The morphological distribution of molecules within the organic lattice can significantly influence the efficiency of this mechanism. Additionally, the phenomenon of exciton annihilation, involving the interaction between two excitons, can also impact device efficiency [2]. In this study, we investigate how different morphologies of the organic film influence exciton dynamics, considering the potential role of exciton-exciton annihilation. Electronic structure calculations were performed on two typical organic polymers, poly (p-phenylenevinylene) (PPV), polythiophene (PTh), using Density Functional Theory (DFT). Subsequently, photophysical properties were obtained using the nuclear ensemble method. These features were used in a Kinetic Monte Carlo algorithm that simulated exciton diffusion across various morphologies. Our findings demonstrate that exciton dynamics are significantly influenced by morphological variations, and such variations can mitigate the annihilation process in optoelectronic devices. This research makes significant contributions to the field of organic photovoltaics, with a focus on reducing annihilation effects and thereby enhancing energy transport.

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Interfacial Properties of MXene $Ti_3C_2T_x$/Polypropylene Nanocomposites from Multiscale Simulations

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Tribology, the study of friction, wear and lubrication, plays a critical role in a wide range of industrial sectors, whose impacts on the global economy and environment are complex and multifaceted. Therefore, there is a growing need for developing innovative materials with improved tribological properties. MXenes are a class of 2D nanomaterials, which one promising approach is the incorporation of MXene Ti_3C_2 nanoparticles as reinforcement in polymers, polypropylene (PP) in particular, a material of interest for engineering applications. In many engineering problems involving lubrication, there is great complexity in the existing interactions at the nanoscale (nanotribology), which requires a more pragmatic approach through the Integrated Computational Materials Engineering (ICME), based on multiscale implementation. Atomistic simulation techniques, such as Density Functional Theory (DFT) and Molecular Dynamics (MD), have been used to investigate the tribological properties of these nanocomposites. MD simulations were applied to study tribological interfaces at nanoscale through empirical potentials. In DFT calculations, recent studies are focused on understanding the effects of MXene functionalization, where the functional groups typically are T_x = O, S, F and OH, on the adhesion of the polymer, which can be done more efficiently through High-Throughput DFT (HT-DFT) methods, reducing costs and research time. This work aims to study the interfacial characteristics of MXene $Ti_3C_2T_x$/PP nanocomposites through atomistic multiscale HT-DFT/MD simulations.

Investigating Loading Frequency's Impact on Time to Fracture in W-9Cr Steel under Creep-Fatigue Conditions

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Predicting the lifespan of high-temperature materials such as the novel W-9Cr steel poses a significant challenge, especially in conditions involving creep-fatigue [1]. This study investigates the correlation between loading frequency (f) and time to fracture (tf) in W-9Cr steel, essential for comprehending the intricate interaction between time-dependent and cycle-dependent mechanisms. Establishing a relationship between f and tf through experimental creep-fatigue testing at a frequency of 1 Hz and holding times (th) of 0, 5, 60, and 600 seconds. Allowing estimation of time-dependent and cycle-dependent mechanisms. Results indicate a transition zone where the mechanisms interact, influencing crack growth. For high holding times (60 and 600 s), the relationship tends to start parallel to the log f axis, indicating dominance of the time-dependent mechanism. In contrast, for shorter wait times (5 and 0 s), corresponding to frequencies of 1.7E-1 and 1 Hz, the relationship exhibits some gradient at 45°, suggesting influence from the cycle-dependent mechanism. Yokobori et al.'s (2004) [2] theoretical framework provides insights into this phenomenon, demonstrating good agreement between calculated and experimental results (for th=5, experimental tf=88:35, while calculated tf=105:20).

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Large-scale Atomistic Investigation of the Interplay of H-embrittling Mechanisms in Nickel

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Hydrogen embrittlement (HE) remains a persistent challenge in metallic materials, posing a significant barrier to the advancement of a sustainable hydrogen economy. Nickel (Ni), with its single-phase microstructure, is a prominent model for HE studies in fcc metals. HE in polycrystalline nickel is characterized by a transition in fracture models from ductile transgranular (TG) to brittle intergranular (IG). Ongoing debates center around the individual contributions of the various HE mechanisms like hydrogen-enhanced decohesion (HEDE), hydrogen-enhanced localized plasticity (HELP), and hydrogen-enhanced strain-induced vacancy (HESIV), besides the formation of hydrides at the crack tip to IG fracture. Atomistic simulations have allowed the detailed study of these mechanisms. However, atomistic studies related to H-embrittlement mechanisms usually focus on a single mechanism and are limited to idealized pseudo-2D setups.

Here we report on large-scale, fully 3D atomistic simulations of cracks in the presence of dislocations and grain boundaries (GBs) with different concentrations of hydrogen introduced by a Monte-Carlo (MC) approach. The setup allows us to systematically vary the crack system, type and orientation of GBs, as well as the character and position of pre-existing dislocations. Interplay of different HE mechanisms and the occurrence of defect phases are also included in this work. These are compared with predictions from Density Functional Theory calculations of H segregation in small atomistic models, enabling the creation of so-called defect phase diagrams. Such diagrams have the chemical potential of hydrogen as the underlying variable.

Local softness indexes as an alternative to find chemical paths

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Producing a specific chemical compound from another often involves multiple steps, with multiple short-lived intermediates that are difficult to study (and predict) once they cannot be observed under reaction conditions. In this context, computational studies could be considered as relevant tools to provide a mechanistic rationale for the reaction’s chemical pathway [1]. Usually, the Intrinsic Reaction Coordinate (IRC) method is the tool used to search for different pathways and calculate their energy and the formation enthalpy, however, it is commonly a very expensive and user-dependent approach. In this study, we set out to explore the use of local softness (LS) indexes [2] as a chemical pathway prediction tool. The advantages are that it is an inexpensive method and does not require the user's previous knowledge of the system. The molecule 1-azafuvenallene and its pathways towards phenylnitrene was considered as a model system. The results show a great correlation between IRC and LS, putting the latter as an interesting primary tool to find which 2 atoms are prone to interact, which can be further studied by IRC.

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MAGNETIC PHASE TRANSITIONS IN VS4 NANOWIRES INDUCED BY MECHANICAL DEFORMATIONS

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Abstract

The natural material Patronite is composed of vanadium sulfides with stoichiometric composition VS4 and nanowire morphology bonded through van der Waals interaction. Recently, synthesis methods of this material have emerged on carbon nanotube or graphene oxide substrates. Studies of the fundamental properties of an isolated VS4 nanowire show that the material is a semiconductor with antiferromagnetic (AFM) magnetic order. Non-zero magnetic moments in V4+ cations alternate in the lowest energy configuration. However, other magnetic orders can be stabilized in this nanowire. Here, we will investigate four different magnetic orders: two antiferromagnetic (AFM1 and AFM2), one ferrimagnetic (FI), and one ferromagnetic (FM), and the energy variations of each phase with the application of mechanical deformations. We found two magnetic phase transitions with strains, including a transition from AFM2 to FM order. It was also observed that the material is a semiconductor in all investigated magnetic orders, with energy gaps ranging from 1.60 eV to 1.17 eV. Although VS4 nanowires are being recently synthed mainly for applications in lithium-sulfur battery cathodes, we found that the fundamental properties of VS4 nanowires may be interesting for other applications, including technologies with magnetic semiconductors.

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MOFs Learning : a data-based platform to accelerate functional MOF discovery

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Metal-organic frameworks (MOFs) are highly porous crystalline solids researched for applications in gas storage, separations, catalysis, sensing, and biomedicine. Their synthesis and the vast array of building blocks (metal precursors and organic linkers) allow for structural tuning to specific needs. The systematic cataloging in the Cambridge Structure Database (CSD) and other databases facilitates property characterization using molecular simulations, covering adsorption, thermal, mechanical, and electronic properties. However, synthed materials often exhibit more complexity than 0K crystal structures resolved by X-ray diffraction, and synthesis conditions are challenging to extract from literature due to lack of metadata and standardized data formats.

The "MOFs Learning" project, part of a national French consortium, sets best practices for managing and digitizing data in materials research. Collaborating with synthesis (IMAP), molecular modeling (IRCP), and materials testing laboratories (CEA), the project utilizes a broad range of measurements (volumetric and gravimetric adsorption, TGA calorimetry, XRD, FTIR, column adsorption, simulations, ...) to characterize materials. This work presents our management strategy and the tools developed to create a library of functional porous materials. We replicate materials like MIL-53, MIL-160, and CAU-20, ensuring accurate identification and property comparison with existing databases (NIST, synthesis mining). We design computational workflows to compute in-silico properties using FAIR practices, including containers (Apptainer) and workflow environments (AiiDA). A workflow for calculating the thermodynamics of adsorption is highlighted. The final project architecture will be presented as a database of standardized Sample Identity Cards (SID) integrating synthesis, characterization and simulation data and will eventually be available hosted on a web platform.

Molecular Engineering for Optoelectronic Device Design Through Computational Analysis of Excited States

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Organic materials are pushing numerous breakthroughs in materials science. Uncovering comprehensive methodologies to determine photophysical properties and characterizing said materials may be essential to further reduce costs and optimize the design processes. Understanding how light absorption and light emission takes place in these materials is of paramount importance. In that sense, the employment of computational methods to simulate the aforementioned spectra is of major interest. The nuclear ensemble method is often used to simulate molecular spectroscopy and consists of the excitation of an ensemble of geometrical conformations around the optimized energy for a certain electronic state[1]. It also makes use of the normal mode frequencies obtained from the same geometries. Nevertheless, some normal modes may provide more important vibrational contributions to the formation of the spectrum. In this work, we investigated how each isolated normal mode affects the energy range, absorption and emission intensities and spectral profile of a group of small organic molecules. Employing density functional theory and its time dependent extension[2], we analyzed the vertical transition energies and the associated oscillator strengths when normal modes are individually activated. We used an ensemble of 200 geometrical conformations for each normal mode. Our results indicate spectrum intensity may remain unaltered if certain normal modes are made inactive. For instance, in naphthalene’s absorption spectrum less than 20% of the normal modes show a variation of more than 26 meV (1kT) in its vertical transition energy. Our findings indicate a new path to engineering UV-Vis spectra, potentially inspiring innovative technologies in organic electronics.

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Molecular modeling of two-dimensional covalent organic structures for application in toxic gas detection: a case study for TBQP-COF

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Covalent organic structures currently define systems of great interest for diverse applications. Such materials combine the interesting properties of two-dimensional structures, like graphene, with semiconductor characteristics, that enable their use in electronic devices. In the present work, computational modeling tools based on a molecular approach were used to analyze the basic properties of these compounds in order to establish possible structure-activity relationships for the proposition of new derivatives with improved properties, especially regarding their application in gas sensors. Reduced structures and building blocks of 2, 7, 13, 18 - tetrabromodibenzo [a,c] dibenzo [5,6:7,8] quinoxaline - [2, 3-i] phenazine COF (TBQP-COF) [1] were investigated in the framework of the density functional theory. The presence of side groups were also evaluated. The study analyzed the local reactivity of the systems, to identify more reactive regions and relevant sites for interactions with external species. Adsorption studies and comparative analysis of the optoelectronic response of the systems were also conducted for selected toxic gases. Our results show that the local reactivity of COFs can be predicted from their building blocks. Additionally, the reactivity patterns identified for small model structures are maintained in more complex ones. The inclusion of selected side groups on the TBQP-COF lead to significant effects in the local reactivity and optoelectronic responses. We show that most of the systems can be employed for detection/monitoring of toxic gases.

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New penta-octa structure based on silicon carbide

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The structural engineering strategy of inorganic analogs of 2D carbon lattices has increased the potential applications and offers an alternative to the main properties of carbon-based structures. In this way, our interest is devoted to the penta-octa-graphene (POG) structure formed by pentagonal and octagonal carbon rings lattice, hosting type-I and type-II Dirac line nodes due to its sp^2 and sp^3 mixed hybridizations [1]. In this way, this study proposes penta-octa-graphene based on silicon carbide (POG-Si5C4) by means of density functional simulations with the HSE06 functional. The POG-Si5C4 structure has a square unit cell with lattice parameters a = b = 8.061 Å, belonging to space group P4/nmm, which has a negative cohesive energy of -5.22 eV/atom. Also, the phonon dispersion analysis confirms it dynamic and thermal stability up to 1020 K. The structure of the electronic analysis indicates that it is a semiconductor with an indirect band gap transition of 2.02 eV, which has potential for applications in photocatalytic water splitting due to its band edge alignment. The mechanical properties exhibit anisotropy, with Young's modulus ranging from 38.65 to 99.47 N/m and an unusual negative Poisson ratio of -0.09.

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On the water interaction with functionalized (110) diamond surface: A Molecular Dynamics study

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The good optical and electronic properties, chemical inertness and high biocompatibility [1,2] of diamond make it an excellent material for sensors, electrodes, field effect transistors, substrates for biological activity, among others. However, it is observed that many electronic and tribological properties of diamond depend directly on its interactions with the environment [3]. It is known that, when in contact with water, a significant change in some properties of diamond occur, such as in its conductivity of dielectric permittivity [3]. Theoretical and experimental works have been done in order to better evaluate the effect of the diamond surface chemical composition on the water behavior on it. In this work, we performed molecular dynamics simulations in order to study the interaction of the water molecule in contact with five different (110) diamond surfaces functionalized with: (i) ~30% of fluorine; (ii) 50% of hydrogen; (iii) ~8% ether and ~16% hydroxyl; (iv) ~8% amino, 8% ether and 8% hydroxyl; and (v) ~8% N-N, ~8% ether and ~8% hydroxyl groups. The main conclusion of our work is that the more diverse the functional groups present on the diamond surface, the more disorganized and slower will be the closest water molecules to the surface, which can have a direct impact on allowing other molecular species to reach the diamond surface. Our results can help experimentalists to find new diamond applications, such as coatings for anti scaling application.

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OPTIMIZING THE ANALYSIS AND CHARACTERIZATION OF ATOMIC FORCE MICROSCOPY IMAGES USING A GRAPHICAL INTERFACE IN MATLAB

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Advancements in science requires reliable tools for characterizing materials and devices at micro, nano, and atomic scales. Atomic force microscopy (AFM) and its different modes of operation are a versatile tool that allows information to be obtained on the morphology and topography of the surface, along with the mapping of charge distribution, local electronic properties, among other properties in high-resolution space (Da Silva, 2001). While AFM provides rich data, existing analysis software lacks clarity on parameter derivation. MATLAB, a numerical computing language, emerges as a valuable tool for manipulating matrices, plotting functions, data and creating program interfaces (GUI) (MathWorks). Leveraging AFM's native file export capabilities, MATLAB facilitates surface structure quantification through statistical analysis, yielding crucial parameters like roughness and height distribution. Autocorrelation functions and power spectra enable assessment of surface fractal behavior. Moreover, MATLAB supports mathematical operations such as Fourier Transform and correlation calculations, enhancing surface analysis capabilities. To streamline AFM image analysis, a MATLAB-based graphical user interface (GUI) was developed, offering improved usability compared to established software like Gwyddion. Its accessibility caters to a broad user base, from novices to experts, across diverse applications.

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Phase transitions in ferromagnets at zero external field, a Monte Carlo simulation of the classical 2D and 3D Ising model

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Investigations into critical phenomena in phase transitions are of paramount importance for studying the physical properties of a wide variety of materials. Phase transitions may occur due to variations in parameters external to the samples of interest, changes in their properties can be observed, for example, by subjecting them to a thermal bath or by varying an applied external magnetic field. Critical phenomena are also objects of interest for current study, near the critical temperature Tc of transition, a thermodynamic system undergoes fluctuations due to changes in its physical properties[1]. We intend to study the magnetic phase transitions (ferro-paramagnetic). To this end, we will modelate the Ising model at zero external field, which describes the nearest-neighbor interaction between spin–½ localized magnetic momenta on 2D and 3D lattices. The model phase diagram contains the ferro and paramagnetic phases and a phase transition between them. We use the Monte Carlo method[3] to measure average quantities of energy and magnetization, as well as their respective derivatives: specific heat and magnetic susceptibility, that can determine the critical point. One of the possible practical applications of second order phase transitions, involves the critical behavior of the cubic Laves compound ErNi2 near the ferro-paramagnetic phase transition[2]. Monte Carlo simulations are of great importance for simulating critical phenomena in magnetism, as well as in a variety of systems, and their physical properties.

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Plasmonic Properties of Hybrid Systems: Impact of Grating Parameters on MoS2 Monolayer Exciton emission.

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Hybrid systems formed by semiconductors and metallic nanostructures have been widely investigated as options for more efficient optoelectronic devices. Therefore, understanding how the geometric properties of the nanostructures alter parameters such as plasmonic resonances and the magnitude of the generated fields is crucial for comprehending and manipulating plasmonic platforms that are more suitable for a given semiconductor [1]. In this work, we studied a hybrid system consisting of a gold metallic grating coupled with a monolayer of MoS2 (ML-MoS2), whose emissions are predominantly dominated by excitons. Using the FDTD method from Lumerical, we simulated the reflectance spectra of this system composed of square arrays with slits 50 nm wide and 90 nm deep, exhibiting periodicity from 200 nm to 900 nm, with ML-MoS2 deposited on them. We examined the effects of these geometric parameters for two different contexts: illuminating with a white light source, analyzing across the entire visible and near-IR region; exciting at specific wavelengths close to surface plasmon (SPP) resonances and analyzing the distribution of the generated fields for two different polarizations of radiation. From these results, it was possible to determine the properties of the SPPs of each metallic grating, observing a redshift in the SPP wavelengths when the grating periodicity increases. Experimental two-photon confocal microscopy analyses were performed on real samples to corroborate the simulation data. This study adopted an integrated approach, combining experimental observations with numerical simulations to understand the observed optical phenomena [2].

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Scanning of potential catalytic sites in $M_{13-n}N_n$ nanoparticles (M, N = Pt, Pd or Ni with n = 0, 3, 6, 9, 13) for the water gas shift reaction.

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The technological transformations experienced by humanity have generated several challenges, such as the search for renewable and sustainable energy sources. In this context, hydrogen gas stands out, as its combustion generates water as a product. The occurrence of water-gas shift reaction (WGSR) illustrated in equation 1 is a reversible and non-spontaneous exothermic process[1].

$CO + H_2O$ $CO_2 + H_2$ $\Delta H = -41{,}09$ kJ/mol (1)

Catalysts are crucial for this reaction due to its high activation energy (~274 kJ/mol). Bimetallic PtM nanoparticles (M = d-block metals) offer advantages such as high chemical activity and resistance to water-induced oxidation[1,2]. To mitigate the cost and undesirable characteristics of Pt catalysts, Ni and Pd are added to form bimetallic alloys of $M_{13-n}N_n$ (M, N = Pt, Pd, or Ni, with n = 0, 3, 6, 9, 13). This study aims to identify the efficiency of these catalyst compositions for WGSR. Low-cost computational tools, including the semi-empirical methods of the GFN-xTB family[3] and the CP2K package[4], were employed to understand the properties of the nanoalloys[5]. Structural and electronic investigations, utilizing techniques like stability analysis and energy assessments, provide insights into nanoparticle behavior as WGSR catalysts. Pd_4Ni_9 nanoparticles exhibit promise due to their low energy barriers and favorable adsorption energies. Reducing energy barriers in the carboxylate formation stage could further enhance catalytic yield.

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Simulation of Electronic transport in Graphenylene nanodevices

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Nanoscience has been driven by the continuous search for materials with exceptional electronic properties. In this scenario Graphenylene, a graphene-like 2D material, stands out due to its unique hexagonal network structure, offering significant potential for innovations in semiconductor devices. In this study, we investigate electron transport in graphenylene nanoflakes of various s and contact and doping formats using the non-equilibrium Green's function (NEGF) method within the density functional tight-binding theory (DFTB). When appropriate, wide band approximation was also used to reduce computational cost. We have shown a significant influence of the contact surface and their electronic nature on the characteristic I-V response. During our study several contact configurations were considered, namely two, three and four terminal devices in order to simulate representative situations. We probed the electric current dependence on the applied potential to characterize possible current rectification, ohmic behavior and the possibility of some dependence of transmitted currents on external applied fields. Our results indicate also the existence of a combined dependence of conductance on the external bias, applied electric field and on doping and geometric configurations. Our results were interpreted combining the influence of the ingredients cited above on transmission plots with potential and local currents maps which will be discussed. We hope this study represents progress in understanding the electronic behavior of graphenylene and can stimulate further efforts in the design and optimization of devices based on this material, contributing to the development of more sustainable and powerful technologies in the future.

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Stability of Ag_2CrO_4 surfaces via first principles atomistic thermodynamics

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Silver chromate (Ag_2CrO_4) is highly studied for its high photocatalytic activity in degrading organic pollutants and biological pathogens, owing to its surface atomic and electronic structures. Therefore, the influence of external pressure and temperatures was studied in terms of surface stability. This was achieved by applying a first principles atomistic thermodynamics model, which relates the surface Gibbs free energies, based on DFT-total energies, with chemical potentials, to seven surface orientations of the Ag_2CrO_4 crystal: (100), (010), (001), (110), (101), (011) and (111), considering different possible terminations for each one, to study its stability dependence on ambient conditions. Key findings show that the types of undercoordinated and coordinated surface clusters play the most important role in the stability of the systems across different temperature ranges. For instance, the $AgCrO_3$ termination of the (100) orientation is the most stable one independently on the oxygen chemical potential, while for (001), the $AgCrO_3$ and $Ag_4Cr_2O_{14}$ terminations dominate at high and low temperatures, respectively. These trends were also investigated in terms of Wulff constructions, obtaining different crystal geometries also as a function of the ambient conditions. In addition, Bader charge analysis, work functions, density of states, and band gaps were also made to the most stable terminations to enrich the comprehension of the results and assist in future studies that can be interested in the photocatalytic mechanisms of the system.

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Structural and Electronic Properties of Axial GaN/AlN Nanowire Heterostructures Grown in the [001] Direction

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According to the International Roadmap for Devices and Systems [1], the limit trend for CMOS devices, is to be reduced to nanowire dimensions. In addition to being the active medium for future CMOS devices, nanowires can be useful in designing future optoelectronic devices, such as nano-LEDs, nanolasers, and nanophotovoltaic devices. In this work, we present our preliminary results for the structural and electronic properties of the axial GaN/AlN interface nanowire grown in the [001] direction in both the wurtzite and zincblende phases, and their dependence on the variation of its radius, as well as on the thickness of the materials to compose the interface. Calculations were obtained using the Tight-Binding approximation for Density Functional Theory [2]. Our preliminary results show that the interfaces between AlN and GaN are smooth, without distortions. However, on the lateral surfaces of all studied nanowires, we observe that cations tend to enter the material, while anions tend to leave it. Additionally, we find that the bandgap due to the presence of the interface is direct, and this system will be useful for new optoelectronic devices. Finally, the band offset obtained for these systems shows that the AlN/GaN interface forms a barrier on the GaN side, resulting in type 2 superlattices.

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Structural and magnetic properties of metallocene molecules deposited on metallic surfaces

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In this study, we investigated the structural and magnetic properties of several molecules of metallocene deposited on metallic surfaces through computer simulations, using Density Functional Theory (DFT). Initially, we optimized the geometries of the molecules and surfaces, taking into account the van der Waals interactions. Then, we calculated electronic properties such as band energies and densities of states, to analyze the behavior of the adsorbed molecules. Additionally, we investigated the magnetic properties of the metallocene molecules adsorbed on metal surfaces. We analyzed how the magnetic moments of the molecules were oriented on the metallic surface and the magnetic interactions between neighboring molecules. Our goal is to understand and control the magnetic properties of metallocene molecules mediated by the interaction with metallic surfaces. The obtained results are relevant to the fields of spintronics and quantum computing, where control of the magnetic properties on a molecular scale is fundamental.

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Study of the Magnetic and Thermodynamic Properties of $LaMnO_3$ using the Gibbs-Bogoliubov Inequality through Mean-Field Theory.

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This study presents a detailed investigation into the magnetic and thermodynamic properties of the perovskite compound $LaMnO_3$, a material of great interest due to its potential applications in magnetoresistive devices and magnetic refrigerators [1]. The theoretical formalism to analyze the magnetic and thermodynamic properties of stable, metastable, and unstable states was carried out using the Gibbs-Bogoliubov inequality. The exchange constants employed in the modeling were extracted from previous studies [2]. The behavior of the system's thermodynamic states was analyzed for different anisotropy constants present in the model. The results obtained reveal insights into the magnetic phase transitions of $LaMnO_3$, with proximity in the critical transition temperature and in the behavior of thermodynamic quantities when compared to works already established by other methods [2]. Continuous and first-order phase transitions, as well as critical points, were investigated. The results were analyzed in relation to exchange interactions and anisotropy in determining the Néel temperature and describing the antiferromagnetic behavior of the material. An increase in the magnetic order of each sub lattice was observed, which was detailed by the Gibbs free energy and entropy curves.

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Study of the Optical Properties of Plasmonic Structures Using Numerical Simulation

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The study examines numerical simulations for the optical characterization of plasmonic structures, varying the polarization of light between 0 and π/2 radians. Specifically, the simulations explore a grating with different periodicities, distinguishing between a grating and a single slit. Initially employing a plane wave source. The primary goal is to determine the Extraordinary Optical Transmission (EOT), which will be compared with experimental data, along with evaluating reflectance and field profiles. Parallel computing and cluster utilization were instrumental in conducting the simulations. These materials hold significant potential in nanophotonics.

Surface-enhanced Raman spectroscopy for L-dopa detection using functionalized gold nanorods: Computational insights

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In medicine or pharmacology there is a need to monitor and/or detect the concentration of medications, hormones and other compounds in the human body, such as the effects of the drug L-dopa. The difficulty in detecting these compounds at low concentrations is still a challenge, with surface-enhanced Raman spectroscopy (SERS) being a promising technique. In particular, gold nanorods (AuNR) functionalized with lipid structures, such as CTAB, have been proposed as a promising substrate for SERS detection of such kinds of negatively charged analytes. To better understand the SERS effect and identify relevant variables for L-dopa, in this study electronic structure calculations were conducted in the framework of the density functional theory (DFT) at B3LYP/6-311+G(d,p) level. Local reactivities were assessed using condensed-to-atoms Fukui indices (CAFI) [2]. L-dopa structures containing a single metal atom (Au) attached to the most reactive sites (identified via CAFI) were also investigated at the same level of theory (with ADZP basis set for Au [3]). Molecular dynamics (MD) simulations with the OPLS-AA force field were also conducted to investigate details on the L-dopa+AuNR/CTAB system. The DFT results show the existence of distinct anchoring sites in the L-dopa structure according to the redox state, as well as the effect of Au adsorption on the compound Raman spectra. The molecular dynamics study showed that the CTAB molecules on the metal surface influences the diffusion efficiency of L-dopa and the creation of defects induces the entry of the solvent into hydrophobic regions. It was found that L-dopa tends to interact more effectively with the N(CH3)3+ groups of CTAB. The proposed model can assist experimental tests.

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Synthesis and characterization of lanthanides complexes with carboxylic chalcone to study spectroscopic properties

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Chalcones, known for their two aromatic rings connected by an α,β unsaturated carbonyl group, are extensively studied for their biological activities, e.g., the inhibition against an Yersinia enzyme by a novel carboxyl chalcones [1]. The lanthanide (Ln) complexes containing carboxylate ligands are the most widely investigated kinds of coordination compounds. The ibuprofen, a non-steroidal anti-inflammatory drug, was used to perform Tb3+ and Eu3+ luminescent complexes, evaluated by semi-empirical methods [2]. Here we propose to study chalcones as antenna ligands to investigate the structure and optical properties. This work focuses on coordinate 4-(3-(4-methoxyphenyl)-3-oxoprop-1-en-1-yl)benzoic acid (C4MOBA) with Ln3+ ions to explore spectroscopic properties. Using the semi-empirical model Sparkle/AM1 and INDO/S-CIS method, the GdC4MOBA ground state structure predicts a triplet state value of 19215.4 cm-1, suitable for energy transfer to Eu3+ ion. GdC4MOBA synthesis involved adding LnCl3 aqueous solution to a deprotonated C4MOBA ethanolic solution, under stirring at ~50°C for 1h, yielding a white powder filtered after one week. In a digital melting point device the complex exhibited a darkening above 190°C and melted at 220°C. Displacement in FT-IR from 1660 cm-1 to 1651 cm-1, respectively from ligand to complex, of the □C=O carboxyl stretching, indicates coordination by this group rather than by the carbonyl group, which showed small variation from 1678 cm-1 to 1682 cm-1. Next steps include synthesizing EuC4MOBA, Ln3+ complexometric titration, CHN analysis, determining the experimental triplet and emission from the complexes by photoluminescence spectroscopy.

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The microstructures and mechanical properties of a nodular cast iron of a railway fastening system shoulder: experiments and numerical modeling

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Nodular cast iron is commonly used in various industrial and engineering applications, including some components of the railway fastening system, such as shoulders and baseplates. The mechanical characteristics of nodular cast iron are influenced by its microstructure and the features of graphite nodules, which can assume spherical or skewed shapes in their distribution. Spherical shapes tend to have lower stress concentrations, but skewed nodules are desirable as they indicate that some graphite nodules are formed late in the solidification process, which effectively combats shrinkage. Additionally, nodular graphite degeneration can occur and has a detrimental effect on material properties. The microstructures of shoulders and baseplates were analyzed using optical and scanning electron microscopy, in order to characterize common metallurgical defects found in the production of ductile cast iron, such as spherical and skewed shapes of graphite nodules, degenerated graphite, and inclusions. Computational image analysis was employed to quantify the of graphite nodules and to determine the volumetric fraction of each phase in the nodular cast iron microstructure. Mechanical properties were obtained through tensile tests, Charpy impact tests, Vickers hardness tests, and microhardness tests. The micrographic images and measured properties were used for microstructure modeling using Finite Element Method (FEM) software, by coupling Object-oriented finite elements (OOF2) and Abaqus, to evaluate the effect of shrinkage defects and the different shapes of graphite nodules, including the graphite degeneration, on the stress field and the elastic and elastoplastic mechanical behavior of the material when subjected to typical railway loads. The results showed that the microstructure has a strong effect on the material's strength.

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Theoretical-experimental approach for studying the reactivity of the $Cu_3Mo_2O_9$ catalyst for CO_2 conversion into Methanol

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One of the major challenges facing the world today is the need to reduce greenhouse gas concentrations to mitigate global warming. One approach to addressing this issue is the utilization of CO_2 for the production of valuable chemical products, such as methanol and ethanol. In this context, metal oxide catalysts have emerged as promising candidates for facilitating these reactions.[1] Copper (Cu)-based catalysts based on crystalline mixed oxides hold significant potential for industrial applications in CO/CO_2 hydrogenation processes, offering an alternative to traditional Cu/ZnO/Al_2O_3 catalysts for CO_2 hydrogenation.[2]

In this regard, the $Cu_3Mo_2O_9$ catalyst was investigated for its potential in the conversion of CO_2 into methanol. Employing a combination of theoretical and experimental approaches, the catalytic properties of $Cu_3Mo_2O_9$ were thoroughly examined. This involved establishing the synthesis of the catalyst, characterizing its structure, and evaluating its physicochemical properties, with a focus on its reactivity towards CO_2 and H_2, leading to methanol formation.

In the theoretical investigation, Density Functional Theory (DFT) calculations were carried out on bulk and slab models to analyze the geometrical and electronic structure. Meanwhile, in the experimental studies, the $Cu_3Mo_2O_9$ structure was characterized using X-Ray Diffraction (XRD) and High-resolution Scanning Transmission Electron Microscopy (HR-STEM). The material was tested as catalyst for methanol production using a batch reactor and the products were analyzed using Gas Chromatography (GC).

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Theoretical investigation of Nb-functionalized silica: a surface investigation based on DFT

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Since the beginning of its existence, human beings have developed numerous technologies to improve their quality of life, facilitating some tasks and make others possible, developing mechanisms and equipment, and providing a better understanding of the universe around them. Technological advancement has become increasingly fast; hence, new technologies have quickly become obsolete, mainly observed for electronic devices, such as computers, cell phones, integrated circuits, sensors, data storage devices, and others.

In this context, technological advancement is strictly connected to the development of materials that enable the improvement of available devices or the creation of new technologies. In recent decades, materials development for technological application has been based almost entirely on semiconductor materials since the same semiconductor can be applied to several electronic devices. It is possible due to the possibility of controlling their properties through the creation of defects, chemical modification, doping, formation of heterojunctions, or morphology control.

This work presents a Density Functional Theory investigation of silica bulks and surfaces modified with Nb to understand their suitability in the development of different electronic devices and processes of environmental or health interest. In particular, the silicas were modified with Nb, a chemical element whose natural reserves are primarily found in the national territory. In this context, their application to developing novel technologies represents an economic advantage. The electronic structure, charge carrier features, band edge potentials, and transport properties are discussed.

Theoretical studies on the photocatalytic activity of silver nanoparticles on Ag_3PO_4 by ab initio calculations

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Silver-based semiconductor materials have been studied for some time due to their photocatalytic and antibacterial effects when irradiated with electron beams and fs-laser. Specifically, electron irradiation causes the absorption of electrons, causing the formation and diffusion of metallic silver from the crystal interior to the surface. Understanding how this mechanism works is essential for a good understanding of catalytic effects in silver-based semiconductors. In this work, we perform a comprehensive study to compare the electronic properties of the Ag3PO4 (110) terminations modified with added Ag clusters with the same terminations exposed to the effects of electron irradiation. The study is based on Density Functional Theory calculations and uses an ab initio atomistic thermodynamics approach to determine the most favorable surfaces. The structural and electronic analysis of the superficial clusters reveals the key factors for the catalytic activity of both systems.

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Theoretical Study of Molecule Encapsulation in Porous Fullerenes

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A class of fullerenes known as porous fullerenes is theoretically investigated in our study. The structure PGC20 was constructed as proposed by Paupitz et al. a few years ago[1], by repeating the porous graphene block to create a C20-like cage molecule. In our work, we perform the encapsulation of molecules such as CO2, H2, and H2O within this macromolecule using DFTB, a density functional-based tight binding method[2]. This approach is applied to describe their eletronic and structural properties. According to our results, the maximum encapsulation capacities for the porous fullerene PGC20 were estimated to be 20 CO2 molecules, 37 H2O molecules and 55 H2 molecules. Additionally, we estimated the potential barriers for the encapsulation process from the first to the last molecule in all three cases. LUMO-HOMO energy gap values varied between the systems with maximum capacity and the empty fullerene, showing a 10% variation for the H2O molecules, while CO2 molecules' gap variation was around 5%. Furthermore, a "locality" of the molecular orbitals in cases of these encapsulated molecules was observed. We also carried out theoretical investigation of stability patterns for different quantities of molecules within the cage structure. Molecular dynamics for encapsulated systems were carried considering temperatures between 100K and 900K.

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Understanding the colorimetric properties of new π-conjugated polymers by tuning their acceptor-donor configuration.

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Conjugated polymers are considered one of the most popular materials for optoelectronic developments, thanks to the unique ability to transport charge and absorb light. Some heterocyclic-based electron-rich polymers are among the most promising materials in various areas such as organic solar cells, organic LEDs, organic field effect transistors and electrochromic displays. The design and arrangement of the polymer structure are the most influential factors affecting their electric and optic behavior. For example, both theoretical modeling and UV-Vis Spectroscopy were used to investigate the dependence of color properties on molecular structure for the series of new donor–acceptor conjugated polymers. In this work, a series of five new π-conjugated donor-acceptor-donor (DADn) copolymers, named P3-X (X = OMe, H, F, COOMe, CN), will be investigated and the UV-VIS spectra will be calculated with the ωB97XD functional. This functional has shown to reproduce experimental spectra with higher precision compared to other Density Functional Theory (DFT) functionals. A comparison between the experimental results and the results obtained with the B3LYP functional will also be shown. [1] These results contribute to the broad understanding of structure-property relationships in π-conjugated polymer films, and also suggest guidelines for the design of essential materials for the manufacture of various devices, such as monitors and sensors. It shows the importance of color and optical engineering in synthed polymers, thus highlighting their implication in the next generation of optoelectronics. These insights can accelerate advances in diverse fields, including electronics, photonics and materials science.

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Understanding the mechanism of photocatalysis for TiO_2, $BiVO_4$, and $BiNbO_4$ materials from a DFT approach based on excited states

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The increase in waste generation is one of the consequences of the current accelerated technological advance, leading to extensive contamination of water, soil, and air. Thus, it is necessary to improve available methods for the degradation of pollutants and, in this context, heterogeneous photocatalysis, using semiconductor materials able to interact with solar radiation, stands out as a potential alternative to decrease water contamination through a fast and efficient process, with low cost and using sustainable energy.[1] Over the years, many experimental and theoretical studies have focused on developing new photocatalysts from empirical or theoretical approaches. In particular, most computational studies only evaluate the materials ground state, neglecting the existence and the features of the excited states, which is an essential step in the photocatalytic process obtained due to the semiconductor interaction with solar radiation.[2]

In this study, the electronic and photocatalytic properties of the ground state of three semiconductor materials are carefully investigated, and a new approach based on excited state properties was proposed. The proposed approach was first applied to two materials well-known in the scientific literature, TiO_2 and $BiVO_4$. Then, the now-validated approach was employed to analyze a potential new photocatalytic material, the $BiNbO_4$. The constructed models were carefully discussed regarding structural and electronic properties, focusing on the influence of defects on the materials properties, electronic structure, and charge carriers stability. Furthermore, the effect of slight structure relaxation during the materials interaction with solar radiation was evaluated. The obtained results provide a broad description of the investigated materials properties, allowing a better understanding of the excited-state features and how the photocatalytic process occurs when semiconductors are involved.

Unlocking the potential of melanin-inspired compounds for nitroaromatics detection

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Nitroaromatic compounds (NACs) pose significant environmental and health risks due to their mutagenic, carcinogenic, and toxic nature. Current detection methods are limited by various factors, including cost, complexity, and practicality. Melanin-inspired compounds show promise due to their unique properties [1], but their potential for NAC detection remains unexplored. In this report we evaluate some electronic and reactivity properties of melanin-inspired polymeric systems (9a and 9b) via molecular modeling techniques to assess their potential applicability as NAC detectors. The calculations were conducted in the framework of the density functional theory (DFT), considering the B3LYP hybrid exchange correlation functional and 6-311G(d,p) basis set. DFT-based condensed-to-atoms Fukui indexes [3] and docking by automated interaction site screening [4] were evaluated to identify relevant adsorption centers. Our results revealed promising optoelectronic responses of melanin-inspired compounds to the presence of NACs, especially di- and tri-nitro aromatics. Effective adsorption and π-π stacking are noticed for select NACs on melanin-based structures, which leads to significant changes in the optical absorption spectra and frontier molecular electronic levels alignment. The results suggest that melanin-based monomers can be used for NACs detection via electrical and optical methods.

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Unraveling the effects of gold surface functionalization and steric hindrance on the detection of acephate and diuron molecules via SERS: a computational study

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The extensive use of chemical products in agriculture affects the environment in a significant way, particularly water contamination [1]. Developing sensitive techniques for monitoring these compounds in water is a crucial and challenging task. In this context, surface-enhanced Raman scattering (SERS) with suspended nanoparticles (NPs) has gained prominence, yet detecting species with negatively charged centers remains difficult due to NP surface charge. Gold nanorods (AuNRs) functionalized with positive species show promise, though additional species complicate interactions [2]. Here we report a series of density functional theory-based studies and molecular dynamics simulations performed to explore details on the interaction between acephate (pesticide) and diuron (herbicide) molecules with functionalized AuNRs with hexadecyltrimethylammonium bromide (CTAB) molecules, as well as evaluate the theoretical Raman spectra of adsorbed model structures. While identifying relevant adsorption centers and predicting effects on Raman activity of the compounds, our results also evidence that intrinsic difficulties related to steric hindrance effects hamper the effective detection of acephate and diuron using CTAB-covered AuNRs, limiting the detection potential of such substrates.

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Unraveling the magnetic ordering in Cu-doped SnO2 nanoparticles at low Cu concentrations

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Doped metal oxide semiconductors (MOS) present an interesting perspective, particularly regarding the emergence of room temperature ferromagnetism (RTFM) without the use of magnetic ions (d0 or f0), which remains a contentious matter requiring further investigation. Recently, there was experimental evidence of the emergence of ferromagnetic properties in d0 semiconducting metal oxides like Na-doped SnO2, particularly noticeable at low doping concentrations [1], which suggests that the magnetic doping ions can not be the key to understanding the RTFM in those systems. Previous research [2] reported magnetic measurements notably due to the presence of ferromagnetic CuO secondary phase primarily observed at higher Cu concentrations exceeding 10% to 30%. Nevertheless, at lower doping concentrations, the manifestation is less apparent, as there is no discernible second phase, and the Cu ions remains confined to a solid dilute solution. The experimental results indicate that our system is characterized by the dominance of paramagnetic and clustered magnetic phases (Bound Magnetic Polaron). The introduction of \ce{Cu^{2+}} ions into a solid solution, replacing \ce{Sn^{4+}} ions, induces the formation of oxygen vacancies as confirmed by our theoretical calculations. This local defect may be responsible for the observed enhancement in RTFM, which is particularly evident at low concentrations, especially at 0.5 Cu. Here, a remarkable increase in the magnetization (M_S) of about 778 times compared to undoped \ce{SnO_2} NPs is observed. Using ab-initio calculations of local point defects, we have identified the conditions under which the material exhibits a strongly ferromagnetic ground state.

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Unveiling a New 2D Semiconductor: Biphenylene-based InN

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The 2D materials class earned a boost in 2021 with biphenylene synthesis, which is structurally formed by the union of 4-, 6-, and 8-membered carbon rings, usually named as (4-6-8) biphenylene network (BPN). This research proposes a detailed study of electronic, structural, dynamic, and mechanical properties to demonstrate the potential of the novel biphenylene-like InN (BPN-InN) via density functional theory and molecular dynamics simulations. The BPN-InN has a direct band gap energy transition of 2.02 eV, making it promising for optoelectronic applications. This structure exhibits maximum and minimum Young Modulus of 22.716 and 22.063 N/m, Poisson Ratio of -0.008 and 0.018 and Shear Modulus of 11.448 and 10.860 N/m, respectively. To understand the BPN-InN behavior when subjected to mechanical deformations, biaxial strains and uniaxial strains in armchair and zigzag directions from -8% to 8% were applied, achieving a band gap energy modulation of 1.36 eV over tensile deformations. Our findings are expected to motivate both theorists and experimentalists to study and obtain these new 2D inorganic materials that exhibit promising semiconductor properties.

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Advancing 4D-STEM and Electron Ptychography for Comprehensive Characterization of Soft/Hard Interfaces

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The elucidation of interfaces between soft and hard phases is essential for the development and functional optimization of hybrid materials, with widespread implications in fields ranging from catalysis and gas storage to drug delivery [1,2]. The characterization of these interfaces presents significant challenges due to their complex structural diversity and vulnerability to electron beam exposure [3]. This work introduces a combined approach employing 4D scanning transmission electron microscopy (4D-STEM) for crystal structure elucidation and optimized electron ptychography for high-resolution imaging to overcome the limitations of traditional imaging techniques. These advanced methodologies provide unparalleled insights into the intricate interfaces of soft/hard materials, facilitating a more nuanced understanding of their properties and interactions.

Optimizing parameters such as electron dose, illumination angle, and defocus is crucial for 4D-STEM and electron ptychography techniques, to ensure the integrity of beam-sensitive materials while capturing their complex interfacial structures with high resolution and contrast. Our integrated approach leverages the strengths of 4D-STEM for its detailed diffraction information and electron ptychography for its phase retrieval capabilities, allowing for a comprehensive characterization of materials at the nanoscale.

Through rigorous simulations and empirical studies, we demonstrate the effectiveness of this hybrid methodology in providing detailed visualizations of soft/hard interfaces. The enhanced imaging capabilities of 4D-STEM and electron ptychography, optimized for soft/hard material characterization, promise to deepen our understanding of material functionalities and to expand the potential applications of hybrid materials.

Nano to Atomic scale TEM Characterization of β Ti-Nb and Mg-based alloys obtained by Selective Laser Melting, HPT and Sputtered Thin Films for Implants.

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New processing routes can be used to obtain metallic biomaterials for implant with suitable properties, such as selective laser melting (SLM) which is a AM process that produce a metal parts by melting the micrometric metal powder layer-by-layer. In this context, the metastable β Ti-15Nb alloy (wt.%) appears, processed through selective laser melting (SLM) and arc melting, since this is free of cytotoxic elements and shows lower Young modulus down to 60 GPa. β Ti alloys are acclaimed for biomedical applications due to their mechanical properties, good biocompatibility and corrosion resistance. Furthermore, for orthopedic applications, there is a considerable difference between elastic modulus of Ti and a+β alloys, from E = 100 to 110 GPa, and that of human bone, around E = 30 GPa. Another approach is thin film by sputtering in order to reduce the surface elastic modulus of stainless steels adopting low modulus β Ti-Nb-based alloy.Characterization of SLM β Ti-15Nb alloy and Thin Films of β Ti-Nb-based alloys obtained by magnetron sputtering were done by optical microscopy (OM), X-ray diffraction (XRD), scanning electron microscopy (SEM) and transmission (TEM) coupled to ASTAR - automatic crystal orientation mapping (ACOM). Vickers microhardness, and elastic modulus via nanohardness and impulse excitation were evaluated. The coating of Ti40Nb20Zr40 alloy (at.%) alloy presented lower elastic modulus of 51 GPa and hardness values, and these were related to the increases in both the lattice parameter and mean nanoscale grain of thin film. For SLM of β Ti-15Nb alloy with a alfa´+ β microstructure, the Vickers microhardness and elastic modulus measured by nanohardness and impulse excitation technique were evaluated, showing suitable modulus of around 60 GPa. Besides that, the microhardness was found around 300 HV and density of 99%, which plays an important rule in mechanical properties. Therefore, AM of β Ti-15Nb showed as a promising material for orthopedic applications.

New directions in electromagnetic field mapping in the transmission electron microscope

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Transmission electron microscopy can be used to obtain quantitative information about not only local variations in microstructure and composition in materials, but also functional properties and switching processes in nanoscale materials and devices. I this talk, I will focus on the use of phase contrast techniques in the transmission electron microscope, such as electron holography and electron ptychography, in combination with model-based and model-independent data analysis, for the measurement of local variations in magnetic field and electrostatic potential within and outside materials with nm to atomic spatial resolution. I will illustrate how such measurements can be made both in projection and in three dimensions, as well as in the presence of external stimuli such as applied voltage, magnetic field, reduced or elevated temperature, reactive gas and light. I will also highlight key experimental issues that need to be considered, including the influence of sample preparation, dynamical diffraction and electron-beam-induced specimen charging. The examples that I will present will include studies of closely-spaced magnetic crystals and nanoscale devices that contain geometrically-confined magnetic skyrmions, sub-100-nm vortex-like spin textures with particle-like properties that are of interest for future energy-efficient memory technologies. This work takes advantage of the recent development of a model-based iterative reconstruction approach, which can be used to retrieve projected or three-dimensional charge density or magnetization distributions from electrostatic or magnetic contributions to recorded electron optical phase images. I will conclude the talk with a personal perspective on possible future developments in instrumentation and techniques in transmission electron microscopy that may allow such measurements to be made with greater reliability, sensitivity, precision and accuracy.

On-Surface Reaction: An Atomic-Scale Design of Functional Organic Nanomaterials

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Materials science in the nanoscale domain has become a reality for several applications, from integrated circuits, sensors, catalysts, medicines, data-storage devices, among others [1]. We achieved the ability to understand materials and, more importantly, command the materials' properties at the atomic level using precise synthesis and growth methods. Therefore, during the last decades, enormous efforts have been made to develop new processes for fabricating, characterizing, and manipulating materials in complex nanoarchitectures with atomic precision, making it possible to express emergent new chemical, electronic, photonic, magnetic, and structural properties [1]. On-surface synthesis becomes a powerful bottom-up technique to fabricate such nanostructures using organic and organometallic precursors as molecular building blocks [1]. In this talk, I will present some strategies we have adopted to produce planar carbon lattice nanostructures, such as porous nanoribbons and nanomembranes [2-5]. For a complete understanding of the atomic and electronic properties of the materials, we have combined scanning tunneling microscopy and spectroscopy (STM/STS), X-ray photoelectron spectroscopy (XPS), and numerical simulations based on density functional theory (DFT) calculations.

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Probing phonons at the nanoscale with electrons

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The development of atom-wide monochromatic electron probes in transmission electron microscopes has enabled the realization of phonon spectroscopy studies in nanomaterials with superb spatial resolution. This capability is permitting to unveil new phonon properties of advanced materials with potential applications in infrared nanophotonics, nanoscale heat transfer, and quantum technologies. In this talk, we will describe progress along those directions by highlighting results involving (i) imaging and spectroscopy of hyperbolic phonon polaritons in twisted low-symmetry crystals, (ii) studies of heat transfer across nanoscale gaps, and (iii) localized phonon behaviour across semiconductor interfaces. These results represent progress towards understanding the role of phonons in physical process involving light-matter interaction and nanoscale energy transfer.

Ptychographic Imaging of Orbital Angular Momentum and Moire Systems

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Electrons play a pivotal role in stabilizing matter, but they are also tools that can reveal the underlying physics of complex systems from high energy physics to condensed matter. Electrons can be used as imaging probes, where properties of matter such as ferroelectricity, magnetism or topology can be observed atom-by-atom. In this talk, I will discuss a new type of electron probe which can image orbital angular momentum, torque transfer and chiral order of topological structures in ferroelectrics. I will also show how electron ptychography, an iterative computation imaging technique, can improve resolution beyond the numerical aperture of the electromagnetic lenses to the sub-angstrom limit in a conventional electron microscope. Using this technique, we essentially develop a 'computation lens' approach to imaging, opening opportunities to explore new physics in emergent materials beyond physical lenses in a cost-effective manner, and thus expanding access to high-resolution imaging approaches to a broader range of institutions.

Resolving the 3D morphology and atomic structure of nanoparticles using a single 4D-STEM diffraction map: application to complex multibranched plasmonic particles.

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Metal nanoparticles (NPs) are an intensively studied nanomaterial due to the possibility of tuning the optical properties by tailoring surface plasmon resonances through changes in morphology and . Discrete tomography represents the most popular method to gather the 3D shape of complex NPs (anisotropic, branched, etc.) although this requires the acquisition of several tens of images and a high total electron irradiation dose. Here we will describe the simultaneous determination of the shape and detailed atomic arrangement of a multi-branched AuAg metallic nanostar (NS) from a single scanning transmission electron microscope nanodiffraction map (4D-STEM) acquired using Precession Electron Diffraction (PED). The applied methodology exploits the 3D crystal orientation information carried by the electron diffraction pattern, where quantitative analysis of the PED intensities has been used to improve interpretability and precision. The high aspect-ratio legs were determined to be decahedral rods located on a high symmetrical icosahedral core; legs were spatially distributed on an almost planar configuration. This anomalous leg distributions provided illuminating new understanding on NS formation along the complex 2-step chemical synthesis procedure, whose deep understating is essential to develop the upscaling NS synthesis aiming practical applications. This work has required total electron dose of ~200 electrons by square Angstrom and it is very promising for the study of beam sensitive nanomaterials.

Cryo-TEM of Self-Assembled Gels and Pastes

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In colloidal systems specimen preparation is still a major limitation of Cryo-TEM, because the plunge freezing method is only applicable for low viscosity fluids and might lead to undesired morphological changes [1]. Alternative methods of vitrification (e.g., cryo jet freezing) and/or of sample application on the grid (e.g., scribing) might be used to overcome the viscosity issue, but if it is too high, as in the case of gels and pastes, cryoultramicrotomy is considered to be the most effective approach [2]. The morphological changes induced by sample preparation is far more complex and somewhat less explored. There are two factors governing these transitions, temperature and concentration. In most cases, temperature-dependent transitions are easily determined by complementary techniques (e.g. rheology or differential scanning calorimetry) that facilitate specimen preparation, as we demonstrated in previous work [3]. Conversely, information regarding concentration-dependent transitions is often unavailable during cryo-TEM specimen preparation. Herein we present a simple method for preparing cryo-TEM specimens of gels and pastes that preserves the native concentration of the sample. This technique consists of applying a small amount of sample on the grid with a syringe needle and dragging it across the surface of the grid with a razor blade followed by vitrification. So far, we have successfully used this method to investigate gels of wormlike micelles; thermoreversible micellar hydrogels; surfactant lamellar phases; and nanocellulose-based gels. The versatility and simplicity of this strategy, alongside with its high success rate and low material requirement clearly demonstrate its potential.

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Effect of adding different percentages of K-PHI carbon nitride on the TiO2 structure

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Herein, we report the effect on the structure of TiO2 photoanodes after modifying with different proportions of potassium poly(heptazine imide) (K-PHI), a PCN structure well crystalline and with good photocatalytic activity [1]. Initially, the photoanodes were produced in the form of films, by spin coating deposition of a paste prepared by adding 2.5%, 5.0%, 10.0%, and 20.0% (wt. %) of K-PHI to a commercial titania paste. From the Raman spectrum of the samples, was possible to observe characteristics TiO2 anatase phase bands, with Eg (~147 and ~635 cm-1), B1g (~400 cm-1), and A1g/B1g (~518 cm-1) modes presenting some shifts with the progressive K-PHI addition. As the Eg modes refer respectively to the interactions between titanium-titanium (Ti-Ti), as well as titanium-oxygen (Ti-O) interaction in the lattice, the gradual redshift of the first mode, concomitant to the blueshift of the second mode with increasing K-PHI percentages indicated a progressive distortion of the TiO2 crystal lattice. This distortion, especially the increase in the Ti-O bond distance, is in line with the increase in d-spacing observed in the TEM images. For the addition of 5% of K-PHI in TiO2, it is possible to observe less organized edges in the particle. The influence of K-PHI in the crystallinity of TiO2 particles is evidenced by the calculation of the d-spacing referring to the plane (101) of the anatase, which presented an increase from 0.367 nm in pure TiO2, to 0.395 nm in the TiO2-K-PHI 5% sample. Furthermore, the SEM images allows to observe that increasing PCN content did not affect the morphology of the samples, however the films becoming more compact due a possible agglomeration of the particles. All the modifications observed may further affect the photoelectrochemical response of the samples to some extent.

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Effects of $4d^n$ Doping on Microstructure and Photoelectrochemical of rutile Titanium Dioxide films prepared by hydrothermal

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Titanium dioxide (TiO_2) nanostructures combine a bandgap (Egbulk) of 3.2 eV and high physicochemical stability, it becomes an excellent candidate material for the photoelectrocatalytic generation of hydrogen [1]. In this work, We report the microstructural and morphological effect of dopping the TiO_2 rutile with $4d^{n+}$ ions (K^+ ($4d^0$), Co^{3+} ($4d^6$), and Ni^{2+} ($4d^8$)). The impact on morphology was evaluated by scanning electron microscopy, exploring top-view and cross-sectional images to understand the growth dynamics of hierarchical structures of TiO2 nanorods/spherulites. The crystalline structure was evaluated by X-ray diffraction (XRD) and the microstructural advancement was verified by Williamson-Hall microstructural analysis. XRD patterns were obtained by the Rigaku diffractometer. The reactions were carried out in hydrothermal using titanium diisopropoxide (TTIP) as a titanium precursor, allowing the formation of TiO2 via acid hydrolysis with the growth on the surface of tin oxide and fluorine. Dopings were carried out in the range between 1.0% and 5% of 4dn ions. From the doping process, no modification of the crystalline structure of rutile TiO2 was verified, and there was no formation of secondary phases, such as titanates. Shifts in 2θ values are observed as a function of the ratio between the ionic radii of Ti^{4+} and its 4th-period pairs, and the W-H plots showed the microstructural advances. Hierarchical structures with growth of spherulite-like structures, such as nanorod continuity were verified for pure TiO_2. But depending on the level of doping, valence electrons, and ionic radii, different morphologies were obtained: larger nanorods when doped with high levels of Co^{3+}, lower growth density of spherulites with Ni^{2+}, and formation of urchins over nanorods for doping with K+.

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Effects of N-acetylcysteine on *Xylella fastidiosa* extracellular polymeric substances: a spatiotemporal microscopy study with implications for biofilm breakdown

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The extracellular polymeric substances (EPS) matrix found in biofilms significantly increases the risk of bacterial infections by shielding bacteria from the immune host response and drugs, ultimately fostering bacterial resistance. Therefore, alternate treatments that disrupt the EPS matrix are required. One alternative that has a variety of impacts on bacteria is N-acetylcysteine (NAC), albeit its various mechanisms of action in biofilms are still unknown. In this work, we investigate the effects of NAC at the single-cell level and early-stage biofilms of the phytopathogen Xylella fastidiosa using fluorescence and atomic force microscopy at micro and nano scales. We show the physical effects of NAC on each type of EPS and on the adhesion surface, as well as the mechanical response of single bacterial cells to NAC concentrations ranging from 2 to 20 mg/mL. Our results show that NAC disturbs the biofilm matrix, changes the conditioning coating on the substrate, and break down the soluble EPS, releasing adhering bacteria. NAC also reduces the volume of loosely bound EPS, and provides structural changes in tightly bound EPS. Furthermore, the use of InP nanowire arrays in bacterial force measurements during NAC action revealed an improved momentum transfer to the nanowires as a result of a larger cell mobility brought on by the removal of EPS. Our findings unequivocally demonstrate that soluble EPS and conditioning film are essential for controlling cell adhesion, and that NAC primarily acts on EPS removal, both at single cell and biofilm levels. These results provide solid evidence for the efficient use of NAC-complexed fertilizers in citrus cultures to protect against bacterial infection, and avoiding the eradication of infected plants.

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Engineering two-dimensional nanoporous networks selected by metal and nonmetal adatom coordination

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On-surface synthesis has been widely explored to prepare low-dimensional materials and control their functionality at the atomic and molecular levels [1]. A plethora of on-surface reactions can be employed to build such nanostructures, e.g., the C-H activation, Ullmann, and Sonogashira reactions, among others [2]. One of the main challenges is synthesizing a low-dimensional material with long-range and defect-free domains. Herein, we investigate the adsorption of organic molecules with pyridyl end groups on Cu(111) and Ag(111) using scanning tunneling microscopy (STM) and density functional theory (DFT). The deposition of (1,3,5-tris[4-(pyridin-4-yl)-[1,1'-biphenyl]]benzene) (TPyPPB) at room temperature on Cu(111) leads to vitreous structures, which rearrange in a honeycomb structure upon annealing at 400 K [3]. After annealing at 420 K a complex arrangement in a flower-like appearance. In addition, a honeycomb nanostructure is composed of low-defect and long-range domains. As observed in the smaller precursor, the hexagonal networks are stabilized only in the presence of Cu adatoms On Ag(111), a highly ordered and low-defect porous self-assembly is formed at RT. Subsequent deposition of Co and Cl, leads to the emergence of new ordered phases at RT. Especially the Cl adatoms leads to the formation of a self-assembly monolayer (SAM) stabilized by unconventional hydrogen bonds involving the halogen adatoms. The use of nonmetal adatoms, such as Cl, is a promising approach for applications in nanodevices due to their small influence in the semiconductor behavior of the 2D material formed.

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Improving Electron Pair Distribution Function (ePDF) for Nanomaterials

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Nanomaterials' properties are imposed by their crystallographic atomic arrangement and characterizing their structure is essential to understand their full potential application. However, standard X-ray diffraction (XRD) fails to elucidate the structures of small nanocrystals due to the elevated peak broadening, a challenge known as the nanostructure problem. Recently, Pair Distribution Function (PDF) analysis obtained by neutrons and X-ray scattering has been used as the main crystallographic tool to solve the nanostructure problem. However, Transmission Electron Microscope (TEM) technique can become an alternative to obtain the PDF from electron diffraction (ePDF), specifically for amorphous and nanocrystals.[1] Electrons have higher scattering power offering the advantage of using small sample amounts, time-efficient data acquisition, and lower costs. On the other hand, electrons have a higher probability of multiple scattering and inelastic scattering leading to a challenging data acquisition in the kinematical regime. Therefore, our team at LNNano have put efforts to study the effect of electron diffraction onto final ePDF $G(r)$ aiming to improve the technique towards quantitative ePDF. Comparing the experimental scattering profile $I(Q)_{exp}$, the structure factor $S(Q)_{exp}$, and the PDF $G(r)_{exp}$ with calculated $I(Q)_{calc}$, $S(Q)_{calc}$, and $G(r)_{calc}$ for spherical nanoparticles, the effect of TEM to final $G(r)$ are calculated. Also, comparing xPDF (synchrotron) with the ePDF, we have studied the influence of the instrumental transfer function to final PDF (peak broadening and damping). Excellent structure refinement has proved that ePDF can become a quantitative crystallographic tool. Allied to other TEM techniques, ePDF can be used to solve the nanostructure problem.[2]

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One-pot hydrothermal synthesis of TT-Nb_2O_5 and $H_4Nb_2O_7$ phase mixture

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Niobium oxides represent a class of materials under active investigation due to their anomalous crystallographic behavior. Among them, the TT-Nb_2O_5 phase stands out for its ongoing structural elucidation, while the pyrochlore phase of niobic acid ($H_4Nb_2O_7$) was first reported in 2008. Both phases remain subjects of debate in the literature, where the TT phase is obtained at low temperatures and the pyrochlore phase via hydrothermal methods using basic media, like ammonia [1,2]. In this study, we produced the nanomaterial via the hydrothermal route using hydrated niobium ammonium oxalate and urea, a weaker base than ammonia, obtaining a phase mixture of TT and pyrochlore for the first time, showing that basicity is key in the synthetic route. XRD, HRTEM, HAADF-STEM, and SAED revealed a phase mixture of $H_4Nb_2O_7$ and TT-Nb_2O_5. Interestingly, TT-Nb_2O_5 exhibited rod-like growth on the surface of $H_4Nb_2O_7$, established through images and FFT analysis, which confirmed the existence of a solid core of $H_4Nb_2O_7$, serving as the initial nucleation site for TT phase growth on the surface. Notably, TT-Nb_2O_5 displayed unprecedented behavior, forming nanorods with an average diameter of 10 nm and featuring bending structures with a high density of microstructural strain, making it a soft nanoceramic. Moreover, synthesis time directly influenced rod length and the fraction of the $H_4Nb_2O_7$ phase, indicating a correlation between synthesis duration and phase composition. The phase mixture showed excellent adsorption behavior, prompting the use of the studied material in several applications, such as batteries, photocatalysis, and adsorption for water treatment.

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Spatial Chemical Distribution Analysis of Sub-10-nm Bimetallic Nanoparticles via STEM-EDS and Machine Learning

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Nanoparticles have immense potential across various fields due to their tunable properties and their possibilities increase significantly for bi-metallic ones (BNPs), where the chemical composition and atoms' location within the BNPs become crucial. Determine their spatial chemical distribution is a challenging task, particularly for BNPs below 10 nm. In this study, we employ scanning transmission electron microscopy coupled with energy-dispersive spectroscopy (STEM-EDS) to investigate AuAg nanoparticles in the 3–10 nm range, produced by gas aggregation. Our analysis reveals robust evidence of Ag enrichment towards the BNPs surface, confirmed by statistical analysis and non-overlapping 3-sigma uncertainty intervals. Additionally, employing principal component analysis (PCA) and non-negative matrix factorization (NMF) machine learning techniques, we extract latent information on subtle composition variations within the the studied nanosystens, validating our experimental findings with simulated data sets. Our results not only contribute to the understanding of spatial chemical gradients in BNPs but also underscore the importance of well planned experimental procedure, data collection, rigorous error bar calculations, and raw data statistical validation for precise structural and chemical investigations of nanosystems.

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Understanding Cellulose Nanocrystal Nematic Phase by Cryo-TEM

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Nanocelluloses extracted from pulps (nanocrystals-CNC and nanofibrils-CNF) are environmentally friendly sourced and biocompatible materials with outstanding properties, like high Young's modulus, and aspect ratio. CNCs readily self-assemble into a nematic phase in water at low concentrations. These structures are promising for the rheological control of formulated products and as photonic pigments.1 Despite increasing interest, insights into the arrangement of CNCs and its impact on mechanical and optical properties are scarce. In this contribution, we used Cryogenic-Transmission Electron Microscopy (cryo-TEM), to understand the organization of CNCs with different surface charges (≈0, 0.25, and 1.2 mmol g-1) in water. The oxidized CNCs were prepared using the method described by Habibi (2006), and images were acquired on a Glacios cryo-TEM (Thermo Fisher Scientific).2 Preliminary results show that the CNC morphology is not affected by the degrees of oxidation. All CNC samples expose a rod-like morphology with diameters of 5-8 nm and lengths of 60-160 nm. Surface charges modulate the organization among nanocrystals, and low charge-density CNCs are better distributed over the TEM grid. Surprisingly, highly charged CNCs tend to agglomerate, possibly to reduce the excluded volume.3 To characterize arrangement in more detail and to understand how this influences the nematic phase, a Cryogenic-Electron Tomography study is being carried out.

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Understanding Nanoscale Sodium Niobate Perovskite Structures grown on Nb substrate by Advanced Electron Microscopy

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Sodium niobate (NN) perovskites are widely studied for their diverse semiconductor, piezoelectric, and photocatalytic properties. They offer facile synthesis and are non-toxic, making them prime candidates for replacing lead-based traditional materials and spearheading novel device innovations [1]. In this study, we use a hydrothermal process and a subsequent vacuum heat treatment, to tailor NN into one-dimensional nanostructures and stabilize the elusive Q phase—which is typically a metastable phase endowed with room-temperature ferroelectricity [2, 3]. This unique phase shows exceptional promise for piezo-phototronic devices (PPD), where the synergistic coupling between piezoelectric and photocatalytic effects enhances the efficiency of devices [4, 5]. To understand the NN microstructure, as well as its crucial features for applications, including surface, substrate interface, chemical composition, and polarization characteristics, we have used advanced techniques such as scanning transmission electron microscopy (STEM), coupled with energy dispersive spectroscopy (EDS), and differential phase contrast (DPC). This study serves as a linchpin for comprehending and optimizing device design tailored for PPD applications, paving the way for innovative advancements in functional materials.

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A model system for “host-guest” chemistry: Pt-based organometallic nanomesh on Ag(111)

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The study of two-dimensional molecular systems on metal surfaces has generated interest in the scientific community in recent decades due to its potential applications [1]. One method to obtain these nanostructures is the bottom-up technique, which involves the manipulation of molecular precursors through reactions on the surface, forming structures such as metal-organic networks. These molecular structures are highly ordered, where metal atoms act as connecting nodes, generating porous structures that exhibit long-range order, offering a favorable environment for the adsorption and reaction of molecules in confined spaces, known as "host-guest chemistry" [2]. In this work, we investigate by scanning tunneling microscopy STM measurements the adsorption of two molecular precursors: 1,3,5-tris[4-(pyridin-4-yl)-[1,1'-biphenyl])benzene (TPyPPB) and dichloro-(1,10-phenanthroline)-platinum(II) (Cl2PhPt), deposited on the surface of Ag(111) at room temperature. The results show the formation of two-dimensional metal-organic porous networks with hexagonal geometry. Our results reveal that by combining these two molecular precursors and using annealing treatments for molecular activation, these two molecules manage to interact with each other to form a series of different ordering patterns before stabilizing in a network with hexagonal coordination geometry. That is, two adjacent molecules TPyPPB are oriented collinearly and are coordinated through their endings Py by a Pt atom. This nanostructure has a regular distribution of its pores, which indicates the ability to confine within molecules that function as rotors and can only be stabilized in positions where there is a coordination point between the TPyPPB molecules and a Pt atom. Acknowledgments

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Analysis of graphene oxide addition on the formation of grass-like alumina films

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Amorphous aluminum oxide (Al2O3) can form structures referred to as "grass-like" or "flower-like" through hydrothermal treatment near the boiling point of water. The presence of the grass-like structure (GL) allows for an increase in the surface area and transparency of alumina films, primarily utilized for functionalizing transparent coatings obtained by aqueous phase [1] or vapor phase [2] deposition techniques. The modification to a GL occurs due to the hydration of alumina in water, through the formation of oxyhydroxide (AlOOH) or hydroxide (Al(OH)3) [3]. The impact of additives in alumina films on the formation of the grass-like structure is a topic that has been scarcely addressed in the literature. Intending to identify the impact of adding graphene oxide (GO) into the system while synthesizing a transparent and conductive film, we synthed films of Al2O3 with GO addition via the sol-gel method using aluminum isopropoxide as a precursor. Films were obtained through the blade coating method and deposited on soda lime glass substrates. The samples were sintered at 400°C and underwent thermal treatment in water at 85°C. Scanning electron microscopy images showed that grass-like structure was formed on the surface of both samples, with and without GO. GL nanostructure removed from the films surface was analyzed by transmission electron microscopy and electron diffraction revealed that they have the Crystal structure of gama alumina (ICSD-99836).

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Assembling porphyrin molecules on a molecular nanoporous network

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Manufacturing diverse two-dimensional (2D) functional nanostructures has appeared as a pivotal strategy in propelling technological advances across various fields. On-surface synthesis methods employing multiple approaches, including metal coordination [1] and Ullmann coupling [2], can achieve this. Previously, the adsorption of 1,3,5-tris[4-(pyridin)-[1,1'-biphenyl]benzene (TPyPPB) molecule on Cu(111) has demonstrated the potential to form a nanoporous network [3] suitable for hosting a variety of different molecules. In this work, we investigated by scanning tunneling microscopy (STM) measurements the adsorption of free-base tetra(4-bromophenyl)porphyrin (H2TBrPP) on the Cu-coordinated network of 1,3,5-tris[4-(pyridin)-[1,1'-biphenyl]benzene (TPyPPB) on Cu(111). We deposited TPyPPB at different rates and at room temperature on Cu(111). Upon annealing at 400 K, two ordered phases were observed: honeycomb and flower-like. The adsorption of H2TBrPP held at room temperature on the TPyPPB network led to the observed partial destruction of the network. After a second annealing at 400 K, the honeycomb and flower-like phases were restored, and some porphyrin was trapped in the TPyPPB network pores, indicating the nanoporous network's ability to host porphyrin molecules.

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Assessment of surface defects with different strain levels in the Al-Zn-Cu-Mg (7075) alloy and Al-4Mg (5083) alloy

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Two alloys with different ductility were analyzed in relation to surface defects generated in plastic deformation under tensile tests, and their characteristics were analyzed microstructurally. The Al-Zn-Cu-Mg (7075) alloy is characterized by its high mechanical strength and structural applications, especially in the aeronautical industry, while the naval alloy Al-4Mg (5083) presents moderate mechanical strength and greater ductility. In a first step, alloy 7075 was analyzed with the generation of microstructural defects through tensile tests under different levels of deformation. The samples were stretched up to 60, 70, 80 and 90% of their total deformation. Analyzes carried out via scanning electron microscopy (SEM) revealed the effectiveness of the procedure used in the formation of microcracks. The quantity and of microcracks were proportional to each applied deformation. With the aid of microscopy imaging software (Image-J), the number of defects was quantified and compared. The results show the formation of several types of defects, such as microcracks in the ductile Al-alpha matrix (CFC), brittle microfractures in the second phase, in addition to the occurrence of several grains of the matrix containing multiple cracks transverse sequences to the applied mechanical stress. A complementary analysis was carried out for the Al-4Mg (5083) alloy, which presents moderate mechanical resistance and high ductility, for a deformation of 80%, where, in addition to the lamination deformation lines of the original sample, the marked presence of microcracks transverse to the direction of traction, mainly in its central region; while in the lateral region the occurrence of a greater number of deformation lines parallel to the tension and the presence of shear deformations at 45°. The deformation mechanisms result from the cooperation between the actions of the ductile aluminum matrix (CFC) and the respective hardening precipitates in each alloy.

Atomic force microscopy used to characterize nanomechanical properties of UHMWPE nanocomposite

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Ultra high molecular weight polyethylene (UHMWPE) is used in several areas, such as in orthopedic prostheses due to its biocompatibility, high impact resistance, low coefficient of friction and great wear resistance. Furthermore, the addition of nanoparticles can improve the prostheses lifetime. The objective of this work was to characterize the nanomechanical properties of three samples that were subjected to wear tests: UHMWPE with vitamin E (UE), UE with aluminum oxide nanoparticles (UEA) and UE with boron carbide nanoparticles (UEB). Atomic force microscopy (AFM) was used to measure adhesion and stiffness through force curves in regions inside and outside of the wear track, totaling 1920 force curves per sample. The methodology was tested and calibrated on silicon surface, a more rigid material. The adhesion and stiffness measured inside the wear track of the nanocomposites was higher than that outside the track, probably due to the modification on the nanocomposite microstructure, like chain alignment, during the wear tests [1]. This work showed that the addition of nanoparticles and mechanical deformation modifies the nanomechanical properties of the UHMWPE.

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Characterization of microstructural banding and the effects on mechanical properties of AISI 9254 steel used for railway fastening clips

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The railway fastening system is used to connect rails and sleepers on a railway track. One of the most critical components in this system is the railway fastening clip, responsible for applying compressive forces on the rail base to prevent it from shifting. The material commonly used for manufacturing these clips is quenched and tempered martensitic spring steels. Since heat treatments are typically developed based on nominal chemical composition, local segregation can significantly influence the quality and conformity of the final product. As steels become cleaner and inclusions play a less significant role on the ductility of high strength martensitic steels, local composition inhomogeneity can result in high local deformations in segregated bands and lead to premature failure [1-3]. Through optical microscopy and scanning electron microscopy (SEM) analysis, coupled with energy-dispersive X-ray spectroscopy (EDS), regions containing micro-segregation, primarily silicon, forming bandings have been identified in the AISI 9254 steel of a railway fastener. Thus, this study aims to characterize the micro-segregation present in railway fastenings using nanoindentation techniques to identify changes in mechanical properties in banded regions. For this purpose, nanoindentation marks were carried out on the longitudinal section of the fastener samples to evaluate the mechanical properties of both banded and non-banded microstructure. Additionally, nanoscratching and scanning probe microscopy techniques were employed, and scratches were observed through SEM, measuring the scratch hardness. The properties of banded regions presented higher dispersion when compared to non-banded structures, which can contribute to localized stresses and failures.

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Characterization of Zircon Sample "PEIXE" from Tocantins, Brazil: A Potential Age Standard for Fission Track Method

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Zircon, a ubiquitous accessory mineral found in diverse rock types, plays a crucial role in dating processes due to its ability to incorporate trace elements like Uranium and Thorium [1]. Our research aims to comprehensively characterize and date zircon grains sourced from the Peixe Alkaline Complex in Brazil. We utilize advanced microscopy and spectroscopy techniques including Raman spectroscopy, optical microscopy, scanning electron microscopy (SEM) with cathodoluminescence and energy dispersive X-ray spectroscopy (EDX), X-ray diffraction and fluorescence (XRD/XRF), as well as mass spectrometry employing Laser Ablation Inductively Coupled Plasma (LA-ICP-MS) and the Fission Track Method (FTM). In addition to these techniques, we employ the External Detector Method (EDM) for fission track analysis. In this method, the zircon sample is bombarded with neutrons to induce fission in 235U nuclei. The zircon sample is attached to a mica muscovite sheet, which serves as the external detector. Following neutron bombardment, the mica sheet is etched to reveal the induced fission tracks in the zircon, which are visible under optical microscopy. This approach provides complementary data to the conventional Fission Track Method, enhancing our understanding of the zircon's thermal history. Our primary objective is to classify the zircon sample and evaluate its suitability as an age standard for FTM within the Brazilian context. The zircon specimens extracted from the nepheline syenites of the Peixe Alkaline Complex manifest as megacrystals with centimeter-scale dimensions. To explore potential anisotropic behavior in track density, these megacrystals will be sectioned into different faces. Additionally, a portion of the megacrystal will be reduced into grains with lengths of approximately 200 µm, possessing random crystallographic orientations. Employing FTM in conjunction with LA-ICP-MS will enable the simultaneous acquisition of fission track age and isotopic characterization, potentially validating its utility as a standard. Geological evidence suggests that zircon megacrystals from the Peixe Alkaline Complex nepheline syenites crystallized around 1503±3 Ma, with indications of a subsequent metamorphic-metasomatic event resulting in lead (Pb) loss around 577 Ma [2]. This research aligns with the scope of the XI Materials Microscopy Meeting, contributing to the discourse on advanced microscopy and spectroscopy techniques in material science, particularly within the context of geological sample analysis.

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Characterizing Apatite Minerals: An Atomic Force Microscopy Investigation into the Anisotropy of Apatite Grains

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Apatite reveals its geological history through the accumulation of fission tracks generated by the decay of U^{238}. We can determine their retention age by analyzing these tracks after etching them with nitric acid, thus identifying significant geological events [1]. Etching of the mineral can reveal different distributions of fission tracks, such as homogeneous, heterogeneous, and anomalous patterns [2]. These different patterns, can indicate alterations in the internal structure of the mineral, represent anisotropy. Therefore, this study aims to investigate the anisotropy of apatite grains from the São José do Campestre domain in the Borborema Province, Natal, RN, Brazil.

Utilizing atomic force microscopy (AFM), we analyze the mineral surface during the process of etching, allowing us to observe changes in surface topography and morphology. This enables us to gain insights into how the mineral's surface structure evolves under the etching conditions. This investigation provides insights into the crystallographic orientation and structural heterogeneity within the grains. Furthermore, characterization techniques, including Scanning Electron Microscopy (SEM) coupled with Energy Dispersive Spectroscopy (EDS) and Micro-Raman Spectroscopy, are employed to further explore the mineral properties. These comprehensive analyses deepen our understanding of the geological history and thermal evolution of the São José do Campestre Tectonic Domain and provide data for correlation with other geological formations [3]. This study elucidates the geological processes and tectonic dynamics shaping the studied domain and analogous geological formations worldwide by exploring the anisotropic properties of apatite grains within this region.

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Copper - Brass laminar structures produced by accumulative roll bonding

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Copper is the material of choice for high electrical conductivity, but this metal presets low yield stress. Precipitation hardening induced by alloying elements and mechanical strain elevate the yield stress but reduce ductility and electrical conductivity. The significant advantage of heterogeneous microstructure projects in metallic materials is the optimization of the stress-toughness dichotomy in structural materials. Altering the distribution and shape of regions of strength and plasticity through harmonic, bimodal, lamellar, or gradient structures allows for the optimization of these properties [1,2]. The accumulative roll bonding (ARB) applied to two FCC alloys with different stacking fault energies can create a structure where grain and twin density vary in a lamellar manner. In this study commercial purity copper and 15%Zn Brass were bonded at a volume fraction of 50% using a reduction rate of 50% and annealing steps of 15 min at 700oC. The bonding procedure was repeated up to 8 times resulting in a lamellar structure with layer thickness that varied between 500 and 15 mm. The microstructure was characterized by optical microscopy, electron scanning microscopy and backscattered electron diffraction. The copper layers contained a coarse grain structure and the brass layers were characterized by a refined grain structure. Because Zn diffuses faster than Copper a chemical gradient transition layer (GTL) appeared, the extension of this region increased with the number of bonding cycles.

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Correlative Microscopy Based on Raman, NanoRaman, Nanophotoluminescence: co-localized physicochemical characterization by multimodal spectroscopy

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This presentation will cover the basic principles of correlative spectroscopy applied to a wide range of physical and chemical characterization of materials, including polymers, ceramics, biomaterials, biological sciences and two-dimensional (2D) materials. Based on the light-matter interaction, we obtain relevant information, such as: particle distribution, homogeneity, grain size, phase changes and several other characteristics of the sample by spectroscopic evaluation of the material. The hyphenation of Atomic Force Microscopy (AFM) and Raman spectroscopy provides a broad understanding of the complex dynamics of diverse sample types, recognizing the crucial role of comprehensive characterization, enabling nanostructural and chemical sample characterization, including contamination analysis and traces of materials. A cutting edge multimodal characterization method will be presented based on the use of an automated AFM platform and integrating a Raman/Photoluminescence spectrometer, allowing true co-localized physical and chemical properties. Raman spectroscopy, within this colocalized approach, facilitates the identification and characterization of diverse compounds, providing essential data on their molecular structures and compositions, including potential microscale contaminants. Simultaneously, AFM contributes vital information about the topographical and mechanical properties of these samples, offering detailed data on surface textures, surface adhesion, roughness, and nanoscale stiffness. Laser-excited photoluminescence and Raman scattering of two-dimensional (2D) crystals reveal the structure of solid state materials. The development of instrumentation makes it possible to hyphenate Raman with other techniques, such as Photoluminescence and AFM, which can achieve nanometer-scale resolutions. The technique can be applied in several areas such as pharmaceuticals, photovoltaics, graphene, cells, nanoparticles and microplastics.

Detailed electron microscopy investigation of hydrogen-induced embrittlement in rough and additive-manufactured nickel-based superalloys

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Hydrogen energy is a promising carbon-free energy source. However, the main challenge is hydrogen storage due to the risk of embrittlement of alloys due to their accumulation inside metals. After several years of study, the mechanisms behind hydrogen embrittlement are still not fully understood. Austenitic steels have small hydrogen diffusion coefficients compared to ferritic and martensitic metals, making them a promising alloy for ammonia crackers and hydrogen storage. This study aims to elucidate Inconel 625 (IN 625) hydrogen charging, focusing on hydrogen pathways, trapping sites, interactions with material defects, and the similarities and differences between rough and additive manufactured materials. The specimens were cathodically hydrogen-charged using an As_2O_3 solution and a current density of 20 mA/cm^2 for 168 hours. During electrochemical hydrogen charging, hydrogen atoms enter steel and preferentially occupy FCC octahedral interstitial sites. After the hydrogen release, the specimens' surfaces were analyzed by SEM, EBSD, ECCI, and silver decoration [1]. The results indicate that some of the H^+ is released as hydrogen molecules. The primary mechanism for hydrogen release is through dislocation slip bands, resulting in surface deformation and the formation of both straight and irregular cracks [2]. The EBSD maps revealed straight cracks come from dislocations slip bands, and irregular cracks due to the lack of space in the grain to support the deformation caused by hydrogen molecules.

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Dimensional Analysis of Graphene Oxide Reference Material by Scanning Electron Microscopy and Atomic Force Microscopy

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Graphene oxide (GO) is a promising candidate for a wide range of applications due to its distinct properties and versatility. The analysis of a graphene reference material is essential for accurately identify its specific properties, enabling comparisons between samples and ensuring consistency and reliability of final products in the industry, thereby promoting safety and efficiency in large scale production. However, to maximize its application field, proper characterization in terms of dimension and morphology is necessary. In this study, dimensional analysis of GO nanosheets was performed from scanning electron microscopy (SEM) and atomic force microscopy (AFM) images, using Image J software for image processing. A protocol for dimensional analysis of GO samples by microscopy was developed prior to data acquisition, testing different conditions of sample preparation to allow a broad visualization of the GO sheets. Results showed that the definition of the protocol for GO sample preparation, encompassing substrate cleaning conditions as well as image acquisition parameters, plays a vital role in the quality of the acquired images concerning particle counting. Thus, several sample preparation methods were explored, and experimental parameters were established to address reproducibility and material quality requirements. Upon analyzing the images obtained by AFM, we observed a graphene layer distribution of approximately five layers in GO reference material, so it meets the rules of the term "few-layer graphene" as described by ISO/TS 80004-13:2017, where the number of layers ranges from three to ten.

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Effect of eletrical charge in electrodeposition process on photoelectrocatalytic performance of $BiVO_4$ nanostructures

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Aiming for energy vectors from renewable sources for the energy transition and the diversification of energy sources towards renewables, green hydrogen stands out for its zero carbon emissions in both its production and combustion. Among the synthesis routes, the photoelectrochemical route has been extensively studied because it uses semiconductors as electrodes, which reduces the cost associated with its implementation. $BiVO_4$ be noteworthy among semiconductors based on metal oxides due to its theoretical efficiency of 7.4 $mA.cm^{-2}$ and solar-to-hydrogen conversion efficiency of 9.2%. From this perspective, the work investigated the impact of the applied electrical charge (-0.2 to -1.0 C) on the electrosynthesis process (nucleation, growth and morphology of bismuth oxyiodide, BiOI) in addition to the photoelectrocatalytic performance of $BiVO_4$. The photoelectrocatalytic performance was developed by linear voltammetry, chronoamperometry, electrochemical impedance spectroscopy and IPCE, quantifying H_2 production by gas chromatography. Being accompanied by structural and morphological advances by XRD, SEM, TGA/DSC and Profilemetry. For the charge studied, the maintenance of the BiOI crystalline phase was reinforced in the applied range, however, the impact on morphology and thickness in the two-dimensional nanostructures was notable, with the growth of nanoplates being evident with increasing charge. Which directly impacts the thermal conversion to $BiVO_4$. Photoelectrochemical characterizations showed a tendency in photocurrent density from 0.8 $mA.cm^{-2}$ to 2.4 $mA.cm^{-2}$, with an increase in the applied charge from -0.2 C to -1.0 C, respectively. Achieving the best photocurrent densities with 3.2 $mA.cm^{-2}$ at -0.8 C, which are associated with film uniformity by cross-sectional SEM images and profilometry. The photocurrent density obtained with the $BiVO_4$ produced corresponds to around 43% of the maximum theoretical photocurrent density of this semiconductor.

Effects of Oxidation on the Surface of Thin Copper Films

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Copper is one of the most used materials in the industry, due to its low electrical resistivity, high thermal conductivity and low cost. Despite its desirable attributes, it is quite reactive to atmospheric conditions, undergoing an oxidation process that affects its properties, especially those related to electrical transport.

In this work, the effect of low pressure oxidation on the surface morphology of copper was studied. For this, a 20nm film of this material on mica was manufactured in a vacuum chamber with the PVD method. It was characterized with scanning tunneling microscopy for different oxidation conditions. The unoxidized and oxidized surface was examined for 3 minutes at E-3[Pa] and oxidized again for 3 minutes to E-1[Pa]. For each state of the sample, 250x250nm2 images were obtained and analyzed with the WSxM software [1] to obtain the correlation function of height differences g(R) of each oxidation condition. Next, the function is fitted to represent a self-affine surface [2], determining the parameters that describe the function. The results indicate that g(R) and its parameters changed when the sample was oxidized, implying a significant increase in the roughness of the film, despite the low value of the pressures to which it was exposed.

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Evaluation of Scale-Up Synthesis in the Production of TiO_2 Nanotubular Structures via Electrochemical Anodization

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Titanium dioxide (TiO_2) semiconductors are widely used in photocatalysis due to their high chemical stability, low cost, non-toxicity and good photoelectric response [1]. Among the various structures formed by TiO_2, nanotubes (TNT) emerge for their high surface area, which enhances their photocatalytic activity. This nanotubular structure can be applied for the photodegradation of emerging contaminants, yielding satisfactory results. Thus, increasing the anodized area of these materials lead the way for large-scale applications, such as effluent treatment [2]. Therefore, we increase the anodized area of TiO_2 nanotubes (TNT), aiming to overcome the limitation of 10 cm² reported in most published works [3]. The nanotubes were produced in 30 minutes, using a titanium substrate with a fluoride-containing electrolyte, applying a potential of 30 V. After anodization, the material was crystallized at 500 °C to obtain a mixture of anatase and rutile phases. Furthermore, the material's properties were characterized by X-ray diffraction (XRD), Diffuse Reflectance Spectroscopy (DRS), and its morphology was analyzed by Scanning Electron Microscopy (SEM). The anodized area achieved was 50 cm², the XRD confirmed the presence of anatase and rutile phases, while the DRS indicated a band gap characteristic of the majority anatase phase. The SEM images showed the formation of TiO_2 nanotubes with uniform morphology, and therefore, the results demonstrate the feasibility of producing TNT on a larger scale by electrochemical anodization, with potential for applications in the photodegradation of pollutants.

Acknowledgements: TiO_2, anodization, nanotubes
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Evaluation of the shear-induced non-isothermal crystallization of polyamide 6 by optical microscopy

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The use of rheo-optical techniques to evaluate crystallization on polymer processing has many advantages, especially when linked with microscopy analysis [1-3]. In this work, shear-induced crystallization of polyamide 6 (PA6) was studied with these techniques. A polarized light optical microscope, with an AxioVision system attached on its top allowing the acquisition of photos at any time during the measurement and a Linkam hot stage device to control shear and temperature, was modified to receive a specially built quantitative rheo-optical detector. Temperature was variable characterizing non-isothermal analysis. The experiments consisted of varying the shear rate on the polymer system while collecting the respective cross-polarized transmitted light intensity response by a LabVIEW software. Shear rates of 1, 10, 100 and 180 s-1 were applied to all samples. The crystallization behavior of the polymer was evaluated by DSC analysis. PA6's crystallization increased with the increase of the shear rate, however, for the PP/PA6 mixtures under the highest rates, the crystallization intensity falls from a specific temperature in which the polymer's viscosity is not enough to maintain the structural integrity. Data related to the PP/PA6 mixtures also showed that shear increases crystallization if the polymer has time to organize itself.

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Factorial design of pulsed anodization on TiO2 nanotubes formation and Hydroxyapatie deposition for dental implant applications

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Titanium is a biomaterial most commonly used in the study and development of endodontics implants due to its favorable mechanical properties, high biocompatibility, low toxicity and corrosiveness. However, it is an inert material and its bonding to bone tissue is hampered by poor cell-implant interaction. This work aims to modify the surface of titanium (Ti cp) by pulsed anodizing [1], with nanotubes formation and electrodeposition of hydroxyapatite, with subsequent in vitro tests with cells, to developing dental implants with characteristics favorable for adaptation of the human body, improving osseointegration and regeneration of bone tissue. Initially, a 23+CP factorial design [2] was carried out to screen for the variables anodizing processes: temperature (25°C/50°C), composition (NaF/NH4F) and solute concentration (0,35%/1,39%m/V). The electrodeposited TiO2 nanotubes were synthed and the samples were heat-treated at 400°C for 3 hours at a heating rate of 10°C/minute. Finally, the physicochemical properties were characterized using X-ray diffraction techniques, scanning electron microscopy and confocal Raman spectroscopy. The results obtained suggested that solute concentration has an effective impact on formation and morphology of the nanotubes. The samples showed the presence of morphologies characteristic of hydroxyapatite electrodeposition and Raman spectroscopy confirmed the presence of the anatase phase of TiO2 and the formation of nanotubes with diameters between 70 and 150 nm. Further experiments are therefore needed to complete the factorial design and quantify the correlations between the factors studied, with a view to future applications in dental implants.

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Fractal analysis of microstructures in Portland cement pastes

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Cement is used for the construction and renovation of structures such as buildings, bridges, and viaducts owing to its cohesive properties, low cost, versatility, and moldability. The conditions and curing time affect the microstructural characteristics and properties of cementitious materials in their various constitutions. Morphological changes occur in the microstructures of cementitious matrices with the progression of the hydration process and according to the type of cure, which affects the mechanical properties and durability of the material. Therefore, cylindrical specimens were fabricated to investigate the effect of curing conditions (ambient or submerged) on the morphology and compressive strength of hardened pastes cured for 7 and 28 days. The samples were subjected to the compressive strength test, and the surface of the fractured samples was analyzed using microscopic techniques. The quantifications of the morphological characteristics of the hydrated cement were correlated with the mechanical tests, and the local and global fractal dimensions were found to increase with time. This increase was accompanied by an increase in the compressive strength, which inhibited the propagation of the cracks and the development of broken fractal figures due to greater resistance to fracture.

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Germanium segregation on hematite-based photoanodes for water splitting

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Ge-doped hematite (Ge-Hem) was recently reported as a promising material for water splitting reaction due to its superior photoelectrocatalytic efficiency compared to pristine hematite and using other dopants.[1] It is well known that Ge is prone to segregate when hematite is formed [1], and it is associated with the control of hematite grain during thermal treatment. However, the homogeneity and extension of this segregation are not still deeply discussed. We have used transmission electron microscopy (TEM) and energy dispersive X-ray spectroscopy (EDS) to look in detail the Ge distribution in the sample. A lamella of Ge-Hem was prepared using FIB milling and analyzed using a Tescan Tensor microscope (100 kV) equipped with dual windowless silicon-drift EDS detectors. Non-negative matrix factorization (NMF) is a widely used tool for denoising EDS data [2], and it was employed to improve the signal-to-noise ratio and reveal hidden features from the Ge-Hem sample. The Ge segregation occurred mainly at the hematite surface and FTO/hematite interface. No significant Ge migration toward the substrate was identified. Different pre-treatment conditions, such as binning and filtering, were employed, and they affected the number of components distinguished from the noise. It highly impacted the quality of the denoised model and retrieval of real sample features. Our results corroborate other studies that discuss the loss of information in the case of low-concentration elements when using multivariate analysis [3]. Also, this approach helped to diminish the effect of undesired elements, such as Ga implanted during FIB milling.

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Growth of thin film of CuZr metallic glass by sputtering

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Metallic glasses materials change mechanical and chemical properties in comparison with the correspond metal and bulk are normally produced by ultrafast cooling [1]. However, a thin film of metallic glass can be produced by growth methods such as sputtering or thermal evaporation [2]. In this study, we have grown thin films of CuZr by sputtering with different compositions. The thin films were characterized by different techniques. The composition was obtained by dispersive energy spectroscopy (EDS) and electron energy loss spectroscopy (EELS). The oxidation state was acquired by electron energy loss spectroscopy. The structural analysis was done by electron pair distribution function obtained by electron diffraction. The roughness and the thickness were measured by atomic force microscopy (AFM). In this way, we have obtained the highest amorphization for 47% of copper and 53% of zirconium. We have observed that the oxidation process is higher for CuZr metallic glass thin film with higher contents of Zr.

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In-Situ Experimental Investigation of Fugurite Crystallization: Influence of the physicochemical composition of the sand

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Fulgurites are amorphous crystalline structures (glasses) naturally formed from atmospheric discharges that reach soil containing sand. Such electrical discharges generate abrupt heating of the silicates in the sand, creating a dendritic crystal structure that has fractal properties. They generally occurs on beaches and deserts. However, the reproduction mechanisms of these structures in laboratories are still the focus of investigations. Several factors can influence the shape of fugurites, one of them is the physicochemical composition of the sand. In the present work, using an arrangement of high-power electrical discharges made from voltage doublers and a metalic capacitor reactor designed to support 0.1-2mA discharges with voltages of the order of 10-400kV, we will investigate the influence of the granulometry of three different sand samples, that also have different chemical compositions. The Sands were collected from the following beaches: Ubu Beach in Ubú-ES; Pontal do Atalaia Beach in Arraial do Cabo-RJ; and Camburi Beach in Vitória-ES. For the purpose of more effective characterization of the sand samples, we calculated the electrical resistivity (used to determine the voltage range used in the discharges), density and x-ray diffraction. The structures obtained are in the characterization phase, and as first analysis, the morphology (volume, total area of spreading of the samples' dendrons) points to a change in the shape of the crystals through a change in granulometry/chemical composition. The parameterization of fugurites via fractal dimension using the mass-radius technique wil be evalueated and possibly allow a more categorical analysis of the influence of the type of sand on the formation of crystals.

Integration of Microscopy Techniques for Zircon Thermochronological Analysis

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The mineral zircon, with the chemical formula $ZrSiO_4$, is abundant in the Earth's crust and possesses the crystallographic property of accumulating heavy chemical elements like uranium within its crystallographic structure. This characteristic makes it a valuable tool in thermochronology studies. When subjected to an etching on its surface, zircon exhibits fission tracks resulting from the spontaneous fission of the U^{238} isotope, observable under optical microscopy (OM). Large-d zircon crystals are rare, with typical usage occurring in small grains measuring less than 1 mm. Therefore, microscopy techniques are indispensable for the analysis of this mineral. This study aims to incorporate microscopy techniques as a means of supporting thermochronological studies with zircon, including micro-Raman spectroscopy, scanning electron microscopy, atomic force microscopy, and OM. The Raman spectra can quantify not just a crystal's bulk radiation damage, but also map intracrystalline variations that are associated with radionuclide zoning [1]. Raman bandwidths results suggests a decrease in the relative percentage of the crystalline/amorphous phases at areas with higher density of tracks. Some SEM/EDS analysis showed chemical differences in intact and damaged regions after etching. Under cathodoluminescence, the mapping in zircon shows micro-domains with high Y, U, and Th concentrations within darkcores, while in bright cores there are deficiency in these elements [2]. Through AFM, it can be observed tracks that cannot be seen under optical microscope [3]. And for OM, it can be used to categorize zircon by the tracks appearence.

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INVESTIGATION OF HELIUM DIFFUSION IN NATURAL ZIRCON

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Zircon contains traces of unstable actinide elements [1], such as U and Th, and therefore undergoes radioactive decay, emitting alpha, beta, and gamma radiation particles in U-Pb and Th-Pb chains, alongside with spontaneous fission events of the U-238 isotope. Among the decay processes, alpha decay significantly contributes to the bulk damage and the loss of radiogenic Pb and He, skewing geological age determinations.

Our investigation focuses on the diffusion of helium from zircon, a product of alpha decay with unique diffusion properties in the mineral. Understanding the alpha emission from different zircon grains from standard samples (Fission Canyon Tuff (FCT) and Kawamoto Granadiorite (KGD)) revealed the inhomogeneity of U and Th concentrations, which can impact measured U-Th/He ages. This heterogeneity in particle emission may originate from imperfections in the crystalline structure, either inherent to zircon crystallization or acquired during its geological history [2].

We conducted an annealing test by exposing CR-39 alpha-particle detectors to the FCT and KGD samples inside an oven at various temperatures (40°, 50°, 60°, 80°, and 100°) and exposure times in order to understand the helium diffusion process due to temperature effects. After the irradiation process, the CR-39 detectors were chemically etched to reveal the alpha tracks, which were analyzed using an optical microscope. As a result, the percentage of track loss attributable to the annealing process was calculated based on the track density in the CR-39 detector.

Understanding helium diffusion from zircon's crystalline structure is fundamental to interpret U-Th/He ages accurately, thus improving the reliability of geological dating methods.

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Microstructural Elucidation of Ce-YAG Transparent Nanoceramics via HR-STEM with SiO_2 and MgO Additives

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This study presents the development of cerium-doped yttrium aluminum garnet (Ce-YAG) nanoceramics with the incorporation of silica (SiO_2) and magnesium oxide (MgO) to enhance optical properties.[1] Utilizing state-of-the-art microscopy techniques, we have detailed the microstructural transformations that contribute to transparency in the material. High-resolution scanning transmission electron microscopy (HR-STEM), with spherical aberration correction, was pivotal in revealing the nanoscale distribution of additives and their effect on the crystal lattice. These microscopic investigations were augmented by precise grain orientation analyses through HR-STEM's double tilt capabilities, exposing a significant reduction in light-scattering sites. Energy-dispersive X-ray spectroscopy (EDS) complemented the imaging data, ensuring a homogeneous dopant distribution and verifying the elemental composition. The combination of advanced microscopy techniques highlighted the role of SiO_2 and MgO in promoting densification and reducing porosity, critical factors in achieving superior optical quality.[2] Simulations using JEMS software confirmed the empirical observations, allowing us to model the optimal dopant concentrations for enhanced transparency. Our findings demonstrate that the strategic addition of SiO_2 and MgO to Ce-YAG can significantly refine its microstructure, thus offering a path to cutting-edge transparent ceramics for high-performance optical applications.

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Microstructure and Performance: A Deep Characterization of Electrofused Magnesia-Chrome

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Complex spinels are the leading contender for replacing electrofused magnesia-chromite aggregates (EMCA) in refractory compositions. This substitution is necessary because the commercial aggregate (which has its microstructure composed of spinel precipitates surrounded by a periclase matrix) releases Cr+6 at high temperatures (an ion toxic and carcinogenic to humans). However, with current developments, there is still no substitute product that performs similarly to EMCA, particularly in properties such as corrosion and thermal shock damage resistance. Previous work[1] shows that the high resistance to thermal shock damage is primarily due to oriented microcracks present in periclase. Hence, understanding its microstructure is crucial for replicating its properties in chromium-free complex spinel compositions. Using transmission electron microscopy and the 'ASTAR' orientation mapping technique on a lamella of electrofused magnesia-chrome obtained by focused ion beam (FIB) preparation technique, the interaction between precipitates and matrix was investigated. This in-depth analysis helps us to fundamentally understand the origin of cracks, particularly in the tension regions between the two phases present. In addition to tensions, the analysis identified nanoscale spinel precipitates present in the matrix, connected by lines of dislocations. These findings provide valuable insights for advancing the selection and development of safer and more efficient refractory materials, contributing to sustainability and innovation in the industry.

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Microwave Microscopy in Aqueous Environments

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The task of creating new methods for microscopy and biology presents itself with several challenges. Often the systems that need to be investigated must be in in vitro or in vivo conditions, which means that cells and other biological tissues must be in a liquid solution. Optical microscopy stands as the oldest tool to investigate living organisms, with numerous applications and results that made it ubiquitous for life sciences research. A recent development on the scanning probe microscopy family has been on microwave impedance microscopy, or microwave reflection microscopy (sMIM). The technique is quite suitable for the characterization of nanostructures and nanodevices, finding an important role in validating other techniques such as Tip Enhanced Raman Microscopy. The challenges in applying sMIM to life sciences stems fundamentally from the deployment of the technique in an aqueous environment, as well as the geometric effect of structures on the capacitance response. Usually, one operates the sMIM at 3GHz frequency, which is quite interesting since the relative permittivity of water at this frequency is over 80, which would correspond to a refractive index of 9. As such, water is an essential component for imaging surfaces. The main challenge is the operation in the near field since the associated wavelength is 10cm. Here we demonstrate the design of a microchamber with an appropriate transparent window for the deployment of the technique in aqueous environment. The microfluidic aspects, as well as the electromagnetic aspects of the chamber design were modeled using the COMSOL Multiphysics platform. The system operates by means of the reflection of the microwaves through the window onto which the sample of interest is adhered to. We will show preliminary results with polystyrene microspheres, demonstrating the feasibility of the technique, and perspectives for the investigation of live cells and other biological tissues and systems.

Modification of Titania Nanotubes with Bone-Like Apatite and RGD peptide to improved titanium biocompatibility

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Surface modification involving nanotube formation is a method that mimics the implant surface, bringing it closer to the nanometric dimensions of human bone and enhancing prosthesis interaction [1]. Additionally, coating with biocompatible molecules, such as hydroxyapatite and peptides, can promote a better cellular adhesion, bone mineralization, and extracellular matrix formation, thus accelerating the osseointegration process [2]. In this study, surface modifications are being developed on grade two titanium, involving the simultaneous formation of nanotubes with apatite and subsequent addition of the RGD peptide. The nanotubes (TiNTs) were obtained through the anodization method, with the electrolyte modified with simulated body fluid (SBF) for apatite electrodeposition, resulting in TiNT/SBF material. The RGD motif has been immobilized by silanization with 3-aminopropyltriethoxysilane and maleimide on TiNT/SBF. The presence of calcium (Ca) and phosphorus (P) was confirmed using scanning electron microscopy (SEM) with energy-dispersive X-ray spectroscopy (EDS). The apatite presence increased hydrophilicity measured by decreasing of contact angle, roughness by atomic force microscopy (AFM), and cell adhesion in MTT tests. These characterizations are also being carried out with samples containing the RDG motif (TiNT/SBF/RGD). After immobilization of RGD, the FTIR spectrum of the sample shows characteristic bands of APTES silanization and suggests peptide immobilization, with stretching at 2918 cm-1 for C-H and 1028 cm-1 for Si-O-Si. SEM images were used to demonstrate the morphology alteration after functionalization. In-vitro tests are being conducted to confirm the peptide's influence on titanium biocompatibility.

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Molybdenum (II) acetate as a precursor for molybdenum trioxide

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Transition metal structures (such as cobalt, nickel, and molybdenium) have been the subject of studies in recent years due to their electrical, catalytic and magnetic properties. Orthorhombic molybdenum trioxide (α-MoO3) is relevant because it is an antioxidant material, leading to its catalytic properties that are influenced by the valence state of molybdenum ions and the local environment where they are inserted. These structures have been investigated in developments of sensors, energy storage and the formulation of gels for the treatment of chronic diseases [1]. In this perspective, the present work proposes the use of the molybdenum (II) acetate as a metallic precursor for obtaining α-MoO3 structures by the thermal decomposition method [2]. The Mo (II) acetate belongs to a group of metal complexes composed of two highly correlated Mo ions, in which each cations are connected to complexes containing oxygen. This reagent could favor, in specific chemical route, the crystallization of MoxOy [2][3]. The syntheses yields were characterized by X-ray diffraction (XDR), scanning electron microscopy (SEM), and energy-dispersive analysis (EDS). The X-ray diffraction results suggested α-MoO3 crystallite of the 77 nm (by the Scherrer equation). By means of microscopy analysis were observed that the obtained morphology is microrod-like, with a of approximately 774 nm and a length of the 37 micrometers. The EDS analysis only showed energies related to molybdenum (Mo) and oxygen (O), confirming the purity of the obtained material.

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Nanostructural study of the nucleation and crystallization process of calcium carbonate and calcium phosphate

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Calcium carbonate (CaCO3) is one of the most abundant minerals in nature. Widely used in industry because it is low cost, abundant and has the characteristic of being harmless to health [1]. Calcium phosphates (Ca3(PO4)2) are one of the main inorganic constituents of calcified tissues of vertebrates and can be used in bone implants due to their high biocompatibility and bioactivity [2]. Controlled synthesis of CaCO3 and Ca3(PO4)2 is an important requirement for different applications and can also be used to understand the mechanism of biomineralization [3]. In this work, the physiochemical and morphological characteristics of CaCO3 and Ca3(PO4)2 nanoparticles were studied using cryo-TEM over time to analyse the precursor phases and the structural modifications of the nanoparticles in formation. Additionally, in situ TEM were performed, to monitor the phase transformation under heating. Aqueous solutions of Ca(OH)2 and H2PO4 were mixed under magnetic absorption. After 15 and 30 minutes of synthesis, the solution were ultrafast frozen (cryo-TEM) or dried on a TEM heating chip (in situ TEM). The synthesis of CaCO3 was carried out in a similar way, but using an aqueous solution of CaCl2 and NaHCO3 and with times of 5 and 15 minutes. Both syntheses were also carried out in the presence of molecules of biological and industrial interest. The results showed evidence of the precursor phases of the nanoparticles, as well as the phase transformation with the supply of energy to the system, proven by electron diffraction patterns.
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New transmission electron microscopy techniques available at LNNano

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The Brazilian Nanotechnology National Laboratory (LNNano) is an open, multi-user facility offering cutting-edge infrastructure, processes, and resources to support research in nanobiotechnology, nano- and microfabrication of devices, as well as synthesis and characterization of nanostructured materials. Our laboratory serves the academic community in Brazil and abroad, providing access to state-of-the-art equipment such as scanning probe microscopy, electron microscopy and various spectroscopic techniques.

LNNano offers a range of advanced and continually evolving electron microscopy techniques, including in situ heating, in situ liquid cell and four-dimensional scanning transmission electron microscopy (4D-STEM).

In order to fully comprehend the potential of these techniques, the principles and instrumentation associated with them, along with recent results obtained in support of both external and internal proposals throughout 2024 will be presented. It will also cover the process of submitting and evaluating proposals that justify the utilization of these techniques.

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Organization pattern of human osteoblasts grown on ceramic surfaces containing macropores with special geometries

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Topography of the substrate can lead to specific cell behavior [1]. Thus, it is expected that topographical features with different s and/or shapes would mimic in vitro, the properties of triggering and guiding the directional growth of cells that would occur in vivo. Here we studied the organization pattern of bone marrow stromal cells (BMSC) grown in vitro on the surface of hydroxyapatite ceramic discs containing macropores with cross-sections of different geometries. Discs with cells after 28 days of culture were analyzed by differential interference contrast (DIC) light microscopy and transmission electron microscopy (TEM). Cells grew onto the free region of the macropores and organized differently in regions near the limit of the ceramic when compared with the inner region of the pore. While near the ceramics contour, cells were distributed more radially, in more inner region where each cell was in contact only with neighbor cells, they oriented tangentially to the limit of the cell layers (usually circular) with a high number of cellular junctions. Tomographic series of images obtained sequentially by DIC showed the 3D arrangement of cells. The comparison of cells orientation with extracellular matrix molecules orientation was performed in order to make possible correlation between cell-to-cell tensions and the disposition of EM molecules. As next steps we expect to analyze potential mineralization in this model and if there is any correlation among cytoskeleton organization/cell organization/EM molecules organization, in a context of tensegrity.

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Particle size characterization of crushed papaya seeds for adsorption of copper (II) dispersed in aqueous medium via DLS-PCS

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Water contamination by copper is common in natural environments due to processes that exploit this metal, but it is also quite common to find high concentrations of copper in residential and commercial pipes that contain devices (valve) and/or copper tubes. Recent studies have been carried out with reusable organic materials that can adsorb copper dispersed in water. One of these materials is dried and crushed papaya seeds. Tests with powder from the same seed as well as the whole seed have already been carried out, indicating that the of the papaya seed particles must have a great influence on the efficiency of the process. The characterization of the of papaya seed particles has not yet been well explored. Therefore, the present work used the DLS-PCS technique developed in our laboratory for the purpose of determining the granulometry of samples in triplets of papaya seeds crushed in 3 different times (1min, 5min, 15min) in a high power blender (1500W) and diluted in 100mL of distilled water. The DLS experiment was carried out after 20 minutes of resting the solutions at room temperature 25ºC. Using the PCS protocols present in the literature, we found different values of hydrodynamic lengths for the 3 different types of crushed seed preparations. This characterization can help explain the improved efficiency obtained for the use of crushed seeds instead of seed powder, and help in defining a critical of the particulate material that can effectively maximize the copper adsorption process from water.

Polymeric film of Latex Dispersion with Silver Nanoparticles

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Latex or natural rubber is a biologically active and biocompatible biomaterial that can induce tissue repair [1]. This polymer is obtained in its colloidal suspension form either through extraction from the Hevea brasiliensis rubber tree or synthsized from hydrocarbon monomers, such as styrene and isoprene [1,2]. In addition to its biorepairing properties, latex possesses excellent physicochemical properties, such as good elasticity and high mechanical resistance , ensuring the durability of this material under unique conditions. The addition of silver nanoparticles (AgNPs) to the colloidal suspension confers antibacterial properties to the latex [3]. Herein, we propose obtaining a bioactive coating from natural latex with silver nanoparticles. Silver nanoparticles were formed in situ within latex dispersion by organic reducing agents, like glucose present in latex. The film was formed by casting and analyzed with profilometry to determine the thickness and Scanning Electron Microscope (SEM) to evaluate the morphology. The formation of nanoparticles was confirmed by UV absorption, and their morphology was obtained by Transmission Electron Microscopy (TEM). Their size and charge were obtained through dynamic light scattering (DLS) and Zeta potential, respectively. The antimicrobial activity of the nanoparticles and film is being tested against gram-negative (Escherichia coli) bacteria

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Probing the effect of ethanol concentration on cellulose-lignin interactions by AFM-force spectroscopy

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Lignocellulosic biomass is a promising source of renewable energy and materials. Cellulose and lignin, the major components of biomass, need to be separated for their further use. The mixture of water and ethanol is a promising solvent for separating cellulose and lignin. However, its effect on the molecular interactions between these molecules still needs to be understood. Herein, we used atomic force microscopy (AFM) in force spectroscopy mode to investigate the effect of ethanol concentration on the interaction between cellulose surface and lignin-coated AFM tip. The adhesion force measurements were performed in water, ethanol, and water-ethanol. Around 1024 force curves were collected for each solvent. Compared to water (~135 pN), the adhesion force exhibited a modest decrease in the mixture (~80 pN), followed by an increase in pure ethanol (~260 pN). The change in the conformation of lignin (more open in ethanol and more compact in water) can be an essential factor for this change in adhesion force. Molecular dynamics simulations are being performed to understand better the molecular interactions between cellulose and lignin in different ethanol concentrations. In conclusion, our results demonstrate the effectiveness of force spectroscopy as a tool for directly quantifying the effect of solvent composition on cellulose-lignin interactions at the nanoscale, providing insights for biomass pretreatment optimization.

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Structural, Chemistry and Electronic State of the Interfaces of Transparent Conducting Oxide and Hematite applied in Photoelectrocatalysis

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The efficiency of ta device at the nanoscale is driven by interface boundary conditions [1]. Changes in chemical concentration or structural arrangements at the interface can be assessed at the nanoscale by high-resolution transmission electron microscopy (HRTEM) images, in addition to electron energy loss spectroscopy (EELS) and energy dispersive spectroscopy (EDS) coupled to a scanning mode microscope (STEM) [2]. In this study, we investigated the interface of hematite with 3% Zr deposited on fluorine-doped tin oxide (FTO). We obtained chemical and electronic state characterization at the FTO/Hematite interface via STEM-EELS-EDS maps, processed using multivariate analysis calculations (PCA and NLLS). The results show a 2.5-nm thick interface region containing a Fe-Sn-O mixture. Structural analysis of the interface region by HRTEM imaging and HRTEM simulations showed that Hematite and FTO exhibit lattice distortions and stress field images were obtained via Geometric phase analysis (GPA). The concentration map revealed that Zr segregated at the grain boundaries of the hematite and in the mixing region of the interface and that Ni is deposited on the free surface of the hematite, not FTO. Zr acts in grain control and interface adjustment and Ni is a co-catalyst, improving the efficiency of the PEC device. The energy maps show a shift towards Sn+4 to Sn+2 and Fe+3 to Fe+2 for both FTO and Hematite grain boundaries, caused by the loss of oxygen from the system.

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Study of thin film of CuZr metallic glass by electron pair distribution function (ePDF)

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Metallic glasses materials present different behavior of the same bulk material such as higher strain deformation and lower corrosion and bulks are normally produced by ultrafast cooling [1]. However, a thin film of metallic glass can be produced by growth methods such as sputtering or thermal evaporation [2] and the films structure can be described by electron pair distribution function (ePDF) [3]. In this study, we have deep analyzed the amorphization local and averaged by electron pair distribution function (ePDF) using electron diffraction for different composition of CuZr thin films. We have obtained the length structure coherence (LSC) and maximum of crystallite (rmax). The composition and oxidation were analyzed by the first peak position and correlated with spectroscopy results, dispersive energy spectroscopy (EDS) and electron energy loss spectroscopy (EELS). We have also used electron pair distribution function simulation to better understand the structure properties of CuZr thin films.

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Synthesis and Structural Analysis: Enhancing CdSe Quantum Dot Efficiency through Electron Pair Distribution Function

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Cadmium Selenide (CdSe) Quantum Dots (QDs) are nanometric semiconductor materials under massive study due to their size-controlled optoelectronic properties. The crystallographic structure of nanoparticles can hinder the efficiency of QDs applications because of defects such as stacking faults and vacancies. Nanometric materials are challenging to characterize in terms of their crystallographic structure using standard X-ray diffraction analysis due to peak broadening[1]. The Pair Distribution Function (PDF) analysis of the total scattering data is an evolving alternative method to solve the atomic arrangement structure for nanomaterials. Specifically, electron diffraction PDF (ePDF) is optimal for characterizing nanoparticles because the strong electron-matter interaction allows for the precise acquisition of diffraction patterns from a known ensemble of nanoparticles. TEM equipment can collect diffraction data from a specific nanoparticle region, enabling the matching of images and elemental composition analysis with ePDF analysis. In this work, we synthesized CdSe QDs by classic routes to ensure reproducibility. Thermal annealing of the QDs was carried out to minimize structural defects. The Reduced ePDF G(r) was obtained by the Fourier Transform of S(Q) using Python scripts. Simulated G(r) for spherical zinc blend CdSe was fit to the experimental data using the DISCUS software[2], introducing stacking faults in the wurtzite structure. We quantified the stacking fault defect probability in the QD samples by fitting the G(r). Electron diffraction data revealed that the synthesis resulted in zinc blend structures with 40-50% stacking faults. G(r) results indicated a smaller crystallite size than those obtained from TEM morphological diameter and the first excitonic peak position.

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Understanding the Role of HP Steel Microstructure in its Magnetic Response

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Ferromagnetic materials exhibit inherent magnetization due to unpaired electrons, generating an internal magnetic field linked to material type and microstructural arrangement. The use of magnetic response identification has been employed as a non-destructive method to inspect and evaluate the integrity of steam-reforming tubes within the petrochemical industry. During operation, these tubes undergo microstructural changes and subsequent mechanical property deterioration, primarily attributed to the aging of HP steel under extreme service conditions. This aging process leads to the formation of precipitates and phase transformations over time, influenced by varying working conditions [1-3]. Dille et al. [4] reported that samples aged at 500-550°C exhibited a magnetic response at the matrix-Cr23C6 precipitate interface. Our study aims to correlate the sample's microstructure with its electromagnetic properties, enhancing non-destructive inspection sensors and deepening understanding of magnetic response evolution during HP steel aging. Using focused ion beam and transmission electron microscopy with energy-dispersive X-ray spectroscopy, we identified notable changes, including increased Nb concentration at certain interfaces and accumulation of Si and Ni-rich nanoprecipitates (~10 nm) at others. A full understanding of ferromagnetic behavior such as the one observed in the aged HP steel is crucial for the development of non-destructive techniques.

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Utilization Of X-ray Microtomography And Scanning Electron Microscopy Techniques For Characterization Of Alumix Matrix Composites Reinforced With Zirconium Tungstate

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The automotive industry prioritizes lighter components, prompting the study of Al-Si alloy (Alumix 231). Maintaining properties like thermal expansion coefficient (CTE) is crucial. Composites with zirconium tungstate ceramic reinforcement (ZrW2O), possessing a negative CTE, were developed to counter Alumix's high CTE. [1] [2]

Two samples were analyzed: pure Alumix (AZ00) and Alumix with 20% ceramic reinforcement (AZ20). Microstructural analysis employed X-ray computed microtomography (microCT) for volumetric analyses and scanning electron microscopy (SEM) for comparing results.

Pore percentage in AZ00 was 2.84% measured via Archimedes method, contrasting with 0.54% from microCT, attributed to resolution limits. MicroCT revealed pores ranging from 5.11 µm to 129.65 µm, averaging 9.16 µm, while SEM showed pores of 0.61 µm to 8.55 µm, averaging 1.27 µm. SEM's pore measurement (2.31%) aligned better with Archimedes.

In AZ20, microCT overestimated reinforcement percentage, indicating limitations. Despite smaller sampling, SEM's higher resolution enables more precise segmentation.

Ongoing efforts involve assessing matrix and reinforcement morphology and quantifying their distribution, alongside obtaining more SEM images to increase statistical robustness. This microstructural characterization is crucial for correlating thermal and mechanical properties of the composite.

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AC07-Surface Engineering - functional coatings and modified surfaces

Designing Multifunctional Coatings and Engineered Surfaces for Next Generation Technology Applications

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Surface engineering is a powerful technique to produce multifunctional coatings that can be used in many application fields. Modifications to surfaces could be on inorganic or organic materials, depending on the application, operational environment and required flexibility. In the case of inorganic materials, one of the most challenging sectors is in space, where extreme environments are present. Within the coatings we have developed, we will discuss how plasma based bespoke CVD systems have been developed for both moisture barrier and UV-radiation protective coatings in next generation satellites and space structures. These coatings have been extensively tested for robustness, space qualification and longevity. A new platform technology has been built to enable this novel form of 'space-skins' with multifunctional capability including energy scavenging and emissivity control. Some of these ideas can now be applied to terrestrial buildings where energy saving coatings can be produced to control heat flow and control habitable environments.

A further innovation is in using some of the large area techniques for flexible electronics, which allows for "human-wearables" and "building-skins" to be produced. These can then be used to monitor both humans and buildings such that we can better assist society in the health and well-being of our people and assets. To achieve this non-invasively with sustainability in mind nano-scale designs are being developed that are manufacturable and inexpensive. This talk will expand on the nanoscale design of systems for future wearables including the IoT plus its synthesis for human compatible bioelectronics.

A future with engineered coatings and multifunctionality will enable assisted living to support modern society. We hope such systems can be now designed and produced to improve the quality of life in everyday activities.

Finding ways to control the electronic and optical properties of single-walled carbon nanotubes towards their applicability

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The advances on the science and application of carbon nanotubes within the last three decades have brought to reality the production of materials approaching the theoretical predictions. Single-walled carbon nanotubes (SWCNTs), in particular, have outstanding electronic and optical properties. For instance, enhancing the photoluminescence (PL) of can bring to reality more than one ground breaking application in fields like biology and optoelectronics. However, the optical properties of these materials are strongly related to their morphology and intrinsically to their diameter. A potential way to gain control of properties like PL is the encapsulation of molecules or nanostructures in the tube´s hollow core but there are very small diameter tubes where this is not straightforward. In this presentation, I will show an overview of how new hybrids of SWCNTs and confined linear carbon chains have been developed toward the goal of gaining tunability of the tubes' properties. Examples of observable phenomena will be shown, such as how a diameter-dependent enhancement of the PL induced by energy transfer can be found in some types of nanotube-chain hybrids.

Nanoparticle-assisted radiosensitization of human glioblastoma cells using high-energy photon and proton beams: Surface engineering for the enhancement of cancer radiotherapy

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Metal nanoparticles are a promising new class of sensitizer agents in cancer treatment using radiotherapy. When colocalized with biological tissue, NPs may augment cell kill induced by high-energy radiation due to specific physical, chemical and biological effects elicited by the particles, which are closely related to their surface properties. In spite of the positive results reported in a large number of pre-clinical studies, the underlying mechanisms behind NP-assisted radiosensitization are not yet fully understood. In this contribution, recent results from our group on the sensitization effects produced by metal nanoparticles of different formulations in human glioblastoma cells irradiated by high energy photons and proton beams will be presented. We explored three classes of NPs: superparamagnetic iron oxide coated with dextran (SPION@DX); gold coated either with dextran (GNP@DX) or PEG (GNP@PEG), and Bi nanoparticles. Two cell lines (U87 and M059J) were exposed to the NPs at various concentrations and subsequently irradiated with either x-rays from a 6 MV linear accelerator, 662 keV γ-rays from a 137Cs source, or 150 MeV H+ beams. Several markers were used to monitor the sensitization effect (NP uptake in the cells, cell viability, post- irradiation cell survival via clonogenic assay, production of reactive species, and DNA damage and repair). Enhancement sensitization ratios at 10% survival (SER10%) varying from 3.5 down to 1.0 (i.e. no effect) where observed, depending on the NP´s characteristics and type of cell. We will discuss the effect of the surface coating and nature of the metal core of the NPs and the type of beam on the sensitization effects, and present mechanistic insights derived from such studies.

Recent Advances related to R&D&I of Diamond-CVD and Diamond-like Carbon (DLC) at INPE and CVD Vale Diamante

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CVD Diamond and DLC films growth have been in evidence by scientific and technological studies due to their demand in terms of scientific research and a lot of applications. More specifically, the DLC films with its superior properties such as low coefficient of friction, high chemical inertness, high hardness, high wear resistance, biocompatibility, bactericide, etc., and CVD Diamond, also with its set of singular properties that qualifies them for immediate and near future applications of high value-added. In this presentation, for DLC films a modified PECVD (Plasma Enhanced Chemical Vapor Deposition) technique with the new concept of additional cathode as an ion and electron confinement system will be presented. It will be shown some results from first stage of research up to scaling up process for industrialization of different DLC coating with superior proprieties on metals, composites and plastics, with very high adhesion, lower coefficient of friction, high hardness, very low growth temperature and very low pressure. Applications on Space, Aeronautics, Metallurgical and Health areas will be presented. Regarding CVD Diamond, a remark of HFCVD (Hot Filament Chemical Vapor Deposition) and MWPACVD (Micro Wave Plasma Assisted Chemical Vapor Deposition) Techniques, for CVD diamond Poly and Single Crystal will be discussed. Also, studies from first stage of growing up to scaling up for industrial application with a lot of examples already in the market and for near future will be shown. Application on metallurgy, health, semiconductor, nuclear batteries, quantum computer devices will be exemplified.

Advanced Nitride Coatings Deposited by Magnetron Sputtering as Enhanced Sensing Units in Impedimetric E-Tongues

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Magnetron sputtering enables precise deposition of thin films, crucial for various scientific and technological applications. Dynamic Glancing Angle Deposition (DGLAD) further refines hard coatings by controlling substrate oscillations [1], adjusting properties like hardness and texture. High-entropy nitride (HEN) films, consisting of multiple metallic elements in near-equimolar ratios, offer superior hardness, wear resistance, and corrosion protection, ideal for advanced sensing [2]. In this study, HEN thin films were applied as functional coatings on e-tongue sensing units to enhance sensitivity, selectivity, and durability of the sensor. Three films were deposited on a printed circuit board (PCB) using DGLAD, varying angular positions and nitrogen content. The deposition process used a multi-metallic target of Ti, Ta, V, Zr, and Nb, resulting in films approximately 150 nm thick on interdigitated electrodes (IDEs) at room temperature. Preliminary results showed significant improvements in sensor array sensitivity and robustness due to the coatings as well as the differentiation of solutions mimicking the basic tastes relevant for human gustatory perception (sweet, salty, sour, bitter, and umami) in a threshold below the human tongue perception. In conclusion, integrating magnetron sputtering with HEN thin films advances sensing technologies, paving the way for next-generation e-tongues with enhanced sensitivity and reliability for environmental monitoring, food quality assessment, and medical diagnostics.

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Application of high-energy ion bombardment for a degradation study on PVC films using the MeV-SIMS, PIXE and RBS techniques

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The study of polymer degradation induced by radiation is an emerging area with versatile practical applications. The dynamic of this sputtering process offers opportunities to deepen our comprehension of material’s resilience and aging mechanism, and also improves the understanding on more stable polymeric materials [1]. Polyvinyl chloride (PVC) experiences a notable loss of chlorine (Cl) atoms when exposed to radiation. The damage can be generated by a wide spectrum of energy, from low (such as visible light or heat) to high intensity [2]. Modifications in the chemical structure of polymers are associated with multiple processes, influenced by factors such as dose rate, oxygen presence, polymer composition, functional groups, crystallinity, and even the nature of radiation; properties such as linear energy transference and cross section define the damage mechanism velocity [1].

The purpose of the present research work is to investigate the degradation of PVC thin films induced by swift heavy ions. Techniques like Particle-Induced X-ray Emission (PIXE), Rutherford Backscattering Spectrometry (RBS) and Secondary Ion Mass Spectrometry induced by MeV ions (MeV-SIMS) were employed. The experiments were carried out with 2.0 MeV protons (PIXE), 1.2 MeV He^+ ions (RBS) and copper ions (MeV-SIMS) ranging from 300 keV up to 6 MeV. The methodology was based on previous studies of PVC degradation with charged particles, applying sequential measurements at the same position [2,3]. The PIXE and RBS techniques enables the verification of Cl loss as a function of irradiation fluency, while MeV-SIMS provides the fragmentation of PVC. The findings allow a proper characterization of the Cl depletion in PVC caused by radiation exposure.

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Comparative Analysis of Thermal Barrier Coatings Produced by Different Spraying Techniques on Aerospace Components

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Improving aeronautical materials properties is paramount. Thermal Barrier Coatings (TBCs) are crucial for protecting components like gas turbines from high temperatures, consisting of a metallic bonding layer (BC), an external ceramic layer (TC), and a thermally grown oxide layer (TGO). Application techniques, including atmospheric plasma spray (APS) and high-velocity oxygen fuel (HVOF) thermal spraying, influence coating morphology and microstructure, affecting properties such as porosity, adhesion, roughness, and thermal conductivity. This study compares TBCs produced with BCs from APS and HVOF on Ti-6Al-4V alloy substrates, focusing on microstructures and mechanical properties. Characterization, through optical and scanning electron microscopy was done aiming to understand its layer thickness measurement. Instrumented indentation tests assessed microhardness, modulus of elasticity, and elastic indentation work, while roughness tests examined coating surface morphology. The results underscored the impacts of different thermal spraying methods on TBC microstructure, with comparisons made to literature data. The study's outcomes are expected to aid in the development of optimized coatings for aerospace applications.

Corrosion Resistance of FeCrMnSiB Austenitic Stainless Steels Processed by Plasma Transferred Arc

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Boron-containing austenitic stainless steel with low stacking fault have been developed for superior wear [1] and cavitation [2] resistance applications. However, few studies have addressed the corrosion behavior of these steels. This investigation assesses the collateral effect of boron additions (0.2 and 0.5wt%B) on the corrosion resistance of FeCrMnSiB coatings deposited by plasma transferred arc (PTA) on AISI 304 stainless steel substrates, in naturally aerated NaCl 3.5 wt% media. The performance was benchmarked to those of similar coatings processed by other manufacturing techniques. The microstructure of the resulting coatings was characterized by optical and scanning electron microscopy, phase analysis by X-ray diffraction and chemical composition by energy dispersive X-ray spectroscopy. Corrosion resistance was assessed by electrochemical cyclic polarization and the corrosion surface mechanisms were investigated by scanning electron microscopy. Results show that the presence of boron leads to the formation of Cr-rich borides, whose fraction increases with boron additions, depleting the surrounding austenitic matrix in Cr and making it a preferential site for pitting corrosion. Boron increments accounted for a decrease in the corrosion potential of approximately 85mV and for an increase the corrosion rate of about three times, but the pitting potential was not significantly affected. Still, FeCrMnSiB coatings processed by PTA developed low corrosion current densities, greatly outperforming similar coatings processed by HVOF.

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Deposition of graphene incorporated DLC film via enhanced PECVD process

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The need to modify DLC coatings is on the increase to provide tailored mechanical, tribological, lubricating, electrical, and other functional properties by exploring emerging doping elements or compounds. In this works, the incorporation of graphene into DLC matrix is explored to improve the mechanical, tribological and electrical properties by using the enhanced PECVD process. The deposition system was prepared with an additional cathode, placed inside the PECVD reactor, to confine the plasma, and an injector compartment attached to the top of the reactor, to introduce the dispersed graphene in distilled water. Furthermore, the graphene incorporated DLC film was grown on 316L stainless steel, glass, and Si substrates, the voltage was varied from 0.7kV to 1.0kV, and concentration of graphene dispersed in water used was 0, 0.01, 0.05, 0.1, 0.5 mg/ml. Structural changes, mechanical, tribological and electrical conductivity properties of the graphene incorporated DLC film were evaluated. The results presented in this work indicate the presence of graphene in the DLC matrix in all samples. SEM and AFM images reveal the surface morphology of the coating. The Raman spectrum, XRD pattern, and electric resistance measurements are evidence of the presence of graphene in the DLC matrix, which increased as the concentration of the graphene increased and as the voltage increased. The nanoindentation test, adhesion test (VDI 3198 standard), scratch test, wear test revealed improved mechanical and tribological properties. Our results showed that the voltage and concentration variation resulted in a progressive graphitization of the diamond-like carbon incorporated with graphene. Other analyses are in progress.

Evaluation of friction and adhesion behaviors in photoresponsive and photoactive materials under different radiation conditions: implications on the state of matter movement

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Tribology is the science that studies the interaction between surfaces in contact. Thus, this area encompasses the study of phenomena such as friction, lubrication, adhesion, and wear [1]. Friction is the resistance to relative motion between two bodies, with contributions on various scales. In the industrial scenario, significant energy expenditure is observed in overcoming the frictional force between moving parts, demonstrating the importance of scientific development in understanding tribological effects. One established way to reduce the coefficient of friction is through surface modification, chemically or geometrically. Another way to vary the existing frictional force is through the application of light, interpreting the action of radiation as a potential fourth body in the friction between two surfaces [2]. A series of photoresponsive inorganic oxides have their physicochemical properties altered when exposed to radiation, with the advantage of being a reversible process. The general objective of the current research is to quantify the behavior of friction and adhesion in samples of photoactive and photoresponsive materials, in the presence and absence of specific wavelength radiation, and to understand the physicochemistry of interfaces that generate material movement through intermolecular forces and their relationship with phototribology. When irradiated with a specific wavelength, an increase in friction force and a variation in the sample's contact angle were observed, without variations in surface temperature. This occurs because electronic excitation generates an accumulation of electronic charges on the surface. This increase in surface electron density will influence the droplet deposited on the sample, as well as the friction force.

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Exploring properties of TiO2 nanotubes: a comparative study on different alloy substrates

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TiO2 nanotubes (TNTs) are generally grown on titanium alloys through electrochemical anodization. These nanotubes exhibit interesting interfacial properties for biomedical implant coatings, facilitating osseointegration and, consequently, the adhesion and restoration of implanted prostheses. Among the characteristics that make nanotubes useful in the biomedical field, the low elastic modulus of the nanostructures, their biocompatibility, high degree of ordering, and high volume/surface area ratio stand out. In addition, it is possible to manipulate their chemical composition. Although previous investigations have predominantly focused on commercially pure titanium as a substrate, this study examines the growth and compositional and mechanical properties of TNTs grown on alloys of different phases. The alloys studied include Ti-29Nb-13Ta-4.6Zr (TNTZ), Ti-6V-4Al (Ti64), and Ti-CP2, which are respectively beta, alpha + beta, and alpha alloys. After the electrochemical synthesis of the nanotubes, SEM and TEM analyses were performed. These analyses revealed the formation and high ordering of the structures formed on the three alloys, with emphasis on the TNTZ, which allowed the highest tube growth rate. In addition, the TEM allowed the observation of different structures related to the adhesion of the nanotubes to the metallic substrate, including the presence of pores at the nanotube/substrate interface. Through nanoindentation, it was found that the nanostructures grown on the TNTZ presented the lowest elastic modulus (17 GPa), attributed to the ordering of the tubes. Finally, the XPS depth profile analysis revealed the presence of various oxidized states in addition to Ti4+, such as Ti3+, Ti2+, Nb3+, Al3+, and V5+, associated with the O2- availability gradient during the growth of the nanotubes.

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Exploring the antimicrobial action of zinc oxide microparticles in surface paints against multidrug-resistant Staphylococcus aureus

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Multidrug-resistant (MDR) bacteria are pathogenic organisms capable of producing opportunistic infections and causing systemic diseases in healthcare environments. The literature already discusses the use of zinc oxide as antimicrobial agent. However, the application in building materials with antimicrobial properties it is still innovative [1]. We evaluated the antimicrobial capacity of zinc oxide microparticles (ZnO-Mps) in acrylic paints against MDR Staphylococcus aureus (ATCC-33591). The ZnO-Mps of 1.5 µm, with flower-like morphology by FE-SEM. Minimum inhibitory Concentration (MIC) tests were performed with the control drug Ciprofloxacin (CIP) and ZnO-Mps against S. aureus. MIC results of CIP were equivalent to ≤1 µg/mL, compatible with the concentration established in the CLSI M-100 [2]. The bacteria showed sensitivity to ZnO-Mps in the range of 0.19-12.5 µg/mL and resistant between 0.02-0.09 µg/mL. Then ZnO-Mps were added in paints for testing against S. aureus by Kirby-Bauer method [3]. The halo diameter of the inhibition zone was 0mm for the control and 11.71±0.63mm for ZnO-Mps additions. The main antimicrobial mechanism may be related to the generation of reactive oxygen species, in addition to the release of Zn2+ cations. It is concluded that ZnO-Mps can inhibit the activity of the bacteria.

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Functionalization of PA66 through in-situ polymerization of PVAc in supercritical CO2

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To mitigate the impacts of organic solvents and high temperatures in polymer synthesis and modification, there has been significant attention drawn to the use of supercritical CO2 (scCO2)[1]. This fluid is cheap, recyclable and can reduce the carbon footprint of a process[2]. In this context, this work aimed to functionalize a textile fiber of polyamide 66 (PA66) though the in-situ polymerization of polyvinylacetate (PVAc) in scCO2. The fibers mesh of PA66- 60F60 and PA66 78F23, supplied by Rhodia Solvay, were treated in a 10 ml reactor at 100 bar of scCO2 and 80 °C for 1 h using 0.3, 1 and 3 g of VAc. The results showed a mass gain from 1.4 to 51 wt%. Through FTIR analysis, it was possible to observe the presence of PVAc in all mesh fibers (C=O peak at 1725 cm-1) which the peak intensity increased with the rise of mass gain of PVAc. The DSC analyses was used to verify the plasticizing effect of scCO2 on the functionalized PA66 fibers. The functionalization process via scCO2 can result in a decrease in the hydrophilicity of the PA66 fiber surface, protecting it against moisture and expanding the range of dyes that can be used in this textile fiber[1].

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Keywords: scCO2; PA66; in-situ polymerization; textile fiber.

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Growth of $Hf_{1-x}Ti_xO_2$ thin films by co-sputtering process aiming their application as a CO_2 gas sensors

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Hafnium dioxide (HfO_2) has emerged as a pivotal material in various technological domains, such as in gas sensing applications. Its remarkable properties, such as a high dielectric constant [1], render it proficient in storing significant electrical energy under the influence of an electric field. This attribute proves invaluable in capacitive gas sensors, where alterations in dielectric constant owing to gas adsorption can be discerned. Moreover, HfO_2 exhibits commendable thermal and chemical stability, ensuring the preservation of its structural integrity and sensing efficacy even at elevated temperatures a requisite for dependable gas sensing applications. Doping HfO_2 with titanium (Ti) yields a solid solution termed $Hf_{1-x}Ti_xO_2$, where in 'x' denotes the Ti doping concentration. This formulation presents a promising platform for advancing gas sensor technologies, offering enhanced sensitivity, selectivity, stability, and compatibility. Consequently, it stands as a compelling contender in meeting the escalating demand for dependable gas detection methodologies. In this study, we undertake the deposition of $Hf_{1-x}Ti_xO_2$ via co-sputtering deposition (using Hf and Ti targets), adjusting the Ti concentration by varying the positioning of the Ti target. We comprehensively investigate the structural, morphological, optical, and electrical properties of the resulting thin films. Furthermore, to assess its potential efficacy in gas detection, particularly towards CO_2, we conduct preliminary tests. Our findings indicate a promising response to CO_2, underscoring the potential of $Hf_{1-x}Ti_xO_2$ as a robust gas sensing material.

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How to Get Published in a Scientific Journal

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In this talk, Prof. Aouadi will share with you his insights on how to write a successful manuscript to be published in a peer-reviewed journal. He has been an editor of Surface and Coatings Technology (Impact Factor = 5.5 and Citescore = 9.2) for 11 years. His presentation will include topics such as an introduction to scholarly publishing, journal organization, building a strong manuscript, what editors want, and the ethics of publishing. He will provide concrete examples on papers that he has handled.

Improving the corrosion resistance of the 316L SS by using sputtered-niobium oxide and amorphous carbon coatings

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This work aims to investigate the influence of niobium and carbon nanostructured coatings on the corrosion resistance of the 316L SS. The coated and uncoated specimens were morphologically and structurally characterized by using OM, SEM/EDX, DRX, FTIR, Raman spectroscopy and XPS techniques. The corrosion behaviour was assessed by OCP, PPc, EIS as well as immersion tests in 0.6 mol L^{-1} NaCl solution. In addition, the average contact angles were used to evaluate the surfaces free energy by the Van Oss interfacial tension component theory approach. Results showed that the surface treatments positively influenced the corrosion resistance of the 316L SS and the coatings act as a protective barrier against corrosion process [1]. The reactive sputtering technique increased the wettability of the surfaces in relation to the base material [2]. Considering applications in aggressive media, the 316L SS/Nb_2O_5 specimen exhibits superior performance when compared to the base material and 316L SS/carbon.

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Kinetic characterization pack-aluminizing surface treatment of AISI316L stainless steel process by additive manufacturing techniques

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Additive manufacturing offers advantages in producing stainless-steel (SS) singular or a few parts with various geometries and sizes. However, in high-temperature applications like petrochemical industries, these components also need protection against oxidation or metal dusting. The pack aluminization process is a competitive method to protect these SS components. It can be applied to intricate geometries producing continuous coatings with strong adherence. For powder-pack mixtures with high aluminum activity, achieved at temperatures below 850°C and high concentrations of aluminum and activator, leads to the formation of brittle high-aluminum-concentration intermetallic phases FeAl3 and Fe2Al5 on the coating's outer layer. To avoid these low-toughness intermetallic phases, a high-temperature powder-pack aluminization procedures were used for surface treating additive manufacturing substrates. In this study, coatings were applied to additive manufactured AISI316L stainless steel processed by PTA-DED, L-DED and L-PBF, using a pack mixture of 1%Al, 1%NH4Cl, and 88%Al2O3 at 1000°C for 1-10 hours. The goal was to stablish the kinetics for the growth of aluminide coating for each AM microstructures. The coatings consisted of an outer layer of FeAl and an interdiffusion layer of α-Fe(Al) on all additive substrates. The non-uniform microstructure of multilayer additive materials, compared to the more uniform grain structure of rolled substrate, accounts for differences in coating kinetics. The coarsest structure of the PTA-DED resulted in a thinner outer layer accompanied by a thicker interdiffusion layer. The larger amount of preferential diffusion paths in L-DED microstructures, accounts for a thicker outer layer and a thinner interdiffusion layer. Growth constant values were calculated for FeAl and α-Fe(Al) phases, which are crucial for evaluating the useful life of materials in high-temperature applications.

Mechanical and biological improvement of UHMWPE joint implant with Ti, Ta and Zr thin films

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With the growing exploration of ultra-high molecular weight polyethylene (UHMWPE) as a replacement for cartilage in joint implants, it is essential to overcome problems such as osteolysis and debris formation [1]. Surface engineering, particularly the magnetron sputtering technique, offers a promising solution by allowing the deposition of thin films on the polymeric substrate. This study examined the physicochemical and biological properties of UHMWPE coated with titanium, tantalum and zirconium films. The coatings exhibited enhancements in wettability alongside diminished roughness. The Zr film exhibited a contact angle of 16°, a significant improvement compared to the UHMWPE sample, which has an angle of 102°. Moreover, the roughness of the pristine sample (0.958 µm) was substantially reduced to 0.403 µm with the Ta film. These characteristics prevented the adhesion of fibroblasts, minimizing the risk of fibrous encapsulation surrounding the implant [2]. Micro-abrasion tests demonstrated that the coatings reduced the wear coefficient, making them ideal for increasing the longevity of the implant in the human body. Transitioning from a wear coefficient of 0.47×10^{-12} m^2/N for UHMWPE, values as low as 0.21×10^{-12} m^2/N were attained, particularly in the sample with the Ti film. Therefore, the coatings exhibit favorable characteristics for the intended biomedical application.

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Micro-Raman spectroscopy characterization of graphene-coated textile yarns and membranes for wearable electronics applications

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The development of wearable electronics and electronics textiles has increased in the recent years the demand of innovative materials able to satisfy the stringent requirements of electrical conductivity, flexibility and compatibility with textile production processes. With this concern, several approaches, exploiting carbon-based fibres, have been adopted in the aim to induce a conductive path useful for smart textiles applications. To this aim, this kind of substrates are then covered by a functional material regarding the specific application. The coating can be performed by means of a variety of wet or dry methods. Anyway, in view of the practical applications it is mandatory to characterize the carbon forms, with specific reference to graphite oxide and reduced graphene oxide, embedded textile yarns and membranes. In this presentation we report on the results of micro-Raman spectroscopy investigations carried out on pristine graphene layers, obtained either by exfoliation or by CVD, as well as on the graphene oxide deposited onto the surface of two different commercial fabrics, consisting respectively of a very dark coloured polyvinyl (PV) membrane and of a polyester (PES) sheet, with a small one-side graphene amount. Highly spatially resolved micro-Raman spectra were carried out at room temperature in backscattering geometry, under excitation of the 488.0 nm or 514.5 nm line of a mixed Ar-Kr ion gas, using a triple monochromator (Horiba-Jobin Yvon, model T-64000), set in double subtractive/single configuration. The filtered radiation was detected by a charge-coupled device (CCD) detector, with 1024 x 256 pixels, cooled by liquid nitrogen. Typical graphene spectra, characterized by a very high signal-to-noise ratio, were observed from pristine layers, while the spectra recorded from the two commercial fabrics suggest the occurrence of highly disordered nano-crystalline graphitic carbon, characterized by very broad D and G bands of comparable intensity.

Nanomaterials applied in the development of smart sensing devices for soil analysis.

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The urgency of optimizing agricultural practices and the rational use of natural resources, without a proportional increase in production area, is keen due to the increasing global demand for food. It implies in the development of advanced tools for precision agriculture to facilitate the judicious application of fertilizers/herbicides, aiming to reduce costs and environmental impacts [1]. However, the precise application of agricultural inputs requires efficient mapping of macronutrients in cropping areas. Traditional physicochemical analysis often falls short due to time and costs, resulting in insufficient sampling density and excessive nutrient dispersal. Smart sensors, especially e-tongues, streamline in situ detection, enabling field sampling and remote monitoring with rapid quali- and quantitative results in liquid media [2]. Our focus is on enhancing the electrical and mechanical properties of the sensing units composing microfluidic, impedimetric e-tongues with metallic nitride coatings via dynamic glancing angle deposition. The technique provides control over film thickness, porosity, and surface roughness, thus improving the robustness and lifetime of the device. Moreover, the controlled thickness and porosity of these nitrides facilitate their use as molecular sieves, capturing chemical species of interest at the electrode/electrolyte interface. This advancement aims to simplify soil macronutrient detection, potentially improving device selectivity for broader applications. Initial tests demonstrate successful discrimination between NaCl and KCl at equimolar concentrations. Our current focus is on surmounting experimental obstacles to streamline nitride formation on substrates, thereby facilitating data acquisition.

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Niobium Pentoxide-based Composites for Visible-light Photocatalysis

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ABSTRACT

Niobium-based materials have been described as promising photocatalysts in the search for sustainable solutions for chemical processes, like green hydrogen production. Nevertheless, the most common niobium precursors, Nb2O5, have wide band gaps and thus are often active under ultraviolet radiation only. Considering this scenario, and taking advantage of Brazil as the niobium worldwide leading producer, the present work focuses on tuning the absorption of niobium pentoxide materials towards the visible region, to obtain promising sunlight-active photocatalysts.

Organometallic colloids were prepared by solvothermal synthesis using low-cost inorganic salts and natural/innocuous organic compounds. The materials were later deposited onto crystallographically different Nb2O5 samples. Experimental conditions and characterization data have not yet been disclosed due to intellectual property protection issues. The photocatalytic activity of the materials was initially tested in the decomposition of rhodamine B in an aqueous medium using either a 100 W white LED.

Characterization data, especially diffuse reflectance spectroscopy, indicated that the surface of all three Nb2O5 materials could be impregnated with the colloids, observed as a sharp rise in the absorption capacity of the surface-coated materials in the range 350-600 nm relative to the pristine oxides. Regarding initial photocatalytic assays, the RhB decomposition upon light exposure is enhanced in the presence of the composites, with catalytic effects of ca. 4-fold in observed first-order rate coefficients compared with precursor materials.

The different composites obtained by the decoration of niobium pentoxide using low-cost and economically circular components proved to be promising visible light active catalysts, opening up possibilities for future applications in the field of photocatalysis.

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Pack cementation technique as a tool for interdiffusion investigations

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Halide Activated Pack Cementation (HAPC) is a technique for preparing protective coatings widely used in the field of surface treatment of materials intended for aggressive high-temperature environments [1]. The principle of this technique is based on the interaction of a gas generated from a powder mixture (cement) with the surface of the alloy to be treated (substrate), placing it within the realm of Chemical Vapor Deposition (CVD) techniques. HAPC has been effectively used to design high temperature protective coatings and to study the growth kinetics of aluminide and silicide systems [2-3]. In the present work, it will be presented how the HAPC technique can be used to create diffusion couples and to study kinetic parameters in binary and pseudo-binary systems. The V-Al system was investigated using a cement composed by high-activity Al (a_{Al}=1) diluted by Al_2O_3 and activated by $CrCl_3$. Two substrates were considered in this work, pure V and 66V-44Al (at. %) alloy. The aluminization was performed in silica vessels sealed under primary vacuum, using the “in pack” configuration where the coupons are immersed in the cement, from 800 to 1000 °C for 4 to 25 hours. In this way, the diffusion in the gas phase is not a rate-limiting step and the coating formation can be understood as a classical semi-infinite diffusion couple. The coated substrates were microstructurally characterized by XRD, SEM and EDS. As a result, kinetic data can be calculated and used as a valuable information for estimating the thermal stability of substrate/coating systems.

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PMMA-silica nanocomposite coatings functionalized with carbon dots for active metal surface protection

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The demand for ecological and efficient protective coating is in the focus of present research. Composite materials containing carbon nanostructures such as carbon quantum dots (CDs) have received special attention as inhibitors in this field. This is due to the possibility of tuning the surface properties of CDs by functional groups, with emphasis on the use of nitrogen and sulfur (N-CDs and N,S-CDs) capable of providing inhibitory and self-healing functionality to the coating. In this study coatings with active properties were developed by incorporating CDs, N-CDs and N,S-CDs into poly (methyl-methacrylate) (PMMA)-silica hybrids. The CDs were synthed by the hydrothermal method involving the pyrolysis of citric acid and functionalized with urea and thiourea to obtain N-CDs and N, S-CDs, respectively. The PMMA-silica hybrids were prepared by combining polymerization reactions and the sol-gel process and deposited by immersion on the AA7075 alloy. Among the structural, morphological and mechanical characterization techniques used in the different stages of the study, atomic force and transmission electron microscopies, infrared, UV-visible and X-ray photoelectron spectroscopies, adhesion and contact angle measurements were applied. The structural and morphological results were correlated with the anticorrosive performance of the coatings investigated by electrochemical impedance spectroscopy in 3.5% NaCl solution and salt spray tests. The results demonstrate that the N-CDs, N,S-CDs provide the coatings with long-term protection and self-healing capacity, suggesting that the combination of passive and active protection results in high-performance and environmentally friendly coatings for anti-corrosion protection of aerospace components.

PTA-DED manufacturing of Nb and Nb+ WC multilayers: a preliminary study

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The Additive Manufacturing has been explored as a relevant methodology to process refractory metals [1]. However, little has been explored of the Plasma Transferred Arc Directed Energy Deposition (PTA-DED) that combines the higher energy efficiency compared to laser-based processes, with the flexibility of performing in-situ synthesis starting from elemental powders This study addresses multilayer coatings processed from crushed powders of pure Niobium and of mixtures Niobium with tungsten carbide (WC) for applications that requires good mechanical resistance at high temperatures. PTA-DED was used to process multilayer coatings of Nb and Nb+2.5wt%WC powder mixtures, aiming to evaluate the processability of each material and the impact of second phase reinforcement in the formation of a Metal Matrix Composite (MMC). Furthermore, the study assessed the efficiency of the PTA-DED shielding gas (argon) in reducing oxygen pick-up during processing. Microstructural analyzes were conducted using Scanning Electron Microscopy (SEM) and Electron backscatter diffraction (EBSD). Preliminary results indicate adequate processability of fully dense multilayer coatings, without cracks and porosity. Analysis revealed the formation of grains oriented in the direction of heat flow and a refinement in the microstructure on deposits with additions of WC. Despite the refined grains formed when processing powder mixtures of Nb+WC, a dispersion of carbide particles was not identified, suggesting the dissolution of the carbides might have occurred. Results indicate that either carbon combined with oxygen being removed from the deposited material or a low amount of carbon remain in solid solution.

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Room-temperature corrosion resistance of NiAl/WC (nanosized) coatings processed by Plasma Transferred Arc Directed Energy Deposition (PTA-DED)

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NiAl intermetallic is an ordered compound that have been widely studied due to its low density and chemical resistance to different environments. NiAl is a competitive material to be used in the chemical/gas industry as coatings for protecting steels and superalloys from oxidation because of the formation of adherent and stable alumina (Al_2O_3) on its surface. Furthermore, small additions of Cr can also improve corrosion resistance [1]. NiAl-based coatings have been successfully produced via in-situ synthesis, through Plasma Transferred Arc Directed Energy Deposition (PTA-DED), by depositing Ni+Al powder mixtures on AISI 304 stainless steel substrates [2]. The microstructure of these coatings can be refined by the addition of WC nanoparticles (WC-NPs) in order to improve room-temperature toughness [2]. Due to the significant applicability of these coatings in the industry, the effects of grain refinement on the corrosion resistance must be assessed. In this work, the influence of grain on the room-temperature corrosion rate of multilayer NiAl-based coatings (PTA-DED, on AISI 304 substrates), without and with grain refinement, induced by the addition of 1 and 2 wt.% WC-NPs, is assessed. For this, the corrosion rate is evaluated by means of micro and macro-polarization resistance and Tafel plot analyses in a NaCl solution, using a three-electrode electrochemical cell, carried out on the transversal cross-section of the coatings, in order to establish a comparative analysis evaluating the impact of nanoparticles in the corrosion resistance.

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Self-healing ceramic coatings for extreme environments

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This paper provides an overview of the latest research developments in the design and exploration of ceramic coatings with high temperature adaptive behavior. The adaptive behavior, triggered by thermal or thermo-mechanical stimulus, may be used to create smart surfaces that are able to change their chemistry and structure to achieve the desired functionality. The initial focus of the paper will be to provide an overview on the basics of self-repairing materials. This will be followed by a brief outline of the work that has been reported on self-healing/adaptive mechanisms in bulk ceramics. We will then focus on providing a thorough review on self-healing ceramics with a focus on adaptation/healing in tribology as well as thermal barrier, anti-corrosion, and oxidation resistant coatings. This overview will provide a fundamental understanding of the changes in the structural and chemical properties of these materials and how that correlates to their performance. This review also includes a discussion on anticipated future developments in this important and upcoming area of research.

Surface modification of activated carbon from tucumã by corona treatment

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The state of global climate emergency has instigated the search for more sustainable energy sources, such as hydrogen gas, to replace non-renewable sources [1]. However, obtaining it from natural gas still represents a challenge due to environmental impacts [2]. A promising alternative is biogas, produced from organic waste, but its purification is essential to remove unwanted contaminants, such as CO2 and H2S [3]. In this work, we propose using the Corona treatment to modify the vegetable charcoal surface to produce activated carbon and increase its adsorption capacity. We investigated the influence of this treatment on the structure and properties of activated carbon using techniques such as Fourier-Transform Infrared Spectroscopy (FTIR), Scanning Electron Microscopy (SEM), and surface area analysis. Furthermore, we evaluated the efficiency of these materials in the adsorption of CO2 and H2S, essential for the purification of biogas. At the same time, we explored the potential of Amazonian agro-industrial residues, such as Amazon-tucumã (Astrocaryum aculeatum) seeds, in the synthesis of activated carbon. We investigated the main parameters for producing this adsorbent and its effectiveness in removing CO2 and H2S through Thermogravimetric Analysis (TGA) and Gas Chromatography (GC) analyses. This research aims to contribute to energy sustainability and the sustainable development of the Amazon region, using residual biomass to mitigate environmental impacts and promote more sustainable practices.

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Surface Profiling of Thin and Ultrathin Polymeric Films by the Coulomb Explosion Technique Through MEIS

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The present study aims to determine the thickness of polymeric thin films of poly(methyl methacrylate) with a technique of high resolution depth profiling of the Medium Energy Ion Scattering (MEIS) through Coulomb explosion. The innovation of this work lies in the proposal of measuring the thickness and density of polymeric films by MEIS, as other techniques used in the literature are not able to determine density, assuming it *a priori* as homogeneous over the entire surface, which is not always true. The technique uses the separation time between incident ion fragments to determine the thickness and density of a thin film. In medium energies the loss of energy is partially caused by interactions with electronic and atomic nuclei. This provides a higher sensitivity. Various amounts of polymer have been spin coated over distinct bulks: metallic Au over Ta over Si, Au over Cr over Si, Au over SiO_2 and Si doped with Au. The experiments of coulomb explosion were made by a series of molecular and ionic beams with various energies, though with similar energy per nucleon in comparison with a single H^+ ion. Different molecular beams, such as HeH^+ and H^{+2} , have been used aiming an amplification of the Coulomb explosion. When in interaction with the surface, the fragments are separated by coulomb forces. Hence, the broadening of the two fragments of ions is converted in dwell time of the centre of mass and therefore the traversed thickness is estimated. When compared with the spectrum of a single H^+ beam, the Coulomb explosion is noticed as a fluctuation of the energy edge. The technique proves to be effective in accurately estimating the thickness of different thin films with distinct thickness and was compared with established techniques in the field of nanomaterial analysis.

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Synthesis, characterization, and cytotoxicity of bismuth nanoparticles with different coatings

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Nanoparticles (NPs) have emerged as highly versatile tools in biomedical research, offering opportunities for innovative diagnostic and therapeutic strategies. Among various NPs investigated, bismuth nanoparticles (BiNP) exhibit favorable physicochemical characteristics, making them an attractive candidate for imaging and radiosensitizing. In this study, BiNPs coated with dextran (DX), polyvinylpyrrolidone (PVP), and polyethylene glycol (PEG) were synthesized by chemical reduction (CR) and thermoreduction (TR) methods. The NPs physicochemical characteristics and cytotoxicity were evaluated. In the CR, conducted in an aqueous medium, the focus was on how temperature influences the morphology of BiNPs coated with DX. Since no significant difference was observed, the reaction at 80 °C was replicated to the PVP and PEG coatings. PVP and PEG coatings led to an increase in NP core . X-ray photoemission spectra (XPS) revealed phosphorus on the surface of the nanoparticles (NPs), potentially from the reagent employed to control pH during the reaction. Also, metallic bismuth and bismuth oxide were identified in X-ray diffraction (XRD) and XPS spectra. The TR method used stabilization with alkanethiol and was carried at different temperatures. In this case, only metallic structure was identified in XRD and XPS, indicating better stability against oxidation. This stability could be related to the presence of Bi-S on the NP surface. Cytotoxicity assessment was performed in U87 GBM cells with DX-coated NPs obtained from both methods. Treatment concentrations up to 100 µg/mL were applied. Only BiNPs prepared via CR showed cytotoxicity, starting at 5 µg/mL. Our findings show the importance of the synthesis method and coating for precise control over biological and physicochemical characteristics of the NPs. We will discuss the influence of different coatings on the cytotoxicity profile.

Synthesis of iron-modified porous clay heterostructures (Fe-PCHs) from a raw Uruguayan montmorillonite

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Porous clay heterostructures (PCH) are nanoporous materials that exhibit a high specific surface area, a combined microporous and mesoporous structure, and high thermal and mechanical stability. These materials are of great interest due to their potential application as adsorbents, catalyst supports and porous matrices for the encapsulation and controlled release of drugs [1]. PCHs are obtain by the modification of a cationic layered silicate with a surfactant and a silica precursor, followed by heat treatment to remove the surfactant.The aim of this work was to prepare iron-modified PCHs (Fe-PCHs) from a Uruguayan raw montmorillonite, with potential application as catalysts in Fenton process. Fe-PCHs were prepared by exchange the raw clay with a solution of hexadecyltrimethylammonium and hexadecylamine as co-surfactant, followed by the incorporation of tetraethoxysilane. Finally, the solid was exchanged with a ferric nitrate solution using different concentrations: 1 and 4 mol/L and thermally treated at 650 ºC in air to obtain Fe-PCH-1 and Fe-PCH-4, respectively. The characterization of the clay and the catalysts involved: XRD, XRF, TGA and nitrogen adsorption isotherm techniques.

The Fe content for Fe-PCH-1 and Fe-PCH-4 is 1.55 and 1.75%, respectively, thus confirming the effective incorporation of iron. Due to the generation of the nanoporous structure, the Fe-PCHs have significantly higher surface area (386 and 378 m^2/g) and pore volume (0.294 and 0.306 cm^3/g) than the clay (28 m^2/g and 0.043 cm^3/g). These properties suggest that Fe-PCHs are suitable candidates for catalytic processes that involve iron as active species.

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Tailoring Hydrogenated Amorphous Carbon-based Coatings Deposited by PECVD for Improving Adhesion on PDMS for Medical Applications

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Polydimethylsiloxane (PDMS) is widely used for medical implants. Despite its well-known properties, such as hemocompatibility, elasticity, and mechanical stability, it is susceptible to bacterial colonization which can ultimately lead to serious infections and even device failure. Hydrogenated amorphous carbon (a-C:H) coatings present a novel avenue for creating long-term antibacterial surfaces by acting as barrier layers that control the diffusion rate of silver ions. However, the lack of adhesion of a-C:H coatings on hydrophobic polymeric substrates is often reported to be critical, and for medical applications, this can compromise the clinical success of the implant. In this research, different a-C:H coatings were deposited on PDMS by plasma-enhanced chemical vapor deposition (PECVD) processes. The effect of bias voltage and hydrogen gas was optimized to enhance the adhesion. The bias voltage applied (-300 V or 0 V), as well as the hydrogen content, were varied to obtain either diamond-like carbon type (DLC, DLCH) or polymer-like carbon type (PLC, PLCH), respectively. Substrate biasing markedly impacted the properties of a-C:H coatings. Indeed, DLC exhibited the lowest ID/IG ratio in Raman spectroscopy, indicating a higher sp^3 content and the highest surface roughness. For PLC-type, the ID/IG ratio was increased suggesting the transition from DLC to PLC. The incorporation of hydrogen gas for PLCH and DLCH samples resulted in a decrease in surface roughness and lower crack density after sample stretching during tensile tests. This may be related to the hydrogen's ability to enhance surface interactions and reduce internal stresses within the coating. Overall, PLCH coating showed the lowest crack density after sample stretching, even after 7 days immersed in PBS at 37 °C, indicating improved flexibility and adhesion compared to other deposited coatings. Therefore, PLC-type coating appears to be a promising strategy for flexible polymer devices.

Ti coating on Pure Nb and Nb alloy

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Niobium and its alloys find applications in different areas such as batteries, medical implants and high temperature equipment, yet intermediate temperature, around 600 °C performance is still an open issue for this alloys. At this temperature, thermal energy storage (TES) assumes an important role due to decarbonization of energy, and the transport of hot Solar Salt fluid through pipes in power plants requires appropriate material [1]. However, the oxidation phenomenon in Nb is known to be catastrophic, requiring procedures to prevent that the interaction with oxygen [2]. A possible and widely used technique to protect metallic materials that operate under temperature is pack cementation. This is a competitive e efficient technique to process coatings for high temperature applications. Diffusion of substitutional elements allow to create a reservoir that supplies oxide forming elements such as Ti increasing oxidation resistance [3].

Previous studies have been shown that Ti coating developed on pure Nb and Nb alloy created a continuous and non-porous layer through titanizing pack cementation at 950 °C for 6h. This study aims to assess the formation of Ti based protective layer in particular the impact of the thickness of a Ti protective layer on pure Nb and Nb alloy (NbTiZr) on the protection against oxidation in an intermediate temperature of 600 °C.

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Transformative Advances in Wire Drawing Soaps: Unveiling the Impact of Nanomaterial Integration on Lubricant Performance

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Nanomaterials have been widely explored for the past few years, as their extraordinary physical and chemical properties have shown the ability to enhance material features in diverse fields. In particular, the use of nanomaterials as additives in lubricants has been explored to improve their tribological properties[1]. In this sense, this study proposes a method to separately incorporate graphene oxide (GO), hexagonal boron nitride (hBN) and titanium dioxide (TiO2) into a wire drawing soap powder to obtain solid nanocomposites and analyze their effects on lubrication[2]. The resulting nanocomposites were characterized by high-resolution transmission electron microscopy (HRTEM), thermogravimetric analysis, Raman spectroscopy, Fourier transform infrared spectroscopy (FTIR) and tribo-rheology. The results confirmed an improvement in lubricating properties with the addition of GO, hBN and TiO2, as evidenced by a 39%, 13% and 40% reduction in the mean friction factor of the nanocomposites compared to that of the bare soap, respectively. This reduction reveals a promising application in a more effective process of wire drawing by reducing the energy loss, extending the drawing life cycle, and enabling other applications[3].

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Tribocorrosive behavior of grinding balls materials using the Miller test and electrochemical techniques

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In mining, the grinding stage is of the most importance, since this process involves comminution of the ore to the desired particle for use in the subsequent stages of ore processing. During contact with ore slurries, the components of mining systems, such as grinding balls, are subject to the simultaneous effects of wear and corrosion phenomena. This is why studies about tribocorrosion are extremely necessary in order to minimize operating costs. This work evaluated the tribocorrosive behavior of grinding balls made from white cast iron (A and B) and low alloy steel (C) from VALE S.A. The effect of the pH of the abrasive slurry on the tribocorrosive performance of the materials was also studied. As taking into account that interpretation of the combined wear-corrosion behaviour requires detailed knowledge of the separate kinetics of wear and corrosion, potentiodynamic polarization tests were also carried out to assess the chemical/electrochemical action of the aggressive environment. The tribocorrosion tests were carried out on the Miller Machine, using a methodology based on the ASTM G75 [1] standard, at a standard slurry concentration and pH values of 8.5 and 11. Increasing the pH reduced the mass loss of all the materials analysed. Low alloy steel exhibited the worst tribocorrosive behavior due to its lower hardness and worse corrosion resistance compared to cast iron. Cast iron A showed the best corrosion resistance when compared to cast iron B, due to its more refined microstructure and higher chromium content. The results obtained correlated well with the results of field tests carried out by VALE S.A., helping to validate the procedure adopted in this study.

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Adhesion of tumor cells on Ti6Al4V electrodes produced by additive manufacturing and functionalized with multilayer polyelectrolytes

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Less invasive methods like liquid biopsy show promise in diagnosing and prognosing oncological diseases. Challenges persist in capturing circulating tumor cells (CTCs) and ensuring detection sensitivity. Additive manufacturing (AM) in biosensor production offers greater design flexibility, advancing the analytical performance and addressing these obstacles effectively. This study evaluates electrodes with 3D geometries fabricated using AM from Ti6Al4V alloy and coated with polyelectrolyte multilayers (PEM) of chitosan (CHI) and hyaluronic acid (HA) for CTC adhesion. Electrodes were produced via Electron Beam Melting, plasma-treated, and coated with a precursor layer of polyethyleneimine followed by multilayer deposition of CHI and HA 0.1% (w/v), comprising 3.5 bilayers. To assess adhesion, PC-3 prostate tumor cells were pipetted onto the electrodes and quantified in Neubauer chambers. PC-3 adhesion was significantly higher on electrodes with 3D shapes coated with PEM, indicating that the micrometric 3D structure enhances contact area, thereby facilitating PC-3 cell adhesion through increased surface contact. This enhanced adhesion is attributed to the interaction between hyaluronic acid and the overexpressed extracellular CD44 receptors on PC-3 prostate tumor cells, corroborating findings from previous studies [1]. This study underscores the innovative potential of electrodes manufactured through EBM and easily functionalized with PEM. The facile fabrication process, coupled with the superior performance observed in PC-3 prostate tumor cell adhesion, highlights the potential of this approach for advancing cancer diagnostics and monitoring.

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Adsorptive study of the removal of the Rhodamine-B dye in an aqueous medium using the bioadsorbent sugarcane bagasse incorporated into iron oxide nanoparticles (Fe_3O_4)

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It is now known that the contamination of water bodies by industrial dyes is harmful to the environment and human health [1,2]. Adsorption is an efficient and effective method for reducing the concentration of these dyes [1,2,3]. Sugarcane bagasse has organic groups that capture these molecules and can be used as a biosorbent. The incorporation of iron oxide nanoparticles (Fe_3O_4) facilitates the separation of the dye-laden material due to the application of a magnetic field [1,3]. Therefore, this work studied the adsorption of the dye Rhodamine-B (Rh-B) from sugarcane bagasse *in natura* (SB), calcined (CSB) and incorporated with Fe_3O_4 (MSB). The SB was cleaned, crushed and dried. The SB was carbonized (600°C, 1h) to produce CSB [2]. The SBC was synthed by co-precipitation, from a mixture of Fe^{2+} and Fe^{3+} salts (1:2) and 1 g of SB, precipitated with ammonium hydroxide, under N2 [3]. Characterization techniques were carried out using FTIR, SEM, XRD and pH_{PCZ}. Adsorption was carried out using 10 mL of Rh-B (10 ppm), 50 mg of the biosorbent, under agitation, for 180 min at 25±2°C, with aliquots being collected every 30 min. The characterizations showed that the materials were produced according to the literature [1,2,3]. The pH_{PCZ} values for SB and MSB were 4.1 and 4.02 respectively. The concentration of Rh-B removed was given by UV-vis. The SB showed a maximum Rh-B removal rate of 82%. The MSB showed a maximum Rh-B removal rate of 86%, that is, higher than the SB, as well as being easier to remove the biosorbent from the aqueous medium. SBCAL showed low removal rates due to heat treatment. Therefore, SB and SBC have potential for Rh-B removal, and in-depth kinetic and thermodynamic studies are being carried out.

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Analysis of Molybdenum Oxide Films produced by reactive sputtering having different oxygen contents (MoOx)

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Molybdenum oxide films find many applications in electrochromic, electrocatalytic and solar energy harvesting devices [1]. To control of the oxygen concentrations and structure of the produced films, an investigation of MoOx films deposited using the reactive sputtering technique was performed using different oxygen flow rates. The growth rate, the grazing angle X-ray diffraction, and the optical spectra of the films were analyzed. The results show that the growth rates are high (~ 0.5 nm/s) for the 0.0 – 1.5 sccm O2 flow range, and small (~ 0.2 nm/s) in the 4.0 – 9.0 sccm O2 flow ranges. X-ray diffraction data show that the as grown samples are amorphous. After heat treatment in air at 300 °C, the 4.0 sccm O2 flux sample crystallizes. The diffraction peaks are clearly compatible with the orthorhombic structure of ▯-MoO3 stoichiometry, Pbnm space group. Similar results were obtained for the 450 °C and 600 °C treatments. The optical transmittance and reflectance measurements and calculations indicate that the film grown with 4.0 sccm O2 flow display several and regular interference fringes can be seen in the spectra of as grown samples attesting the film uniformity. The spectra allowed the determination of the thickness (500 nm) and the bandgap (2.98 eV). The latter is compatible with the trioxide composition (MoO3), while for 2.5 sccm flow the sample has much smaller transmittance. The investigation is being continued aiming the decrease of the resistivity of understoichiometric films (x < 3) to favor the electric transport properties, in special for the use in solar cells.

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Analysis of the Use of Intermediate Polymeric Films in Spot Welding of Metal-Polymeric Composite Joints by Thermal Conduction

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Spot welding by thermal conduction is an innovative technique for joining metal-polymer hybrid structures and is based on heat conduction from the metal to the polymer [1]. Using this technique, joints of aluminum alloy 1000 and laminated poly(ether-imide) composite with fiberglass (FV-PEI) were produced with and without the use of a PEI intermediary film. Tensile shear tests demonstrated that joints with films are stronger (±15 MPa) compared to joints without films (±13 MPa). Additionally, fracture surface analyses revealed larger bonding areas for joints with films. For samples with the film, the extent of softening due to heat conduction is greater, consequently, the low viscosity achieved with polymer fusion promotes wetting of joint component surfaces by softened PEI, resulting in better adhesion between the parts. Furthermore, microstructural analyses demonstrated that the formation of the metallic core and the interdiffusion of PEI molecules between the composite and the film are also favored. Therefore, it was concluded that the addition of the film produced stronger joints.

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Application of HMDSO film by PECVD for improvement of composite joints welded by electrical resistance

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Composite materials have become increasingly popular in the aerospace industry, with up to 50% of aircraft structures now made from these materials [1]. This study explores the use of resistance spot welding as an alternative joining method, which has been improved through surface treatments [2]. The effects of PECVD treatment on AISI 304 stainless steel substrates were investigated, and it was found that treatment with argon plasma followed by HMDSO film deposition improved adhesion and weather resistance. SLSS tests revealed an increase in shear strength from 10 MPa to 16 MPa. FTIR analysis confirmed the presence of Si-O-Si and Si-H groups, indicating chemical interactions [3]. Water contact angle analysis showed that the treated material was more hydrophobic than the original substrate. These results demonstrate the potential of PECVD to improve bonding properties in aerospace composites.

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Bacterial Cellulose Bifunctionalized with Mimetic Peptides: Advancements in Cell Culture Platforms.

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The science related to in vitro models have a great importance of biological context and screening of drugs. Bacterial nanocellulose (BNC), is a versatile biopolymer with a variety of biomedical applications due to its biocompatibility, non-immunogenicity and its structural similarity to collagen fibers found in the extracellular matrix (ECM)[1]. BCN has a high surface area and hydroxyl groups that facilitate interaction with biomolecules such as peptides, growth factors and hormones, giving it bioactive effects. In this sense, this study was design to obtain a novel cell culture platform based on BNC with bifunctional peptides [2]. Neat BNC exhibits a paper-like appearance and shows infrared spectrum bands characteristic for its molecular composition. Moreover, BCN demonstrates an exceptional thermal stability, revealed with three main events: the first event (80–100 °C) is attributed to the loss of water. The second (250 - 400 ºC) and third events (> 600 ºC)are attributed to the decomposition of cellulose’s polymeric chains and carbonaceous residues, respectively. Furthermore, the SEM micrographs of BCN show three-dimensional interconnected fiber networks similar to the ECM. The next steps involving the bifunctionalization of BNC with peptides will aim to evaluate the morphology, physicochemical and biological properties of the cellular platforms, in order to prove their support for cell adhesion, proliferation and differentiation, in addition to their antimicrobial property.

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Bias voltage effect on tetramethylsilane-derived interlayer deposition to a-C:H adhesion on ferrous alloy

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Hydrogenated amorphous carbon (a-C:H) is a high hardness and low friction material used in coatings with promising applications in mechanical, medical, electronic and aerospace industries, in addition to decorative applications. However, when applied to ferrous alloys, a-C:H films presents high residual stress, which ends in low adhesion and delamination. To improve adhesion, an intermediate layer or interlayer can be used. In our work, the plasma-enhanced chemical vapor deposition (PECVD) technique was used to deposit a hydrogenated amorphous silicon carbide interlayer through the tetramethylsilane precursor, prior to the a-C:H deposition. In the interlayer deposition, different bias voltages, from -400 V to -800 V, were applied. The films were analyzed by Field Emission Gun Scanning Electron Microscopy, Glow Discharge Optical Emission Spectroscopy, X-Ray Photoemission Spectroscopy, and scratch tests. The interlayer deposition rate reached its maximum at -600 V. Two competing phenomena were considered to explain this behavior: generation of active species by collisions and sputtering of the growing film [1]. The silicon content of the interlayer bulk and the interlayer/steel interface decreased with higher bias voltages. Scratch tests revealed that the delamination occurred at the interlayer/steel interface, and the lowest bias voltages generated the best adhered films, probably due to the higher silicon content in this region. Finally, these a-C:H films can meet requirements for decorative applications.

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$Bi_{19}S_{27}I_3$ Nanoparticles: Synthesis and Photocatalytic Performance

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Bismuth-based semiconductors are of interest due to their potential for applications in radiation detectors, solar cells and photocatalysis. In this research, sought to synthe and characterize $Bi_{19}S_{27}I_3$ nanoparticles with polyethylene glycol (PEG) as a capping agent and evaluate their potential as a photocatalyst [1][2]. Nanoparticles were obtained through the hot injection method in aqueous solution varying the amount of PEG and reaction time. Electron microscopy techniques revealed the presence of two morphologies: rounded particles and nanorolls. Powder X-ray diffraction studies confirmed the crystalline phase of $Bi_{19}S_{27}I_3$ in the nanorolls with an amorphous component observed in samples with the higher proportion of rounded particles. The direct band gap for $Bi_{19}S_{27}I_3$ was determined at 1.00 eV. This nanomaterial was studied as a potential photocatalyst for the Cr(VI) to Cr(III) reduction reaction in aqueous solution. Obtaining a 91% reduction at 255 minutes. The reaction is favored in acidic conditions, and $Bi_{19}S_{27}I_3$ is a compound with high stability, which is advantageous because the nanomaterials reported for such studies often are not estable in these conditions. This compound is proposed as a potential nanomaterial to combat the pollution for toxic waste in water sources caused by human activities. Furthermore, the synthesis method employed is promising from a green chemistry perspective due to the simplicity, the non-toxic precursors and the low working temperature to be carried out in aqueous solution.

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Chromium decorated copper oxide films as resistive gas sensors.

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Sensors can be understood as devices that help human beings to expand their reality-sensing capabilities. Specifically, they collect stimulus or variations in the environment, and transduce them in electrical signals [1]. Copper thin films 20 nm thick were evaporated in high vacuum system on mica substrates. Once fabricated, the samples were oxidized at room conditions by three hours at 300ºC. Raman spectroscopy and UV-Vis spectrometry were performed in all samples. The characteristic peak corresponding to CuO (296 cm^{-1}) clearly appear in the copper oxide films and from Kubelka-Munk function as a function of the photon energy, the bandgap obtained is 1.78 eV [2]. The temperature dependence of the electrical resistance shows a semi-conductor type behavior with an activation energy of 467 meV. Chromium ultrathin films were evaporated on copper oxide surface with different thicknesses (0.5 - 2 nm), and they were oxidized at 300ºC. The characteristic peak corresponding to Cr_2O_3 (550 cm^{-1}) appear in the films. Finally, the performance of the samples as a gas sensor was tested, measuring the electrical resistance of the films in presence of ethanol gas at low pressure (from 10-3 to 105 Pa). Resistance changes of up to 50% were measured. The chromium layer shows an effect on this behavior, and it is discussed from a gas adsorption model in p-type semiconductors.

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Comparison between aqueus electrolytes containing KOH, in the presence and absence of fluoride ions in the formation of TiO_2 anodic film.

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Recent research on titanium anodisation has focused on coupling two or more technologies to modify the characteristics and properties of anodic films. The morphology of TiO2 films formed by anodic oxidation depends on a set of variables, such as the effects produced based on the number of steps in anodisation tests, type of organic solvent, or concentration of fluoride ions in the electrolyte, in addition to other extensively studied parameters, such as potential, current and anodisation time. [1,2] In this work, the applied potential and anodization time were set at 30 V and 60 minutes, with the aim of evaluating the effect of the electrolyte composition on the characteristics of the films. As studies in which alkaline electrolytes used in the production of TiO2 films are rare, we seek to explore this area of knowledge as an interesting alternative to make the titanium surface more bioactive. A comparative analysis of the current-time curves recorded during the anodizing tests was carried out in two different electrolyte compositions: an 1.0 M KOH solution, in the absence and in the presence of NH4F (0.5 wt%). A positive result of this study was the obtaining of hydrophilic surfaces after the anodization tests.

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Competitive sorption of potentially toxic elements using the Fe-MCM-41 material

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Environmental accidents, such as the rupture of containment dams for mining waste, occur worldwide, releasing large quantities of toxic sludge and unrecovered metals[1]. These substances leak and contaminate effluents, similar to the disaster in Bento Rodrigues, Minas Gerais, Brazil, in 2018[2]. The contamination of effluents by metals can be from numerous sources. As a result, it became necessary to implement measures to address these issues. This study evaluated the capacity of a Fe-MCM-41 material to competitive sorption of potentially toxic metals[3]. Competitive sorption tests demonstrated the material's capacity to adsorb various metal ions indiscriminately, except for the Ag+ ion, which exhibited unfavorable sorption behavior when in competition with other ions. It was demonstrated that the waste could be repurposed for Fe-MCM-41 synthesis. The resultant material can be harnessed to adsorb diverse ionic species, presenting a potential application in monitoring and mitigating the presence of metal ions within effluents and environmental matrices. In order to complement the project, sorption studies with actual water samples can be carried out.

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Development of a commercial steel composite reinforced with graphene through rolling

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Design engineers' pursuit of low-cost structural steels requires careful selection of alloys, designs, and processing methods. In addition to specific mechanical properties, they must ensure surface quality, formability, and paintability for economically viable designs, especially in automotive, aeronautical, and aerospace sectors that demand weight reduction, lower emissions, and cost-effective production. Traditional metals and alloys often struggle to meet these demands, prompting the steel industry to develop high-strength, multiphase steels over the years. A promising yet underexplored approach involves developing steel composites by incorporating carbon-based materials, which have shown significant improvements in properties in engineering matrices such as polymers, ceramics, and metals. Research into metal matrix composites with carbon-based materials typically focuses on metals like aluminum, copper, nickel, and iron, using various processing techniques. However, conventional methods face challenges due to high temperatures and density disparities [1]. This study presents an innovative approach: developing commercial steel composites reinforced with graphene through rolling. Samples of 1008 steel were coated using dip coating with a mixture of polyvinyl alcohol (PVA) and nanographite. The number of coating layers varied. Before coating, the steel was pickled with 30% HCl and heated at 600°C for 1 hour, then rolled. X-ray diffraction (XRD) analysis revealed no oxide presence, while scanning electron microscopy (SEM) showed nanographite particles on the steel's surface. Mössbauer spectroscopy confirmed atomic interaction between the iron and nanographite carbon, indicating iron carbide formation.

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Development of a method to incorporate sulfur in CVD single crystalline diamond using MWPACVD

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The growth of Chemical Vapor Deposition (CVD) diamond has been the subject of increasing interest in the academic community due to its unique properties, including high thermal conductivity, low thermal expansion coefficient, and excellent chemical stability. Therefore, the ongoing development of CVD diamond has the potential to pave the way for more efficient and durable devices. Although P-type doping is well studied and currently well controlled using Boron, N-type doping still remains a challenge with several promising candidate elements, such as nitrogen, phosphorus, and sulfur [1,2]. This study investigated the incorporation of sulfur into CVD diamond using dimethyl disulfide (DMDS) as a sulfur source. DMDS was chosen for its structural similarity to methane, a precursor commonly used in the CVD diamond deposition process and its relatively low vapor pressure. The method involved the use of hydrogen gas to evaporate and transport DMDS to the growth chamber. The CVD diamond layers of approximately 10 µm were deposited using microwave plasma CVD over HPHT type Ib seeds with dimensions of 3,0 x 3,0 x 0,3 mm^3, then analysed using photoluminescence spectroscopy, high resolution x ray diffractometry and Rutherford backscattering. The results showed successful sulfur incorporation. This study opens up new perspectives for the manufacture of high-performance electronic devices and sulfur-doped diamond for various technological applications.

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Development of continuous dyeing processes with natural dyes in plasma treated fabrics

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Dyeing with natural dyes is carried out using the immersion bath process, which uses a large amount of water and energy. In this work, a system will be used by impregnating the dye into the foulard and subsequently fixing it by resting or by hot air or steam. Continuous processes are characterized by large-scale production and low water and energy consumption. Plasma was used in the pre-dyeing preparation, which is a unique process that does not use water and chemicals, being faster and without harming the environment. The objective of this research is to: Treat fabrics with plasma and develop continuous dyeing processes with natural dyes. Initially, oxygen plasma was applied to cotton fabrics for 5 min, under a pressure of 100 mTorr with a power of 100 W. Then, solutions were prepared with a concentration of 20 g/l of the following natural dyes: Terminalia Chebulae, Acacia Catechu, Tegetas Erecta + Butea Monosperma, Punica Granatum, Rubia Cordifolia, Mulberry Plant and Kerria Lacca. Afterwards, these solutions were divided into two solutions, with 20 ml/l of acetic acid added to one and 20 g to the other. /l of sodium carbonate, that is, an acidic and basic solution. Afterwards, 3 fabrics were impregnated with plasma for each prepared solution, one of which was left to rest for 24 hours, another was treated for 5 min at 140 ºC and the other was treated with steam at 100 ºC for 40 min. Then, the tissues were washed in water at room temperature and dried in an oven for 5 min at 70 ºC. It was observed that fabrics dyed in an alkaline medium showed better color performance than in an acidic medium. The hot air fixation method yielded better results than other methods and had a low color yield when left standing. The research could generate solutions that provide lower water and energy consumption both in the pre-dyeing preparation and in the dyeing processes with natural dyes and obtain a large-scale dyeing process.

Development of Floating Adsorbent Based on Carbon Nanomaterials and Autoclaved Cellular Concrete

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This work was developed with the objective of developing a floating adsorbent material based on carbon nanostructures and autoclaved cellular concrete (a material that has a lower apparent density than water), which would be less expensive, highly efficient and easy to remove when end of the process. This material was produced by the chemical vapor deposition (CVD) process, using an Eco-friendly carbon source, ethanol. The prepared adsorbent was tested against two model organic molecules, one anionic and one cationic. The results obtained were very promising, due to the fact that, after the end of the experimental observation time, the material had adsorbed more than 90% of the organic molecules tested. It was also observed that for each of the molecules the adsorption times were different and that the variations between such molecules were due to charge factors, of the molecules, and their spatial shape. Finally, the adsorbent's response to reuse was also tested. The material was tested for 10 adsorption cycles, with little loss of efficiency. In conclusion to all the tests carried out, materials used and production methodology, the adsorbent produced in this work had low cost, high adsorption capacity and reuse of the adsorbent, and ease of removal from water.

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Development of glass-ceramic material using discarded glass

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The United Nations (UN) recognized the year 2022 as the International Year of Glass to highlight its importance for sustainability, emphasizing the material's recyclability without quality loss [1]. However, factors such as the low cost of discarded glass and high transportation costs limit its recycling. In Brazil, less than half of the glass packaging is recycled [2], contributing to poor waste management. However, waste materials like this can be used to produce glass-ceramics. Wollastonite ($CaSiO_3$) is the main crystalline phase commercially utilized due to its properties (hardness, low water absorption, and lower density), making it attractive for the construction sector [3]. Therefore, considering the large volume of discarded glass and its chemical composition, this work proposed the development of glass-ceramic material using waste from discarded bottles with wollastonite as the main crystalline phase. Four types of glass (brown, transparent, green, and blue) from oneway bottles were used as precursors. These bottles were initially sanitized, crushed, and then the glass fragments were milled. Subsequently, the material was sieved with a 30 mm (170 mesh) opening and analyzed by different techniques (XRF, XRD, TG/DSC) for sample characterization. With the obtained fine material, cylindrical tablets were produced with the help of a Shimadzu uniaxial press. The tablets were thermally treated at different temperatures. The XRD results revealed that the desired crystalline phase was obtained through heat treatment at 1000°C, as indicated by the JCPDS 43-1640 reference card.

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Development of SiO2-BaF2 hydrophilic and antireflective coating applied as solar glass

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In this study, we present a methodology for developing a broadband antireflective coating deposited on a glass substrate, which incorporates porosity in the films. We evaluate the film's application as solar glass in covering a monocrystalline silicon solar cell, and we examine the increase in transmittance of the film compared to the glass substrate. Additionally, we investigate the influence of the films on the photovoltaic parameters, such as the fill factor (FF) and power conversion efficiency (PCE). We synthed SiO2-BaF2 by sol-gel and dip-coating deposition, where we varied withdrawal from 1 mm/s to 4 mm/s, followed by thermal treatment at 200°C for 1 h. We characterized the films by analyzing their transmittance and reflectance spectroscopy, and scanning electron microscopy. We also performed electrical characterization of the solar cell covered with the different films and the glass substrate to obtain the parameters of short circuit current density (Jsc) and open circuit potential (Voc), which allowed us to determine the FF and PCE. The results of the transmittance in the visible range (400-800 nm) show that the films with different thicknesses had the following transmittances 1 mm/s with 94.3%, 2 mm/s with 96.2%, 3 mm/s with 98.0%, 4 mm/s with 98.2% and the glass substrate with 91.6%. The film shows a 7.2% improvement in transmittance compared to the glass substrate. The increase was due to the introduction of porosity associated with the in situ formation of hydrofluoric acid (HF). The contact angle was around 20° for all samples. The porosity contributed to the graded refractive index in the SiO2-BaF2 film and these conditions influenced the reflection suppression. We also evaluated the PCE and FF of the solar cell with the device covered with the glass substrate and the film with the best transmittance.

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Development of Thermal barrier coating (TBC) by laser cladding using Al2O3 as coating under structural steels for low-cost aeronautical parts and automotive brake discs

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The last 20 years advances have imposed industrial conditions: an efficiency with less expensive materials. In face of a commercial competition and environmental restrictions increasing [1]. As a result, the parts processing becomes crucial. However, advanced surface treatments, such as ceramic coatings are currently costly. Thus, restricted to aerospace, aeronautical industry and advanced automobility parts; such as Formula 1 braking discs. In this context, this paper aimed the investigation of alumina TBC under structural steels by laser cladding. Considering that the alumina is notoriously cheapness than others; such as Zirconia and WC. In addition, the steel natural ageing oxide layer (SNAL) could provide the thermically growing oxide's (TGO) covalent bonding for ceramic anchoring [2,3]. Therefore, for this research were used for coating an Al2O3 powder and substrates of 2 years naturally aged 1045 steel and stainless steel. In comparative way, NiCrAlY powder was also used as conventional TGO. For the deposition, was used a laser cladding system consisting of an Ytterbium laser (1500W, 6mm spot and top-hat headstock) carried by a robotic arm. Imbued with a powder feeder. Straight tracks were made, with defined parameters of velocity of scanning "vs" (mm/s), powder feed rate "µ" (g/min) and beam power "P" (W). The samples were sectionally evaluated with optical microscopy (OM), scanning electron microscopy (SEM) and X-ray spectroscopy (EDS). The results shown optimum parameters of: vs = 3mm/s, µ = 2g/min and P = 1125 W.

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Effect of Atmospheric Plasma Jet on the Wettability of PDMS Surfaces

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The study of the internal change of polymeric tube surfaces after treatment with plasma jets, such as functional coating, deposition or activation, has been studied for more than a decade. The surface changes that a given polymer can undergo are essential for new biocompatibility methods to be discovered [1-2]. Through a dielectric barrier discharge reactor (DBD) the plasma was produced and then connected to a long and flexible probe, with a copper wire inside[3]. The gas stream flows into the reactor, and the plasma that is generated is then transferred to the end of this probe. In the reactor, high voltage pulses with a damped sinusoidal waveform, with a maximum amplitude of 20 kV for positive polarity and -19.0 kV for negative polarity are then applied to the electrode of the DBD reactor. A primary discharge is generated inside the DBD reactor, which is responsible for polarizing the copper wire. In this work, an atmospheric pressure plasma jet (APPS) with the working gas Argon was applied inside a PVC pipe coated with Dimethyl Polysiloxane (PDMS) material, in order to verify the change in the wettability of this material. The FTIR spectrum of the sample was obtained before and after exposure to plasma, in order to monitor the appearance of groups to verify changes in the sample's functional groups. The temperature of the plasma jet inside the tube was also measured, with the aim of verifying the internal temperature inside the tube coated with PDMS. FTIR spectra showed the emergence of OH functional groups in addition to CH bonds. The contact angle reduced after exposure of PDMS to plasma. Temperature measurements showed low values of 34.0 ºC.

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Effect of Cooling Rate on Microstructure and Corrosion Behaviour of 248.0 Aluminium Alloy

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Current design specifications for the manufacturing of components, from metal-matrix composites, require that aluminum alloys have known and stable properties, able to withstand severe application conditions. This work aims to develop an experimental analysis of the influence of Ni content on the microstructure arrangement and corrosion behavior of an Al-5Cu-1.5Mg-1.0Ni alloy subjected to a unidirectional solidification technique, which allowed a wide range of cooling rates to be attained. Traditional metallography techniques, optical microscopy, and scanning electron microscopy (SEM/EDS) were applied for microstructural characterization. Potentiodynamic linear polarization tests were performed according to the ASTM G3-14. An essentially dendritic morphology was shown to characterize the Al-rich matrix and IMCs containing Ni were detected in the eutectic mixture as a ternary eutectic. It was observed that higher corrosion resistance is associated with a refined Al-rich matrix and with a homogeneous distribution of intermetallic compounds in the interdendritic regions. In the Al-5Cu-1.5Mg-1.0Ni alloy, the reaction of the corrosion process occurred by diffusion control. The Al-5Cu-1.5Mg-1Ni alloy showed a higher i_{corr} = 3.2 µA/cm^2, corresponding to the most active condition, that is, less resistant to the corrosive process, but with attempts at passivation and possibly breakage in the anode branch of this passive film. Up to the potential E_{Pite}= -0.565 V, the process is controlled by activation. After carrying out the corrosion tests, Microscopic analysis showed corrosion in the form of pits.

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Effect of metallic oxide nanoparticles on corrosion in 1020 steel

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Films of metallic oxide nanoparticles have been employed as corrosion inhibiting layers on 1020 carbon steel obtained through different deposition methods. Parameters that have shown importance on the quality of the films and their inhibiting effect include solution composition, concentrations, time, and temperature of heat treatment. The objective of this study is to investigate whether silicon dioxide (SiO2), titanium dioxide (TiO2), and zirconium dioxide (ZrO2) nanoparticles act as inhibitors of the corrosive process in 1020 carbon steel. Nanoparticles were synthed via the sol-gel process and a 25-2 factorial design (SiO2; TiO2; ZrO2; Time and temperature of heat treatment) was used to investigate the method of obtaining thin films on steel via dip-coating. Open circuit potential (OCP) and polarization curves (Tafel) measurements were conducted to determine the corrosion rate (mm/year). The results showed that the temperature of heat treatment significantly affects the corrosion rate, and that under certain combinations of nanoparticle films at certain temperatures, the corrosion rate of the steel with deposition is lower than that without deposition. This effect has been attributed to crack formation processes under certain film formation conditions.

Effect of nitrogen optical centers after irradiation with high energy electrons in single-crystalline CVD diamond

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Monocrystalline CVD diamond holds great promise due to its exceptional thermal conductivity, hardness, and optical transparency [1]. However, its response to ionizing and non-ionizing radiation, especially concerning nitrogen optical centers, is crucial for understanding its stability in high radiation environments, such as in radiation sensor development. This study investigates from the development of the CVD diamond seeds themselves, the deposition process [2], diamond color transformation through the use of electron beam radiation, to the change of nitrogen optical centers in Single Crystal Diamond. Samples were grown via microwave plasma deposition, irradiated with varying doses, with PL used to examine changes in optical centers and FTIR to determine the diamond type. The integration of these techniques provided a comprehensive understanding of radiation-induced changes, crucial for the development of radiation sensor devices and suggesting possible quantum devices.

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Electrocatalytic Hydrogen Evolution Reaction (HER) at in-situ hierarchical self-doped Ti@TiO_2 nanotubes

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Titanium dioxide (TiO_2) is a promising inorganic material for water purification, power generation and Hydrogen Evolution Reaction (HER), for example. TiO_2 is a semiconductor with band gap energy (E_{bg}) of 3.20 eV for anatase phase, which limits its photoactivity at low wavelengths. However, recent developments in the field of doping and nanostructure engineering have led to a renewed interest in the application of TiO_2 in catalysis [1,2]. Recently, sd-TiO_2NT (self-doped TiO2 nanotube) has been developed by simple cathodic polarization and it does not require foreign impurities. In the process, Ti^{3+} dopant states are created resulting in a material with excellent catalytic activity [3]. Therefore, the purpose of this study was to investigate the electrochemical properties of the sd-TiO_2NT in HER. TiO_2NT electrode was prepared by anodization in glycerol solution and calcined at 450 ºC to attain anatase crystal. Sd-TiO_2NT electrode was subjected to cathodic polarization in PBS 1.0 mol L^{-1}. The surface of the electrode was successfully characterized by Scanning Electron Microscopy (SEM), X-ray diffraction (XRD) and cyclic voltammetry (CV). The results showed that, compared to bare titanium and TiO_2NT, sd-TiO_2NT has significantly higher active surface area and HER activity, presenting a typical electrocatalysis profile in CV. Increasing pH and scan rate shifted HER $E_{1/2}$ to more negative potential, possibly due to the poor H^+ concentration on the substrate surface. Furthermore, parameter such as overpotential, charge transfer coefficient, stability and reaction mechanism will be evaluated.

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Evaluation of an Epoxy Self-Healing Coating by Encapsulated Linseed Oil in Poly (Urea-Formaldehyde-Melamine) Microcapsules

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Microcapsules with urea–formaldehyde-melamine as the shell and linseed oil (LO) as the healing agent were synthed by in situ polymerization technique. The characteristics of synthed microcapsules were studied by Fourier-transform infrared spectroscopy (FTIR), thermal gravimetric analysis (TGA), and scanning electron microscopy (SEM) for chemical structure, thermal stability, and surface morphology investigations. The synthed microcapsules presented a range of 20 - 220 µm diameters. LO loading efficiency was 81%. To understand the curing performance of LO as a self-healing agent and the progression of corrosion processes, the microcapsules were added in an epoxy coating and applied on carbon steel, and their self-healing effect was investigated in 0.1 M NaCl solution. The long-term corrosion performance of scratched epoxy-based coating samples containing microcapsules was evaluated using Electrochemical Impedance Spectroscopy (EIS) and optical microscopy imaging throughout 1000 h. The EIS results showed that LO significantly improves the anticorrosive performance of the damaged coating. However, a better protection performance was observed in the short term, as after a period of exposure to the corrosive environment it was possible to observe corrosion in the samples, indicating that the efficiency of protection decreases over time.

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Evaluation of annealing temperature on the properties of $AgBiS_2$

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In recent decades, a form of sustainable energy that has been studied and applied in many countries is solar energy in photovoltaic and photocatalytic forms. Highlighting inorganic semiconductor materials, such as germanium, silicon, oxides, binary compounds and alloys. Some of these solution-processed inorganic photovoltaic materials have stood out due to their reduced manufacturing price compared to conventional production of photovoltaic materials, such as perovskites [1]. However, these materials generally use heavy metals such as lead. An alternative that is being studied to solve this problem are ternary compounds, materials free of heavy metals. Among them, bismuth silver sulfide nanoparticles are being studied. These nanoparticles have a high absorption range, high mobility and high absorption coefficient [2]. The present work aimed to develop and study the ternary compound $AgBiS_2$, as a light-absorbing layer, obtained through solvothermal synthesis, aiming to study the influence of the annealing temperature when the $AgBiS_2$ powder is subjected to temperatures of 100, 200 and 300 °C [3]. The thin films of this material were obtained by spin-coating deposition, being characterized by XDR, FTIR, UV-Vis, XPS and SEM. The solar cells will be manufactured to evaluate the quality of the materials and verify the potential use of the developed materials.

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Evaluation of automobility brake discs wear improvements using a laser cladding system for nickel coating, implemented by a mathematical model

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The general perception highlights the industries and cars (with combustion engines) as the main PM2.5 generators; a particulate matter with a diameter of less than 25 µm. In fact, they account for almost 80% of this generation. However, more than 20% is generated by brake disc/pad friction; into motorcar's braking system. These numbers contribute significantly to health and deaths related to MP2.5'S carcinogenic and its long-term suspension into air. Therefore, brake discs surfacing treatment could to reducing these numbers; due to its wear resistance improvements; such as the laser cladding methods. In this context, this paper aimed a mathematic model proposition. In order to describe a spiral path for brake disc Nickel deposition by laser cladding. To this end, was considered the following experimental set-up: brake disk remaining in rotation with the laser beam and Nickel coating aspersion (Ytterbium laser with a powder system) moving linearly from "A" to "B" points. With this, the math-model aimed the planning of a certain spiral-path planning. In order to assure a most uniform and well executed deposition. Based on laser parameters for its tangential velocity of vs=9-11mm/s, laser beam power of P=1350W and nickel powder feed rate of mi=9.6g/min. The obtained model was able to correlates the path direction with linear laser trajectory; according angular velocities variation and A to B distance. In addition, two case of studies; using the model; were put into practice. These case studies determined trajectories that produced a final nickel coating. The coat path-lanes were analysed macro and microscopically and under an optical microscope (OM). Concluding that the coating presented an apparently uniformity; with few defects. Thus, was confirmed the viability of this process, which could contribute to MP2.5 emissions reducing.

Evaluation of Bone Cells (MC3T3) Behavior on Plasma-Treated Titanium Surfaces

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The search for new surfaces that promote biocompatibility in bone implants has been a topic of increasing interest in the biomedical field. In this context, the titanium surfaces were treated with an argon plasma jet for 1 hour, without heating, and heated to 100°C and 200°C [1]. The jet was produced in atmospheric air using dielectric barrier discharge (DBD). The effects of these treatments on surface roughness, cellular stiffness and live/dead cell immediately after treatment were analyzed [2] It was observed that the average roughness values (Sq) increased as the treatment temperature was elevated without heating, 100 and 200°C, respectively, (1.7 ± 0.4 vs 3.3 ± 2.0 vs 7 ± 1.7), compared to untreated samples (1.7 ± 0.2). Cellular stiffness data demonstrated that cells cultured on surfaces treated without temperature and at 200°C (1.5 ± 7.8 vs 0.9 ± 4.8) had a lower Young's modulus, indicating lower cellular stiffness on treated surfaces compared to untreated samples and treated at 100°C (2.5 ± 0.9 vs 2.0 ± 1.1). Additionally, cell's live counting showed that surfaces treated at 100°C and 200°C (1735 ± 1002 vs 1803 ± 1041) had a higher number of cells live compared to untreated and treated (1495 ± 863 vs 1433 ± 827) without temperature surfaces. Analyses revealed that surfaces treated with plasma at different temperatures exhibited higher roughness and cell number, as well as lower cellular stiffness compared to untreated ones. This suggests greater biocompatibility.

Evaluation of Corrosion Resistance of Galvalume® Steel used in Electric Transmission Towers

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In the electric power sector, corrosion expenses reach the order of US$ 1 billion, and the use of techniques to combat corrosion could save 20% of the annual cost. Considering the significant growth of wind power generation and transmission lines in Brazil coastal areas, this research addresses the corrosive behavior of Galvalume® steel in such environments, with a view to enhancing the stability and reliability of the Brazilian electrical system. For this purpose corrosion resistance of zinc, aluminum and Galvalume® samples were studied through open circuit potential, potentiodynamic polarization, and electrochemical impedance spectroscopy at different immersion times in 3.5% NaCl solution, and also previous microstructure analysis by optical microscopy. The metallographic analysis revealed that steel coated with 55%Al - 43.5%Zn - 1.5%Si, weight percent (AZM150-ASTM A792) presented a uniform layer of this coating, with dendritic regions of aluminum and interdendritic regions of zinc. In open circuit potential experiments, zinc displayed less noble potentials, confirming its sacrificial metal suitability, while Galvalume® showed a mixed potential. Moreover, electrochemical impedance spectroscopy detected migrational ionic transport phenomena in the first seven days, followed by diffusional phenomena after fifteen days in an aggressive environment, for Galvalume® steel. Additionally, there was a decrease in polarization resistance after seven days of immersion in saline solution, from 6.1 kOhm.cm^2 to 0.2 kOhm.cm^2, followed by stabilization of Rp after fifteen days, possibly due to the formation of aluminum oxide (Al_2O_3) on the surface, which acts as a protective barrier against corrosion. In summary, Galvalume®, produced through hot-dip immersion, combines the microstructural properties and corrosion resistance of aluminum and zinc, offering a stable sacrificial coating for substrate protection.

Evaluation of laser cladding contour parameters for additive metallurgy manufacturing with H13 powders under stainless steel substrates

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Industry 4.0 advancement imbues a rapid dynamic and optimized production strategy under parts manufacturing chains sector. In face of demanding consumer and competitive scenario increasing [1]. In this context, 3D printing (3DP) or manufacturing additive (MA) stand out. Where, in the case of metal parts, this field extends to metallurgy manufacturing additive (MMA); with a similar processing of 3DP. In this horizon, from some consolidated techniques highlights laser cladding systems (LCS). These operates by instantaneous fusion of injecting powder and below metal base; by a laser beam emission. With this, the LCS promote a metallurgical bonding; between interest materials. In addition, these promotes a well densification between overlapped layers for three-dimensional part obtaining [2]. Although, for each metal alloy and desired prototype geometry the LCS parameters must be adjusted. Of these, stand out the beam parameters of: laser power "P" (W) and beam diameter "bd" (mm). Likewise, the execution parameters of: velocity of scanning "vs" (mm/s) and powder feed rate "µ" (g/min) [3]. In order to produce successive well-densified layers; presenting a minimal of defects, such as macro-pores, cracks, etc. Therefore, this paper aimed the obtention of a process-chart; correlating LCS parameters and MMA microstructural quality. To this end, were used an Ytterbium LCS, transported by a robotic arm. With H13 steel-tool powder under a stainless-steel substrate, as materials. The optical microscopy (OM) analyses revealed the µ as the main influence parameter; considering fixed P and vs parameters. Thus, the results of obtained process-chart obtained shown an optimum $\mu = 3.2$g/min; with fixed $P = 1275$W and $vs = 3$mm/s. Presenting a macro-pores and flaws decreasing as function of µ decreasing. Nevertheless, low µ (< 2.6g/min) implies a low part growth rate; generating energy accumulation that culminates in the remelting of layers.

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Evaluation of Passion Fruit Peel (Passiflora edulis Sims) Extract as a Natural Corrosion Inhibitor for Carbon Steel in Acidic Media

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The usage of inhibitors is a relevant alternative for preventing loss of metallic materials due to corrosion in acidic media. Nowadays green inhibitors or natural organic inhibitors are drawing the attention of researchers because of its low toxicity, biodegradation, reduced cost and easy acquisition. Green inhibitors are capable of reducing the dissolution of metals through the antioxidant action of extracts from plant leaves, fruits, seeds and peels. In this study, the inhibitive action of passion fruit peel extract in the corrosion of carbon steel in 1 M HCl solution was investigated using electrochemical impedance spectroscopy, potentiodynamic polarization curves, weight loss measurements and surface analysis. It was found that with increasing inhibitor concentration, there was an increase in inhibition efficiency. When it comes to the weight loss test, the maximum inhibition effectiveness of passion fruit peel extract is 94%, which is promising. SEM morphology reveals that the presence of a green inhibitor reduced corrosion on the carbon steel surface. The adsorption mechanism of inhibitor molecules on the carbon steel surface is considered as physical adsorption and the adsorption isotherm was matched with the Langmuir isotherm model.

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Evaluation of the addition of polyethylene glycol and boric acid as a flame retardant in paints

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Paints are dispersions which generally have four main ingredients: pigments, binders (generally polymers), solvents (mostly high-volatility or flammable) and additives. The flammability index of these mixtures can be determined by the flash point (FP), the minimum temperature in which the vapor of the paint can be ignited and the flame spreads over the surface of paint emulsion. A formulation with lower FP means it is easier to ignite. Additives such as halogenated flame retardants are widely used, but there is a great deal of concern regarding their harmful effects [1]. This study investigates the potential application of polyethylene glycol (PEG1500) or boric acid as flame retardants (additives) for paper ink. The mixtures based in nitrocellulose, alkyd resin, toluene, N-methyl-pyrrolidone and red dye were prepared in a mechanical agitation system with PEG or acid boric in 5% (w/w) of the total composition. The flammability index was evaluated according to ASTM D4206-96 (2018) [2], and the tests were conducted in triplicate. The average FP temperatures were 68.0 ± 0.7 °C to a mixture without additive, 80.7 ± 2.7 °C using PEG as additive, and 75.0 ± 7.2 °C with boric acid. An increase in FP of 19% was observed using PEG 1500 and 10% with boric acid, resulting in the reduction of the flammability of the samples. Therefore, the efficacy of the proposed flame retardants was confirmed, demonstrating their utility in reducing the flammability index and serving as a basis for industrial applications involving mixture with flammable liquids.

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Experimental study of chalcone derivatives as new corrosion inhibitors for carbon steel in acidic environment

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Mild steel is widely used in civil and industrial engineering for its cost-effectiveness, strength, and ductility. However, exposure to acidic substances leads to corrosion, posing environmental risks. Organic corrosion inhibitors, with heteroatoms and conjugated pi systems, offer protection by adsorbing onto metal surfaces, forming a protective layer [1]. The study investigated if three chalcone derivatives, named DPP (-H), DTP (-CH3) and DIP (-I), could act as corrosion inhibitors for mild steel in HCl 1 mol L^{-1}. It was employed experimental methods such as weight loss tests, electrochemical impedance spectroscopy (EIS), potentiodynamic polarization (PP) and surface characterization. The molecules demonstrated strong anticorrosive effects, with efficiency values of 84.4% for DPP, 89.3% for DTP and 94.1% for DIP at a concentration of 1 mmol L^{-1}, with their adsorption to the mild steel surface following the Langmuir model . The high value of the adsorption equilibrium constant (K_{ads}) of molecules in solution suggests that the equilibrium tends to favor the adsorption of these compounds on the metallic surface, through a physicochemical interaction with the surface, seen by the value of ΔG_{ads} [2]. EIS analysis showed an increase in resistance to charge transfer. PP results suggested that the compounds acted as mixed type inhibitors, decreasing both anodic and cathodic reactions in the metal . Surface morphology techniques such as SEM and AFM confirmed the metal preservation with maximum inhibitor concentrations, highlighting the formation of a protective film against acidic solutions [1, 2].

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Exploratory research on carbothioamide compounds as corrosion inhibitors for mild steel in acidic medium

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Mild steel is one of the most widely used metallic materials in civil and industrial engineering due to its attractive features, such as cost-effectiveness, high mechanical strength, and ductility. However, when exposed, for example, to acidic substances, whether during transportation of low pH substances or during chemical pickling processes, this material becomes susceptible to corrosion, posing a risk to the environment and surrounding lives. Therefore, one way to protect this metallic material is through the use of organic corrosion inhibitor molecules. These molecules, characterized by the presence of heteroatoms with lone pairs of electrons (P, S, O, N) and conjugated pi systems, have the ability to adsorb onto the metal surface and form a protective layer against aggressive environments [1]. In this study, three molecules derived from carbothioamide, addressed as MTCT (-OCH3), PTCT (-H) and CTCT (-Cl), as corrosion inhibitors for mild steel in an acidic medium (HCl 1 mol L^{-1}) was evaluated. Through the use of the weight loss test, it was possible to observe the good and increasing performance of these molecules in the concentration ranges studied. At the maximum concentration (1.0 mmol L^{-1}), the molecules obtained 87.2 (MTCT), 90.4 (PTCT) and 94.1% (CTCT). It was also seen that, the adsorption of the molecules follows the Langmuir model, proposing the formation of a monolayer of inhibitors on the surface that block the contact of the acid with the active sites of the metal[2] . The calculate K_{ads} indicated a shift in the equilibrium of the system that favors the adsorption of molecules on the metallic surface and ΔG_{ads} suggests that adsorption is of physicochemical nature [1, 2].

Acknowledgments: UFF, CNPq, CAPES, FAPERJ.

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Fatigue-corrosion studies on the 2198-T851 and 2524-T3 aluminium alloys containing Nb2O5 coating

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2xxx series aluminium alloys are extensively employed by the aircraft industry owing to their exceptional mechanical and corrosion-resistant properties, as well as their low density, and ease fabrication. Nevertheless, when aluminium alloys are subjected to corrosive environments such as sodium chloride solutions, their fatigue life becomes compromised [1, 2, 3]. Addressing this, one potential solution to extend the fatigue life is through the functionalization of the 2198-T851 and 2524-T3 alloys by using the reactive sputtering technique. This study aims to investigate the positive effect of Nb2O5 coatings on reducing the fatigue crack growth rates (FCGs) of both aluminium alloys. For this purpose, FCG tests were conducted in air and aggressive medium (0.6 mol L-1 NaCl solution), with a loading ratio of 0.1 and frequencies of 10 Hz (air) and 0.1 Hz (0.6 mol L-1 NaCl), employing sinusoidal waveform. The morphological fracture surfaces of the 2198-T851 and 2524-T3 aluminium alloys were accessed after the corrosion-fatigue tests by optical microscopy (OM) and scanning electron microscopy (SEM). Results demonstrated the corrosion process occurred in the vicinity of the crack tip, where stresses are elevated, and significant plastic deformation prevails, notably influenced by slip bands that induce micro-cracks, exposing fresh material layers to the corrosive surroundings. The Nb2O5 coatings enhanced the fatigue-corrosion resistance of both studied aluminium alloys. This study marks an initial step towards more comprehensive investigations into the impact of Nb2O5 coating on improving the mechanical properties of the 2xxx series aluminium alloys.

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Fatigue Defect Analysis in Railway Wheels

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The damages caused by wheel-rail contact is a major problem on the railway, entailing large maintenance expenses and resulting in accidents with loss of materials and the death of passengers [1]. The objective of this research was to analyze, understand and describe the various wear mechanisms of the wheel-rail tribosystem, using bibliographical review and data collection of railway companies to verify how the defects appear and investigate their possible causes. In the analysis, the premises of the AAR (Association of American Railroads) were used as a parameter.

For the study, a defect found in a railway company was collected, a case of material detachment in some wheels of a railway composition, that is, superficial RCF (Rolling Contact Fatigue), which can be classified as spalling or shelling, both characterized by scaling of the wheel track with material detachment. In order to be precise in classifying the defect, it would be necessary, in the case of shelling, to cut the wheel to check if there was plastic deformation; and for spalling, the use of ammonium persulfate, which in contact with the martensite reveals a clear region and allows the identification of thermal damage [2]. It was not possible to perform these tests, therefore a visual verification was conducted according to the AAR 2022 standard and data from what happened during the operation were collected. Given that the detachment was located around the entire circumference of the wheel, parallel to the tread, the defect was classified as shelling, as it is a characteristic of this type of defect. With the result of the inspections, suggestions were made to the company in order to mitigate these defects.

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Graphene Characterization via LPCVD on ASTM A36 Steel Substrate

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In this work, graphene synthesis via low-pressure chemical vapor deposition (LPCVD) on ASTM A36 steel is investigated using different surface preparations and operational variables. Currently, chemical vapor deposition (CVD) is recognized as a viable technique for the large-scale production of graphene films. Challenges associated with controlling graphene growth to achieve large flake dimensions, uniform layers, rapid growth rates, and minimal synthesis temperatures are noted. In particular, the graphene domain increases concerning growth time. Steel surface morphology, and growth conditions significantly affect graphene quality, highlighting the need to understand operational parameters, such as substrate preparation protocol (mechanical polishing, ultrasonic cleaning), and optimal growth conditions (heating, pre-growth annealing, liquid precursor pressure, after-growth cooling). Characterization techniques include scanning electron microscopy (SEM) and energy dispersive spectroscopy (EDS), which reveal homogeneous graphene layers with increased carbon mass and reduced iron content. X-ray diffraction (XRD) analysis shows no significant changes in crystal structure. Raman spectroscopy and mapping indicates low disorder effects in graphene flakes, as well as a higher monolayer yield than multilayered graphene growth. Steel surface morphology and CVD conditions significantly affect graphene quality, highlighting the need to understand operational parameters for optimal growth.

High temperature oxidation and stability of NiAl-based single and multilayer coatings processed through PTA-DED

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Nickel Aluminide (NiAl) is an intermetallic compound with interesting properties for high-temperature conditions, such as high resistance to oxidation, good stability, and low density [1]. It has an ordered structure and sufficient Al content to form a stable continuous protective film of alumina (Al_2O_3), known for its good adherence and low growth rate [2]. This research is part of an ongoing project that aims to evaluate the impact of carbide content on the single and multilayer NiAl-based coatings processed by Plasma Transferred Arc Directed Energy Deposition (PTA-DED) technology to deposition of Ni+20 wt.%Al elemental powder mixtures (via in-situ synthesis), without and with additions of 10 wt.% and 30 wt.% tungsten carbide (WC-Co), respectively. The study focuses oxidation resistance and high-temperature stability of the coatings, particularly, on the understanding of microstructural changes, oxide mass gain and type of oxides formed during cyclic oxidation at 800ºC and 1100ºC for 10 hours. The observed phenomena are also associated with the reduction of subtract elements, typical of multilayer coatings. A comparative analysis of "as deposited" and "oxidized" specimens is carried out to assess the behavior of each intermetallic coating when exposed to high-temperature, prevalent in different industrial areas. Results also allow to identify and discuss the factors that negatively affect resistance in these aggressive environments.

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Image-based density analysis for indirect Selective Laser Sintering (iSLS): applications & limitations

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Indirect selective laser sintering (iSLS) is an additive manufacturing technique, in which the powder bed is filled with metal-polymer particles in order to accelerate deposition by reducing the required laser energy to melt the powder. Green parts are submitted to a sintering process to remove polymer and strengthen metallic bonds. Such step in the indirect AM chain leaves considerable voids inside the fabricated volume. Therefore, image-based density analysis comes as an effective tool to inspect iSLS complex geometries that cannot be properly addressed by conventional methods, such as Archimedes. The present work aims to develop an algorithm for image based density analysis, highlighting possible limitations of such method for indirect selective laser sintering. To fulfill that objective a Matlab code was written aided by the Image Processing toolbox. Samples made by iSLS were submitted to optical microscopy analysis and then used as input into the developed code. Otzu’s threshold was used and its sensitivity evaluated in terms of final density. Results showed a validated density for the investigated chains, density was in the order of 75%. Variation on the threshold sensitivity highlights that micropores may not be considered on the density calculated by image, especially when compared to L-PBF and M-FDM. This work has provided enough data to conclude that image-based density analysis may be an useful tool for complex geometries, however image threshold must be set carefully according to the AM analyzed process.

Influence of topography of Ti6Al4V electrodes functionalized with multilayer films on tumor cellscapture

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In the oncology area, several techniques have been evaluated with the aim of capturing circulating tumor cells (CTCs) for the purpose of cancer detection, diagnosis, and treatment. Biosensors employing electrode topography have been proposed as a promising approach to isolating CTCs. Furthermore, the identification of CD44, a glycoprotein expressed by tumor cells, through bio specific interactions with hyaluronic acid-based films has been applied to increase the sensing specificity. This study evaluated the capture performance of CTCs in three-dimensional Ti6Al4V alloy electrodes, obtained by additive manufacturing (AM) and functionalized with multilayer films obtained by the layer-by-layer technique. The influence of topography, for the Sch geometry, was investigated by varying the of the cellular units by reducing their edges. The electrodes were produced using the Electron Beam Manufacturing technique and underwent plasma pretreatment for 15 minutes, followed by the deposition of a monolayer of polyethyleneimine. The multilayer coatings were made up of chitosan and hyaluronic acid, by deposition of 3.5 bilayers. This functionalization was promoted by alternating immersion in 0.1% (w/v) polyelectrolyte solutions for 10 minutes, followed by 3 consecutive washes. Adhesion of CTCs was analyzed with prostate tumor cells (PC-3) cultured on the electrodes at a density of 6.25 x 104 cells, with indirect counting after tripnization of the electrodes. The results showed that increasing the of the cell unit had an influence on the capture of cancer cells, as a decrease in the number of adherent cells was observed. This effect may be related to the reduction of the exposed area, since the adhesion of PC-3 cells may be mediated by surface contact [1]. In addition, CHI and HA multilayer films promoted an increase in cell adhesion in relation to Ti6Al4V, due to the interaction between HA and CD44, regardless of the geometry evaluated.

Interaction of oxygen plasma activated water with calcite

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This study deals with the interaction between plasma activated water (PAW) and calcium carbonate, aiming to enhance the dissolution of mineral components into water. Calcium carbonate precipitation, a ubiquitous phenomenon in hard water systems, poses a significant impediment to operational efficiency and product quality [1]. PAW was synthed by activating deionized water with a plasma pen (PlasmaPen, PVA Tepla) supplied with O2 gas, kept at 5 mm over the water surface, for 15 minutes. 10µL droplets of PAW were applied to calcite (CaCO3) crystals freshly cleaved surfaces and left to air-dry. Samples were analyzed via atomic force microscopy (AFM) and UV-Vis spectrophotometry. As reported in literature [2, 3], the incidence of plasma jet on water creates a high-energy environment that promotes the generation of reactive oxygen and nitrogen species (RONS). Thus, the results obtained showed a slight decrease in the pH of PAW, though with remarkable stability for a long period of time. AFM topography of cleaved calcite surfaces initially presented a smooth appearance. However, following contact with PAW, subsequent topography revealed a distinct transformation characterized by calcite regrowth on the crystal surface as well as substantial roughness increase. This result prompts the idea that during contact with PAW, the material started to dissolve, but regrew as the droplet dried. This implies PAW’s ability to dissolve calcite.

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Investigation of alterations on glass fiber and effects on the final properties of glass fiber reinforced composites

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A composite is defined as the combination of two chemically distinct materials with an interface separating them. They are used to obtain specific properties, different from those found in each constituent alone. The glass fibers are widely used in polymer reinforced composites due to their competitive qualities. Glass/Epoxy composites are the most used systems to support impact loads. A composite with fiber/matrix interfaces with cohesive strong bonds usually has high stiffness and high mechanical strength. These properties can be achieved from a surface treatment of the fiber improvement the interfacial properties and, as a result, the durability of the composite from a mechanical and environmental point of view. Adhesion promoters are chemicals that act at the interface between an organic polymer and an inorganic surface to increase adhesion between the materials. A properly coupling agent that forms stable chemical bonds between the matrix and the reinforcement can thus limit the diffusion of water at the interface and consequently the impact on mechanical properties. Characterizing the interphase regions is difficult due to their dimensions and the various interactions between their components. An important condition of these reinforced is that they can be affected by storage. After storage, before use, they may have modifications with a significant impact on the final performance of the composite.

The objective of this work was to characterize glass fibers that will be used for epoxy matrix composites. The focus of the work is on the effect of the storage time of the fiber under different temperature and humidity conditions and how this may have affected the surface of these to modify the chemical bonds of the interface. Characterization tests were carried out on the surface of the glass fibers such as FTIR, MEV and EDS, as well as on some composite samples to evaluate the matrix/fiber adhesion.

Investigation of significant voltage oscillations during niobium plasma electrolytic oxidation (PEO) and their correlation with porous morphology

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The technique of plasma electrolytic oxidation (PEO) has been widely studied due to its ability to produce thick and adherent anodic films from various valve metals [1]. This study observed an unusual electrochemical behavior characterized by voltage oscillation transients during the anodization under the galvanostatic PEO regime of niobium substrates. To investigate this phenomenon, we anodized the substrates in three different electrolytic solutions (H_3PO_4, KOH, and $C_2H_2O_4$) and examined the effect of temperature on each oscillation. Additionally, we tested three different current densities to observe their impact on the voltage oscillations. The results indicate a correlation between the exposed surface area and the morphology of the pores during the film growth in the oscillatory regime, suggesting a simultaneous process of oxide dissolution/pore filling and micro-discharges observed during the PEO process.

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Methylene Blue degradation and adsorption onto Yb3+ doped TiO2 surface during photocatalysis process

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Adsorption and degradation mechanisms of methylene blue are widely studied and used as model to remove a variety of organic pollutants. Photocatlysis aims to accelerate biodegradable process. Thin-film of titanium dioxide were prepared using sol-gel dip-coating method and doped with ytterbium (ranging from 1at% to 8at%) of trivalent Yb and deposited on soda-lime glass substrates. Annealing temperature procedure of 500°C was enough to assure anatase structure formation as the predominant phase. Rare-earth doping showed significantly influence on sample structure and overall crystallinity. Higher doping concentrations were observed to increase levels of anatase and reduce crystallinity. Films were prepared for evaluation as samples for photocatalytic activity and tested specifically for methylene blue (MB) degradation.

Comparative analysis with undoped samples and control runs showed high adsorption rate on the doped film's surfaces. At 4at% Yb, the sample was predominantly anatase, and showed highest adsorption of MB outside photocatalysis (darkness). While 1at%Yb showed fastest degradation of MB in the first hour of photocatalysis (incident UV).

Raman spectroscopy of doped samples showed a high percentage of adsorbed products during MB degradation, which indicates sites of Yb3+ on the surface of samples. These sites are recognizable for adsorption in doped films yielding peaks at 1051, 1086 and 1354 cm-1 and have shown to be responsible for a high rate of interactions during photocalysis.

It was also observed that the photocatalytic efficiency of the material was enhanced upon doping compared to undoped samples. This work represents a significant stride towards developing more efficient methods for carbon capture and organic pollutant degradation.

Microstructural and Mechanical Characterization of Tribological Behavior of Copper Alloy C93900 Through Testing and Failure Analysis

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Copper and its alloys find wide application across various branches of engineering, including thermal, electroelectronics, and sugar-alcohol industries. With over 400 known alloys, those containing lead are particularly noteworthy for their use in sliding bearings. Lead is insoluble in solid bronze alloys, remaining isolated in the form of small nodules within the Cu-Sn-Zn ternary matrix. This study is based on an alloy similar to C93900, with approximate compositions of 75% Cu, 4% Sn, 8.5% Zn, and 12.5% Pb, where lead aids in reducing adhesion. The aim of this study is to analyze the microstructure and mechanical characterization, as well as investigate the tribological behavior of this alloy. Microstructure was analyzed using both Optical and Scanning Electron Microscopy, along with X-ray Diffraction. Brinell Hardness tests were conducted, resulting in an approximate hardness of 60.28 HB. Additionally, Pin-on-Disc tests were performed under dry and lubricated conditions to determine friction coefficient and wear rate, revealing minimal wear even under dry conditions.

Mortar functionalized with silver nanoparticles for antifungal activity

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Building materials are susceptible to fungus attack, leading to structural and aesthetic problems. Nanotechnology has enabled the development of innovative products with unique properties, including antimicrobial capabilities [1]. Although the antimicrobial potential of AgNPs is already known, research on the application of AgNPs in cementitious materials and the behavior in prevention of fungal biofilm formation are still an extremely limited topic. Specifically, against the fungi presented in this work there are no reports. In this work, two types of mortars were formulated using AgNPs (108 µg/mL and 54 µg/mL) and tested against Aspergillus and Fusarium biofilms, fungi causing losses during grain storage. The AgNPs mortars showed strong antifungal capacity, reaching up to 99% reduction of Fusarium and 57% of Aspergillus biofilms. The reduction in the amount of Fusarium biofilm (AgNPs 108 µg/mL) is proven by SEM images. No Ag leaching was observed. Thus, a promising solution is presented for applications in agribusiness. Its significant role in preserving the integrity and quality of stored grains contributes significantly to food security and sustainability.

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Nafion-Induced Alterations in Protein Stability and Functionality

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Given the intricate nature of protein bioelectrochemistry, the immobilization technique adopted shows utmost importance to crucial factors such as biocatalytic activity and stability[1]. Entrapment methods are widely used due to the easy immobilization, including the possibility of simultaneous immobilization of multiple layers, besides reducing direct contact with the reaction medium, which contributes to minimizing leaching effects[1]. Despite the widespread use of the technique, with emphasis on the use of Nafion, an ionomer with sulfonated and perfluorinated groups, the literature still presents many gaps regarding how the characteristics of the polymer interfere with the protein activity, as pointed out by recent discussions[2]. Therefore, in order to understand the effect of pH on proteins due to their high sensitivity to medium conditions, electrochemical and in-situ spectroscopic studies were proposed to relate the effects on the secondary structure of alcohol dehydrogenase enzyme and how this affects its catalytic performance. With the advantage of extensive literature on the chosen protein, initial studies already show significant variations in electroactivity under different pH Nafion conditions, consistent with alterations in the proportions of beta-sheets and alpha-helix, as expected due to the high dependence between the enzyme's secondary structure and its bioelectrochemical activity[3].

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Nanoalumina as Active Material for VOC Sensors

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Air pollution poses a global threat to both human health and the environment. Toxic volatile organic compounds (VOCs) like isopropanol and ethanol have been identified as significant contributors to adverse effects on human health and the environment. Detecting these compounds effectively and selectively under ambient conditions is important for environmental pollution monitoring. Using metal oxide nanostructures as sensing materials for these vapors detection holds promise for enhancing sensor sensitivity and selectivity, especially when these materials are modified or as part of a composite. This study aims to explore the sensing characteristics of alumina nanostructures (aluminum oxide nanoparticles) in the presence of chemical vapors, alcohols, under controlled conditions. It is expected that the nanoparticles have small crystallite s and high surface areas, making them suitable for the detection of these VOCs. The morphological, structural, and electronic properties of the nanoalumina have been explored. To investigate its sensing properties, the materials were deposited onto interdigitated electrodes, and their sensor responses toward ethanol and isopropanol vapors investigated at room temperature by electrical impedance spectroscopy. The findings from this research could serve as a valuable guide for designing sensor prototypes for the real-time monitoring of toxic chemical vapors.

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Nanostructured oxide layers for osseointegration of additive-manufactured titanium alloys

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Titanium alloys are suitable for hard tissue repair, mainly because of their high mechanical strength, biocompatibility, corrosion resistance, and low elastic modulus [1]. Besides the inherent properties of the bulk, the alloy surface properties are also important because they affect the material osseointegration. Electrochemical anodization processes are often used to induce the formation of nanostructured layers on titanium surfaces and improve their biocompatibility. These layers are mainly composed of Ti (IV) oxides, which provide similar properties to the hydroxyapatite [2], with good osseointegration. Laser powder bed fusion (LPBF) allows the obtention of Ti-based alloys with functional chemical gradients, improving their mechanical properties. Nonetheless, composition gradients can also affect the electrochemical response and, consequently, the obtention of nanostructured oxide layers by anodization. In this study, additive-manufactured materials were utilized for nanostructured oxide growth by anodization. Dual-layer composites were synthesized by LPBF technique from commercially pure Ti and Ti-6Al-4V (wt.%) alloy. The oxide layers were characterized by scanning electron microscopy, atomic force microscopy, X-ray photoelectron spectroscopy, and glazing-angle X-ray diffraction. In the studied systems, the anodization efficiently produced self-organized oxide layers. Physical properties, such as morphology, size, and presence of defects, of the Ti (IV) oxides depended on the chemical composition of the dual-layer composite. Even though osseointegration was not studied, this dependence on dual-phase composition may affect it.

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Nb:Ce:La ternary catalyst: synthesis, characterization and potential application for the environment

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The study aimed to create a ternary catalyst using Nb, Ce, and La, intending to modify graphene and utilize it on an EDG cathode for enhancing the electrogeneration of hydrogen peroxide in solution [1-2]. The catalyst synthesis involved diluting 700 mg of Nb_2O_5, $CeCl_3$, and La_2O_3 in 20 mL of distilled water, in a Teflon capsule, followed by the slow addition of 10 g of NaOH diluted in 5 mL of distilled water, stir for 30 minutes. After this period, the capsule was closed and placed in a hydrothermal reactor maintained at 100°C for 24h. After the hydrothermal stage, the catalyst went through the process of 3 washes (water, 50% isopropyl alcohol, water), followed by centrifugation (5000 rpm) and was subsequently dried at 80°C for 10h and calcined at 500°C for 3h. The catalyst was characterized by Raman spectroscopy, showing a characteristic displacement of Nb_2O_5 of 230 cm^{-1}, CeO_2 of 500 cm^{-1}, and a displacement of around 850 cm^{-1} characteristic of La_2O_3. In XRD, a peak was noted at 20° corresponding to Ce, at 32° corresponding to Nb, and at 55° corresponding to La. In the SEM, one could observe the formation of nanorods, evident in the EDX analysis revealing their composition of cerium and lanthanum, with niobium present alongside these filamentous structures.Graphene demonstrated a hydrogen peroxide electrogeneration rate of 67%. This catalyst was used to modify graphene using the impregnation method, in quantities of: 1%, 3% and 5% by mass. in solution, following the 2-electron mechanism. Graphene modified with 1%, 3% and 5% of the catalyst showed about 99% of electrogeneration of peroxide in solution, respectively. The modification was aimed at increasing the electrogeneration of H_2O_2 in the solution during the oxygen reduction reaction (ORR).

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Obtaining optimized TiO_2 nanotubes on biomedical Ti cp

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TiO_2 nanotubes have attracted significant research interest due to their high specific surface area, high charge transfer, and in the biological area, the nano modification of titanium surfaces has the potential to induce osteogenic activity on the implant surface [1]. TiO_2 nanotubes can be obtained by different techniques such as sol-gel, electrophoretic deposition, and electrochemical anodization. For biomedical applications, adhesion and mechanical integrity are very important, in this sense, the anodizing method is the one that presents the best results, and also, under optimized conditions, it is an efficient and economical method for obtaining self-organized nanotubes [2-3]. According to the literature [1-3], the characteristics of TiO_2 nanotubes (such as geometry, length, diameter) obtained by electrochemical anodization, depend on various experimental conditions. Thus, obtaining nanotubes on Ti requires extensive optimization of the electrochemical parameters used. Therefore, the aim of the present study was to obtain self-organized nanotubes, with optimized characteristics (diameter, geometry, and length) on the surface of biomedical Ti cp by electrochemical anodization. The nanostructures were obtained applying different potentials, from 10 to 60V, during 1h to 6h, using aqueous and organic solutions. SEM analysis showed that highly organized nanotubes could be obtained on all studied experimental conditions, with different characteristics, while using organic solutions, the nanotubes presented a well-defined geometry.".

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Optical and morphological characterization of Nb/Al mixed oxide films obtained by Plasma Electrolytic Oxidation (PEO)

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Plasma electrolytic oxidation is a metal surface treatment technique derived from anodizing. In this technique, plasma discharges on the metal surface, and a high electric field produces a thick layer of oxide on the metal [1]. During the synthesis of the oxide film, ions can be incorporated on the metal's surface, forming mixed oxides. Niobium could enhance photocatalytic properties using niobium pentoxide on the semiconductor's surface [2]. In this study, samples were treated under a galvanostatic PEO regime in different experimental conditions of electrolyte solution concentration and temperature, composed of ammonium oxaloniobate (NH4H2[NbO(C2O4)3].3H2O) and ammonium hydroxide (NH4OH). The oxide films were characterized by diffuse reflectance spectrophotometry (DRS) and scanning electron microscopy (SEM) to investigate possible band gap and surface morphology variations with the variation of synthesis parameters.

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Optimization of ultrathin silver-based transparent electrode

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In optoelectronics, functional ultrathin (< 100 nm-thick) metal films based on trilayer architecture may act as transparent electrodes (TEs) due to the combination of an unprecedented high visible light transmittance and electrical conductivity [1 – 3]. In this work, we optimized the thermal evaporation parameters (deposition rate and thickness) to produce a dielectric-metal-dielectric (DMD) structure consisting of single-silver (Ag) layer sandwiched between oxygen-deficient tungsten trioxide (WO3-x) bilayers. By evaluating the optoelectrical properties of symmetric WO3-x/Ag/WO3-x (WAW) electrode, we established that deposition conditions have fundamental limits for each material. For instance, the inner WO3-x layer strongly influences the morphology of the subsequently deposited Ag film. We determined that thermally evaporated Ag directly on the silicon substrate forms only small island-like unconnected Ag grains, which are not conductive below 10 nm thickness. Adding a WO3-x as inner dielectric and seed layer, the same Ag thickness forms a continuous, smooth and conductive layer. At 6 nm Ag thickness such WA bilayer electrode exhibits a sheet resistance of ~ 50 Ω/□ and a transmittance of ~ 70 % at 400–800 nm wavelength, which is superior compared to Ag alone with the same thickness. Further deposition of optimized outer WO3-x layer improves both transmittance and conductivity of the resulting WAW electrode. The optimum structure was confirmed by optical simulation and it consisted of a WO3-x (20 nm)/Ag (6 nm)/WO3-x (20 nm) with total thickness of 46 nm characterized by a plateau shape with average visible transmittance exceeding 90 % and a low sheet resistance of less than 15 Ω/□. The figure-of-merit of the WAW investigated here exhibits the conventional high-cost ITO enabling its use as TE in optoelectronics and photovoltaic devices.

Paints with Zinc Oxide Nanoparticles and Evaluation of Antimicrobial Activity

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In this work, we used commercial paint incorporating zinc oxide nanoparticles (ZnONP) for construction and health purposes. Zinc Oxide nanoparticles exhibit antimicrobial properties, making the paints safer and more effective in healthcare and construction, especially in eliminating pathogens that can cause diseases or engineering pathologies. Zinc oxide nanoparticles were synthed mixing through a process of sodium hydroxide and zinc sulfate precipitation followed by thermal treatment, resulting in nanoparticles with less than 45 nm . Images shown rod-shaped nanoparticles characterized by Scanning Electron Microscopy (SEM). The antimicrobial effects of ZnONP were evaluated through broth microdilution and minimum inhibitory concentration against S. Aureus (54 µg/mL). The evaluation of the paint containing 5% nanoparticles was done using the Disk Diffusion experiment. The inhibition halo of the paint containing nanoparticles was up to 55% larger in diameter than the control samples. Therefore, the incorporation of nanoparticles into paints is a technological alternative for antimicrobial treatment of surfaces in hospitals and the construction sector.

Photoelectrochemical characterization of Nb_2O_5 films obtained by Plasma Electrolytic Oxidation (PEO)

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The environmental risks associated with water pollution demand solutions for non-biodegradable organic pollutants, such as advanced oxidation processes (AOPs), that are applied for water and wastewater treatments [1]. AOPs can be defined as procedures aimed at producing an oxidizing agent, like hydroxyl radicals, that will result in the degradation of pollutants in water [1]. Photodegradation using heterogeneous photocatalysis principles is one such procedure. It utilizes an oxide semiconductor to absorb light, resulting in the migration of electrons from the valence band to the conduction band, forming the electron-hole pair and promoting the formation of radicals. In this work, niobium pentoxide (Nb_2O_5) films are obtained by plasma electrolytic oxidation (PEO) to investigate photoelectrochemical properties for their application in photocatalytic degradation. The anodic oxide films are prepared with different electrolytic solutions, resulting in divergent microstructures and surface compositions. Photoelectrochemistry experiments are performed under a pulsing UV-A light source (λ = 365 nm) to investigate the electronic oxide structure under polarization and light stimulation.

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Preparation and characterization of polyurethane/Ag-TNT nanocomposite with antibacterial activity

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Hospital-acquired infections are an important cause of mortality and morbidity worldwide. Furthermore, the emergence of multidrug-resistant bacteria and new microorganisms has been a challenge in the healthcare ecosystem [1]. Since pathogens adhere to surfaces, the use of coating materials with antibacterial properties has been a promising alternative [2], as biopolymers functionalized with antibacterial-active fillers. This study aims to prepare polyurethane (PU) films using silver-modified titanate nanotubes (NT-Ag) to evaluate antibacterial activity. The Ag-TNT synthesis was performed from a TiO2 aqueous suspension and NaOH solution by hydrothermal method obtaining sodium titanate nanotubes that were modified with AgNO3 solution leading to Ag-TNT. The preparation of PU/Ag-TNT nanocomposites films will be carried out using in two steps: first, the PU will be obtained by synthesis between polycaprolactone diol and hexamethylene diisocyanate, after a determined content of filler will be added by physical mixture. The morphology and thermal and mechanical properties of the nanocomposites will be evaluated. Antimicrobial evaluation of the nanocomposites will be assessed through in vitro tests using well-known gram-positive and gram-negative bacteria associated with hospital-acquired infections, such as Staphylococcus epidermidis and Klebsiella pneumoniae and the cytotoxicity of the nanocomposites will be assessed through a combination of cell culture methods, cell counting, and clonogenic assay.

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Production and characterization of Ni-Co layered double-hydroxide electrodes on stainless steel substrate for alcohol electrooxidation

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All sectors of society are highly dependent on energy, which mainly comes from non-renewable fuel sources [1]. Therefore, reducing the dependence on fossil fuels and their use for energy production is a consensus in the scientific community. The project proposes the production of electrodes modified with nickel and cobalt hydroxide nanostructures for the electrooxidation of alcohols as a model for organic materials, with the aim of producing hydrogen through an electrocatalytic process. For this purpose, the synthesis of a nickel and cobalt catalyst electrolytically deposited on a stainless steel electrode was proposed. A commercially available stainless steel (SS) substrate is activated by an alternating acid etching/alkali hydrothermal treatment to form a hydroxide layer at the interface. [2]. Subsequently, a seamless integrated electrode with Ni-Co bilayer hydroxide (NiCo-LDH) nanoarrays and SS substrate was successfully synthed. The fabricated electrodes were characterized by transmission and scanning electron microscopy, XPS and electrochemical techniques to determine their morphology, structure and electroactivity. Preliminary results show that the pretreatment of the steel mesh altered the surface of the material, which served as a support for the growth of the double-layered hydroxide structure. The deposition was confirmed by scanning electron microscopy measurements and an increase in current was observed by cyclic voltammetry. The modified electrodes exhibit higher electroactivity in the oxidation of methanol and glycerol. It can be concluded that the modification of electrodes with nickel and cobalt hydroxides is a promising strategy for the electrooxidation of organic compounds.

Acknowledgements:
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ROS production induced by gold nanoparticles and its implication in the radiosensitization of tumor cells

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Radiotherapy is fundamental in cancer treatment, using ionizing radiation to target tumors while sparing healthy tissue. Metal-based nanoparticles (NPs) may act as radiosensitizers, enhancing therapy efficacy by promoting reactive oxygen species (ROS) production among other effects. Controlling the surface properties of these NPs is important for product stability, biocompatibility and enhancing cellular uptake. This study investigates ROS production induced by gold NPs (GNPs) and its influence on the radiosensitization of glioblastoma (U87 and M059J) and HaCat cells treated with x-rays from a clinical 6 MV-accelerator. Naked gold nanoparticles (GNP) were obtained by chemical reduction of sodium borohydride, and the dextran-coating was perfomed in situ. Subsequent cross-linking and amination of the dextran layer resulted in (GNP@DX-NH_2). The GNP and GNP@DX-NH_2 showed a mean core diameter around 10nm and zeta potential of –22,9 ± 0,74 and –20,3 ± 0,44 nm , respectively. NP treatment concentrations varied from 0.1 to 100 µg/mL . Initially, acellular ROS production due to the presence of the NPs only in aqueous media was quantified by fluorescence spectrophotometry, using the marker DCFH-DA (2'-7'-dichlorofluorescein diacetate). For the biological assays, cells were incubated with doses of NPs for 24h. NP cytotoxicity was evaluated using the 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT) assay, and no toxicity was found up to the maximum concentration tested. Cells incubated with NPs were then exposed to radiation doses ranging from 2 to 8 Gy. To quantify NP-induced cellular ROS production, DCFH-DA was also used. Acellular ROS production increased strongly with increasing NP concentration. The effect is however much reduced in the cells. Moreover reduced ROS production was found for GNP@DX-NH_2, probably due to the coating, acting as a chemical barrier, limiting NP interaction with the medium and highlighting the importance of surface properties.

Self-Healing Oil/Superplasticizer proportion affects the Mechanical Strength AndHy dration Kinetics Of UHPC

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The aim of this work is to analyze the self-healing action of tung oil (TO) in order to prevent pathologies in Ultra-High Performance Concrete (UHPC) [1,2] monitoring the hydration kinetics, mechanical strength (fcm) and modulus of elasticity of an UHPC in the presence of different ratio of OT and superplasticizer. The hydration kinetics was evaluated by 1H nuclear magnetic resonance (NMR) longitudinal relaxation time (T1) measurements. The T1 essays were performed each hour over a total period of 22 hours in a Bruker model Ascend 400 device, 400 MHz for liquids. The NMR samples were prepared by resuspending 0.015g/mL of a previously fractured (in a granulometric sieve of 75 µm) UHPC, in a mixture of water: deuterated water (H2O:D20), 90:10 (v,v). A control sample was prepared using 4% superplasticizer in absence of OT (0g OT). The control showed a fcm average equivalent to 74.4MPa. This value was compared to the fcm of the sample containing 3% superplasticizer and 8 g of OT, which corresponded to 83.10 Mpa. Thus, the presence of 8g OT and the 1% decrease of superplasticizer increased the UHPC fcm in 6.64 Mpa. The T1 curve also indicated a gradual increase in the gel: space ratio (porous) in the UHPC hydrated cement during the experiment period [3]. The results obtained in this work evidence how promising OT may be in the partial replacement of UHPC superplasticizers.

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Simulation of metallic coating by magnetron sputtering in ceramic vacuum chambers for particles accelerators

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Pulsed injection systems in particle accelerators necessitate specialized vacuum chamber designs, such as ceramic chambers coated with metallic layers on their interiors, to fulfill various functions including the generation of electromagnetic fields. Magnetron sputtering stands as one of the primary deposition methods employed in this context. Ensuring optimal performance of system components demands meticulous control over the distribution and thickness of the metallic coating. This is critical to preserve the integrity of the magnetic electric field and mitigate the formation of eddy currents, which could disrupt the beam stored within the accelerator. Thus, conducting simulations to define the numbers and cathode geometry, and position becomes imperative to meet the specific requirements of metallic coating thickness distribution along the inner perimeter of the vacuum chamber cross-section. This paper presents the parameterization results of cathode geometry derived from simulations using the Monte Carlo method with MolFlow+ [1] software, developed by researchers at the European Organization for Nuclear Research (CERN). The objective was to meet specific requirements within a chamber with an oblong internal transverse profile measuring 30 mm x 12 mm. Particularly, the upper and lower cross-sectional areas were required to maintain a 5:1 ratio compared to the lateral sections in terms of metallic coating thickness. The current study significantly advances the construction of ceramic vacuum chambers with metallic coatings by utilizing simulations and parameterizations of numbers and cathode geometry, and position, thereby playing a crucial role in advancing accelerator technology.

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Structural characterization of an alveolar ballistic-armour structure produced by laser cladding metallurgy additive: an advancing technological sovereignty status for Brazilian Army

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Unfortunately, war conflicts are a reality motivated by territorial and ideological disputes. However, numerous advances and facilities becomes to reality as war resulting; particularity, the security and defence systems. According to historical facts, there was a great development of defence systems in the conflict regions after the First and Second World Wars. Where, European countries becoming into main technologies exponents, especially for kinetic ballistic armour; such as mechanisms and war clothing. In this retrospective, researchers highlight the use of kinetic-armour based on "sandwich" panels. These have simple or complex three-dimensional structures between metal sheets; increasing the vehicle payload capacity (as function of its reduced weight). In addition, they assure a designed ballistic resistance. Nevertheless, according authors, this fabrication are so difficult by conventional way, such as welding and machining. Thus, other authors highlights that the manufacturing by metallurgy manufacturing additive (MMA); using laser cladding systems (LCS); promoting metallurgical bonding (plates/3D structure) and. adequate layers densification. Current literature doesn't show specific studies under this thematic; making it a research opportunity. Based on this context, this paper aimed the sandwich ballistic alveolar structure optical microscopic (OM) characterization; considering its LCS fabrication process: Ytterbium laser; operated by a robotic arm; using pre-established programming routines. With parameters of: laser linear velocity of scanning of 5mm/s, beam power of 1275W and feeding rate of H13 steel-tool powder of 6.4g/min. The OM's morphological analysis shown the 2 layers overlapping with a well-densification. In the same way, defects such as, macro pores, cracks or flaws weren't observed. Concluding the LCS is a feasibility to ballistic armour production. Bringing technological sovereignty to the Brazilian Army.

Study and characterisation of CDW to assess sustainable reuse

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Highliting the high emission of CO2 (carbon dioxide) from the use of conventional concrete, which directly corresponds to 8% of the total emitted globally, the construction industry is also a contributor to the emission rates of greenhouse gases such as NOx, SOx, CO, H2S, VOCs, dioxins, furans and particulate material [1]. In addition to the large generation of waste and residues that are common in this industry, there is also a high volume of waste from earthquakes and armed conflicts [2]. Then the aim of this study was to propose alternative solutions for the conventional construction industry. The project established the characterisation of CDW material (construction and demolition waste) in order to identify its chemical and physical properties, for subsequent use in the production of non-ceramic bricks, which use CDW as their main material. The characterisation of the CDW was carried out after grinding and pulverising it in a Marconi pot pulveriser mill, followed by sieving the material (<150 µm, 100 mesh). The material was then analysed by XRF (Shimadzu XRF-7000) to determine its chemical composition and XRD to identify the phases and then a Casagrande apparatus was used to determine the solid/liquid factor. The CDW chemical composition obtained by XRF is: 18.48% Al and 59.63% Si, and peaks of α-quartz (SiO2). Hydrated calcium silicate (CaH2O4Si) and calcite (CaCO3) were identified by XRD. The CDW solid/liquid factor resulted in 0.32.

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Study of Conductivity in Thin Films of Graphene Oxide

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Graphene is composed of carbon atoms arranged in a hexagonal pattern, exhibiting excellent electrical conductivity. Graphene oxide (GO), on the other hand, presents its conductivity modulated depending on the degree of reduction and doping. Additionally, it can be doped. This nanomaterial can be applied in various areas, such as capacitors, batteries, transistors, sensors, among others.

This work shows the study on majority charge carriers in graphene oxide in relation to its level of oxidation and eventual doping by the presence of metallic nanoparticles. For this purpose, a thin film of GO was deposited on a glass substrate using the spray coating technique, and its sheet conductivity was measured using the Van der Pauw method. Finally, the type of carrier was determined through the Hall effect using a static magnetic field of approximately 1 T.

Study of gas flow in a gas aggregation system to produce nanoparticles

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In recent years, materials science and technology use advanced techniques for production and characterization of nanoscale structures. Metallic nanoparticles (NPs) are notable for their electrical, magnetic, and optical properties, leading to innovative applications in several areas.

In this work, we are conducting a computational study of the nanoparticle production process used in the Magnetic Materials Laboratory of IFUSP (LMM). We use a nanoparticle generator built to operate as a new gun of a commercial magnetron sputtering system (AJA International). This equipment has been used to produce NPs of magnetic or plasmonic materials using the gaseous aggregation method.

Our group has been working on routines to simulate the aggregation process of atoms removed from the target using a Monte Carlo approach. To date, our routine considers basic translation and collision processes of the gas and the metallic NPs. In this way, we are using a simplified model for the pressure and velocity distribution data of the atoms that support the sputtering and gas agglomeration process.

In order to improve our understanding of the growth process, we performed a computational study of the carrier gas flow on the NP generator. Considering this objective, simulations were carried out using Elmer FEM software, which made it possible to improve the design of the NP gun, and resulting in an equipment with a more stable aggregation process. In the current stage of the study, we are integrating simulations of the NP growth process with the gas flow, with the aim of evaluating the compatibility of simulation results in different geometries with experimental data. This analysis will allow us to compare the effects observed experimentally with the results of the simulation routine.

Study of photocatalytic activity of nitrogen doped TiO2NTs

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With industrialization and urbanization, the inappropriate disposal of waste in effluents has become a constant problem. Thus, to minimize the impacts caused by this act, some technologies have been developed, such as those based on advanced oxidative processes (AOP). Belonging to the AOP, the heterogeneous photocatalysis process uses light irradiation on an inorganic semiconductor (for example, TiO2) to cause the excitation of electrons from the valence band to the conduction band, which are responsible for the decomposition of organic pollutants in the aqueous medium through the oxidation process. However, due to its high band-gap value (~3.2 eV), this material presents low catalytic photo-efficiency within the radiation range of the solar spectrum [1]. For this reason, some studies are focused on the doping of these films with nitrogen (N) in order to promote the reduction of the bandgap and increase the radiation absorption range by the semiconductor. Allied with this, nanotubes (NTs) have better photo-energy efficiency than nanoparticles or other dimensional structures. In this way, a study of the production and characterization of titanium oxide nanotubes (NTs-TiO2), obtained by anodic oxidation technique, and doped with nitrogen through immersion in ammonia solution (NH4) besides a study of methylene blue degradation using the obtained nanotube arrays were realized. The nanotube arrays were characterized by Raman, XRD, SEM, EDS and XPS techniques. To evaluate the photocatalytic activity of the nanotubes, the methylene blue (MB) degradation study. It was observed that there was interstitial and substitutional addition of nitrogen in the crystalline network (approximately 0.1%) of the NTs, which promoted an improvement in the photocatalytic activity of the films and may be related to a possible reduction of the bandgap of the material.

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STUDY OF SILICONE OIL CROSS-LINKING PROCESSES BY PLASMA JET TO PRODUCE HYDROPHOBIC COATINGS ON CARBON STEEL

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Abstract:
Siloxanes have been widely applied as liquid-repellent coatings, due to their relatively low surface free energy [1]. It has been recently demonstrated that hydrophobic siloxane coatings can be readily deposited by the plasma activation of silicone oil. This process, performed at room temperature, is a potential strategy for improving the wetting of aqueous solutions or paraffin on the surface of steel [2]. In this work, siloxane coatings were applied on the surface of carbon steel using an atmospheric pressure air plasma jet. The films were deposited in order to minimize contact with moisture, investigating the influence of pre-treatments on the roughness, wettability and free energy of the surfaces. Surface energy of samples was characterized by contact angle analysis in water, di-iodomethane and glycerol, while roughness measurements were performed by AFM. Improvements in the hydrophobicity and oil-phobicity were observed after treatment, with contact angles in water close to 100° and a reduction of up to 10 J/m2 in the total surface energy. These results demonstrate a decrease in the wettability of the surface of the treated specimens, associated with the low surface energy of siloxane chains and a reduction in surface roughness.

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Surface Analyses Approach for a Comparative Study of Reactivity Between Metallic Surface and Degreasing Solutions

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Nowadays, metallic coatings are extremely used in the most diverse applications. The objectives of this type of coating are also varied, from improving the visual aesthetics of an alloy to the search for higher levels of protection against corrosion and erosive wear.

These coatings are often made from different proportions of Zinc, Magnesium and Aluminum. Industrially speaking, this layer greatly improves the performance of various products, such as car parts. However, the three main metals present in these protective layers are relatively easily oxidizable. The metallic oxides formed on the surface, despite protecting the matrix steel, can interfere when applying varnish, paint or other products on the surface.

In order to avoid this behavior, specific degreasers are used to carry out a surface treatment before the product is applied to the coating surface. This work aims to better understand the functioning of these degreasers on different surfaces of metallic coatings produced by Arcelor Mittal. The main goal is to try to correlate their effectiveness with surface parameters of the coating (for example, roughness).

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Surface-enhanced Raman scattering using a bilayer substrate of DLC and Silver for melamine detection

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Surface-enhanced Raman spectroscopy (SERS) is a surface-sensitive technique that enhances Raman scattering by molecules adsorbed on rough metal surfaces or nanostructures. SERS has shown excellent capability for rapidly detecting and identifying analytes at very low concentrations. In this work, SERS-active arrays were constructed with a DLC underlayer nanostructured with a silver overlayer. A previous study using the same structure showed the possibility of identifying R6G in concentrations up to 10-18 M[1]. The present study aimed to investigate the plasmonic enhancement arising from the bilayer (DLC/Ag) hierarchical structure for detecting melamine, a nitrogen-rich compound intentionally used as a protein adulterant in milk for economic benefits [2]. The elevated SERS was attributed to the formation of effective hot spots due to the synergetic effect resulting from the increased roughness of the outer Ag film and the nanostructured DLC film. We show that optimizing the SERS enhancement factor is possible without significantly altering the operating plasmon resonance wavelength. In addition, our bilayered substrates showed long-term stability. These findings demonstrate the potential of using DLC/Ag configuration to morphologically optimize SERS substrates for sensing applications that demand huge SERS enhancement and adequate chemical stability.

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Synthesis and characterization of NaBiS2 for application in energy conversion devices

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The use of solar energy in photovoltaic form is considered a promising strategic alternative for green and sustainable development. In this way, many materials have been studied over decades. Perovskites are materials that have aroused great interest in the scientific community for providing efficiencies above 25% [1]. However, these inorganic materials are unstable and do not provide durability to the manufactured devices, in addition to using lead, which is toxic. The new trend is to modify these structures looking for greater stability or to look for non-toxic materials [2]. In addition to perovskites, chalcogenides, kasterites and ternary alloys are potential candidates [3]. In this work we investigated the chalcogenide, NaBiS2, using the hydrothermal route, known as a simple methodology, varying the sulfur precursors. The films were obtained using the spin coating deposition technique. The developed materials were investigated by various XRD, UV-Vis, FTIR, XPS and SEM techniques. The solar cells will be manufactured to evaluate the quality of the materials and verify the potential use of the developed materials.

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Synthesis and Characterization of TiO2/GE nanocomposite films deposited on AISI 304 stainless steel

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TiO2 and TiO2/exfoliated graphite (GE) films were prepared by the sol-gel method and applied to the surface of AISI 304 stainless steel using the cold spray technique. Initially, natural graphite was subjected to the liquid phase exfoliation process in an aqueous solution containing isopropanol and acetone under UVC irradiation, where expanded graphite was obtained. A solution containing titanium isopropoxide and ethanol was prepared to obtain the sol. The exfoliated graphite, after drying, was then added to the solution in concentrations between 2.5 and 10%, mass/volume ratio. The films were dried in an oven at 100ºC and heat treated at temperatures between 400 and 500 ºC in a tubular oven, under an argon atmosphere. Electrochemical techniques, field emission gun scanning electron microscopy (SEM-FEG), Raman spectroscopy and X-ray diffraction were used to characterize the coatings. The results confirm the formation of the anatase phase in all films and the presence of GE in the composite films. The films have a cracked morphology and TiO2 and GE particles on the surface of the sample were present. The samples were evaluated using potential x time and linear polarization techniques in a 3.5% NaCl aqueous solution at room temperature. The corrosion resistance of the samples increased compared to the substrate, suggesting that the coating act as a physical barrier [1].

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Synthesis of Fe-MCM-41 mesoporous material from mining tailings sludge.

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On November 5th, 2015, the Fundão dam in Mariana/MG broke up, releasing around 50 million m^3 of mining sludge into the Doce River. The sludge, composed of potential toxic elements (PTE) and iron and silicon oxides [1], is an exciting material for synthesizing mesoporous materials such as Fe-MCM-41. The mining sludge was collected in Bento Rodrigues district, near the accident location [2]. Fe and Si were extracted from the sludge using an alkaline fusion process and a heating mix of NaOH and $NaNO_3$. Fe-MCM-41 was synthesized by the sol-gel method, as the sludge extract was added to a hexadecyltrimethylammonium bromide solution. The resulting solution had the pH adjusted to 10.2, heated in an oven, cooled, calcined, and subjected to physical characterizations (XRD, N_2 Physisorption, UV-Vis, and TEM). It is a material made from reuse, so it may have fewer pores and a less defined organization. However, XRD analysis indicated the presence of diffraction planes that can be attributed to a network structure with a hexagonal arrangement of pores, which is characteristic of this type of material. The N_2 sorption isotherm was type IV, characteristic of mesopore filling, with diameters ranging from 2.93 to 4.92 nm and surface area between 291.5 and 494.0 $m^2\ g^{-1}$. The UV-Vis spectra present an absorption band in the 200 to 350 nm range, characteristic of the isolated tetrahedral coordination of Fe^{3+} [3]. TEM analysis showed a tubular characteristic of the pores arranged in a hexagonal shape. Fe-MCM-41, synthesized from the reuse of toxic mining waste, presents advantages from an environmental point of view, becoming helpful in treating water contaminated by EPT from the sludge itself, monitoring, and remediation of contaminants.

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Synthesis of PUF/Epoxy Microcapsules for Self-Healing Coatings Application

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Metals used in the petroleum industry, including electrodes, can undergo mechanical damage and corrosion during transportation, storage, and usage. Hence, the application of polymeric coatings, including those derived from biological sources, can extend the lifespan of these materials [1]. To address limitations such as micro-cracks during application, self-healing microcapsules can be incorporated into the coating matrix, repairing damages and reducing costs [2]. In this study, poly(urea-formaldehyde) (PUF) microcapsules containing encapsulated epoxy were produced via in-situ polymerization using the oil-in-water emulsion technique, to be added to bioepoxy for the production of eco-friendly self-healing coatings. The produced microcapsules were characterized using Fourier-transform infrared spectroscopy (FTIR) and scanning electron microscopy (SEM). The analyses confirmed the production of PUF/epoxy microcapsules with suitable average diameter for use in coatings.

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Synthesis of self-cleaning thin films based on niobium pentoxide: effect of the number of layers on the self-cleaning properties

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Surface cleaning, although crucial for maintaining hygiene, is considered a costly technique. In this scenario, research centered on the development of self-cleaning surfaces has gained visibility, and semiconducting metal oxides have been explored to obtain hydrophilic and photocatalytically active coatings. A potentially promising semiconductor for obtaining these coatings is Nb_2O_5 [1], but there are gaps in its behavior for this application. Therefore, the present work proposes the preparation of Nb_2O_5 thin films via sol-gel deposited on a glass substrate by dip-coating with 3 and 6 layers, in order to investigate the influence of this parameter on the coating's self-cleaning performance. To this end, the films obtained were characterized by Scanning Electron Microscopy, X-ray diffraction, ultraviolet-visible spectroscopy, contact angle measurements and photocatalytic testing. The results suggest that amorphous, nanometer-thick, transparent and homogeneous Nb_2O_5 thin films were successfully obtained. Photocatalytic tests using methylene blue showed that the number of layers had little influence on its degradation efficiency. The 3 and 6 layer films showed maximum UV light transmittance of 75% and 67%, and a reduction in the contact angle from 50.77° to 11.27° and 9.10°, respectively, showing their hydrophilic nature. That said, the Nb_2O_5 thin films synthed were promising as a self-cleaning surface, and the increase in thickness led to an improvement in the hydrophilic performance of the coatings.

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Tin Oxide as Active Material for VOC Sensors

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Sensors based on metal oxides to detect Volatile Organic Compounds (VOCs) at high temperatures (200°C to 400°C) are widely explored in the scientific community. However, research on metal oxide-based sensors at room temperature is still under development and represents a promising area of investigation due to potential commercialization. This study aims to investigate gas sensors, operating at ambient temperatures or below 100°C, based on tin oxide SnO2 nanoparticles to detect VOCs vapors. The material's dispersion is explored through concentration of nanoparticles, composites and solvents, being deposited by casting on top of interdigitated gold electrodes and used as active layer on the studied sensors. The devices are characterized through electrical impedance spectroscopy, from where it is possible to observe significant variations in the electrical response concerning the concentration of different alcoholic vapors, such as ethanol and isopropyl alcohol, in inert atmosphere. This study has the potential to make significant contributions to the field of VOC sensing by reducing the energy requirements for SnO2 sensors without significant loss on sensitivity, offering a more accessible and energy-efficient alternative to high-temperature sensing methods.

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Tribocorrosive behavior of a white cast iron in iron ore slurries using the Miller machine test

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The interaction between corrosion and abrasion could result in material losses greater than those caused by each phenomena individually, highlighting the importance of studying their synergy. In mining environments, abrasion wear and corrosion are common, especially where ore slurry processing takes place. Although it is known that different iron ores have different abrasiveness under dry conditions [2], the effect of ores slurries on abrasion-corrosion behavior is still unclear. In this context, this study investigated the tribocorrosive behavior of a white cast iron in contact with four different iron ores slurries. The main objective was to evaluate the tribocorrosive behavior using the Miller machine test following the ASTM G75 standard. The wear rate of materials is closely related to surface properties and the hardness of abrasive particles. Jaspilite iron ore, which had a high silica content, together with Brazilian normal sand, which has the highest silica content among abrasives, exhibited greatest abrasiveness and consequently promoted the highest wear rate of white cast iron. Additionally, the two ores with the highest abrasiveness were tested in a slurry with the addition of 3.5% NaCl to simulate a more corrosive condition. The results showed that with the addition of 3.5% NaCl, a significant increase in mass losses was observed: 7% for the jaspilite and 77% for compact hematite. These laboratory results showed that corrosion causes an increase of mass losses of white cast iron samples, giving a picture of the situation occurring at mining field, highlighting the importance of further studies of abrasion-corrosion synergy.

Yttrium and Hafnium modified aluminide coatings for γ-TiAl alloy by halide activated pack cementation

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During the last decades γ-TiAl has been investigated due to the combination of its high mechanical strength and low density with a great potential to replace Ni-based superalloys in aircraft gas turbine and turbochargers components. However, the utilization of this class of materials at high temperature exceeding 500°C is limited by their poor oxidation resistance which can be achieved through o modification of their chemistry composition or the use of coating techniques [1;2]. Thus, the aim of the present study was to produce aluminide coating for the TNM-B1 alloy, with nominal composition Ti -43.5Al -4Nb -1Mo -0.1B (at. %), modified by Hf and Y using the halide activated pack cementation technique to improve its resistance against oxidation at temperatures above 750°C. For forming the coatings, the pack mixtures activated by $BaCl_2.2H_2O$ with the coupons to be coated introduced in vacuum sealed silica tubes. The cementation process was performed by placing the sealed vessels in muffle furnace at 1000°C for durations from 9 up to 36 hours. The obtained coating was characterized by means of XRD and SEM/EDS techniques. The microstructure of the substrate consisted of (α;β)-Ti, γ-TiAl and α_2-Ti_3Al phases. The formed coating are multilayered composed of $TiAl_3$ at their outer part and $TiAl_2$ in the inner regions. They are dense, uniform, totally covering the substrate with good adhesion and free of defects. Hafnium and yttrium were dispersed or dissolved in the layers. The coating growth followed with parabolic with rate constants (k_p) of the order of magnitude $10^{-9}cm^2/s^{-1}$.

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AM01-Advanced Materials

Characterization and analysis of leaching routes for iron/nickel reduction slag

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The mining sector is crucial to the country's economy, contributing significantly to technological and scientific development, although it has negative environmental impacts due to the waste generated [1]. This study focuses on designing a possible recycling route for mining waste, using leaching methods in accordance with technical standards, in order to classify the slag resulting from the reduction of Iron/Nickel (FeNi) and achieve the recovery of metallic waste, adding value to the mining process and contributing to the sustainable disposal of mining waste [2]. The sample was first comminuted by jaw mills (primary crushing) until it reached a particle of #0.3mm. According to the recommendations of the standard (NBR 10005) [3], it was shown that the 1 N NaOH solution is the most suitable leaching agent for an aliquot of 100g of the material. A Wagner shaker (18h, 30 rpm) and a vacuum filtration system were used for collection after the test. The materials retained after drying, the filtered and washed solutions were separated for analysis by XRD, XRF and ICP. The XRD revealed the presence of Forsterite, a mineral of magnesium and iron silicates, with elemental concentrations of Si, Mg, Fe and Ni of approximately 19%, 18%, 15% and 0.14%, respectively. With regard to the total chromium parameter, a value below the 5mg/L established by standard NBR 10004 was found. The levels of Al, Fe and Mn were above the standard allowed by the same regulation.

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Deviations in the Relation of Grain Size and Strength for Magnesium Alloys

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Magnesium and its alloys present the lowest density among all structural metals. Consequently, using them in vehicles could be an alternative for reducing carbon dioxide emissions since they could be lighter and save fuel. However, the main drawback of magnesium being widely used in engineering applications is its low mechanical strength. A common way to improve the strength of metals is by refining their grain. Hall-Petch Equation establishes the influence of grain on the mechanical properties of metals as the strength is inversely proportional to the square root of the grain. Then, the mechanical strength of magnesium and its alloys could be enhanced by grain refinement down to nanometers by Severe Plastic Deformation. Nevertheless, there is evidence that pure magnesium shows grain refinement softening at grains smaller than 1 µm and a strength saturation on magnesium alloys. Furthermore, experimental evidence shows that more parameters, such as temperature and strain rate, influence the relation between grain and mechanical strength. Therefore, the validity of the Hall-Petch equation in ultrafine grains for magnesium alloys is not well defined. The present study proposes to investigate this relationship by considering magnesium alloys with different grains at various strain rates and temperatures. Thus, samples of magnesium alloys are processed by high-pressure torsion, and some of them are annealed to expand the grain range. Data from the literature on different magnesium alloys are used to expand the conclusion. The results reveal a different Hall-Petch slope in the ultrafine grains region, leading to an inverse Hall-Petch behavior. The modified grain boundary sliding mechanism proved to be more appropriate regarding grain and strength of grain less than 1 µm. The grain refinement softening was more prominent in low strain rates. The best combination of strength and elongation was detected in grain in the 2 µm and 8 µm range.

Effects of electron beam irradiation on the electrical properties of tin oxide nanopowders for CO detection

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Within the realm of solid-state gas sensors, tin oxide emerges as a significant player, existing in two distinct forms: tin (II) oxide (SnO) and tin (IV) oxide (SnO_2). SnO is intrinsically p-type, while SnO2 is n-type[1]. SnO2 is widely used in chemical sensing, particularly for carbon monoxide detection. Nevertheless, recent attention has shifted towards SnO due to its potential as an alternative to SnO_2 in high-performance gas sensor devices[2]. This study focuses on the electrical characterization of SnO samples subjected to various treatments: (I) pure SnO, (II) thermally treated SnO, (III) electron beam irradiated SnO, and (IV) thermally treated and electron beam irradiated SnO. SnO powder was synthed via microwave-assisted hydrothermal (MAH) method under a reductive atmosphere. A portion of the original SnO powder underwent thermal treatment and electron beam irradiation. Characterization techniques included XRD, Raman spectroscopy, SEM, and UV–Visible spectrophotometry. An alumina wafer with a titanium adhesion layer and a thick platinum film served as the substrate and electrode, respectively. Films were deposited using a screen-printing-like method. Measurements were conducted using an optoelectronic device for semiconductor material characterization under controlled temperature and pressure. The MAH method proved versatile, yielding SnO micro-plates under a reductive atmosphere. Thermal treatment led to the transformation of SnO to SnO_2 nanopowder, while electron beam irradiation induced structural distortions[3]. Electrical characterization revealed enhanced conductivity in air, vacuum, and CO atmospheres post-thermal treatment and electron beam irradiation, attributed to increased charge carriers, primarily oxygen vacancies within the material

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Enhancing Bioprinting Fidelity by Optimized Rheology of CMC/CNC Hydrogels

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This research investigates the cutting-edge in 3D bioprinting, where the integration of advanced materials and precise control mechanisms owns the fabrication of structures that mimic natural tissue properties. In this way, our study focuses on the use of carboxymethylcellulose (CMC) and cellulose nanocrystal (CNC) hydrogels as promising bioinks, owing to their biocompatibility, modifiable mechanical properties, and supportive environment for cell growth. The hydrogels' optimized rheological properties bolster the bioprinting process's precision and stability. A setup with a load cell was used to monitor and adjust the printing parameters to the ink used. This ensures consistent bioink deposition and the printed structures' structural integrity, even when dealing with complex, cell-laden structures. Our finding shows the tuned rheological properties of CMC/CNC hydrogels significantly improve the printability and fidelity of 3D-bioprinted structures. This, in turn, facilitates the creation of tissue constructs with enhanced cellular viability and function. These advancements hold promise in developing tissues for medical use and models for testing drugs.

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Evaluation of the Nematicidal Action of Pectin and Papain Films for Seed Treatment

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Various innovations of interest to agriculture are taking place in the input and processing industries, and in the transportation and storage of agricultural production[1-3]. This work focuses its efforts on the agricultural input production sector. To this end, pure pectin films and their formulation with different levels of papain were produced. Initially, pectin (3% m/m) was dissolved in deionized water and the mixture was thoroughly homogenized in a magnetic stirrer for 2 hours. Glycerol was then added to the biopolymer solution in a proportion of 30% w/w (in relation to the mass of pectin) and stirred for a further 30 minutes. Finally, to prepare the solutions containing papain, different proportions of the enzyme were added (0.5, 10 and 15% w/w) in relation to the mass of pectin and stirred for a further 15 minutes. Finally, 50 mL of the PEC and PEC/papain formulations were poured into Petri dishes (15 cm in diameter). The plates were dried in an air-circulating oven at 35°C for 24 hours. The dried films were removed from the plates and stored in ambient conditions (approximately 4°C and 53% relative humidity) for 3 days before characterization. Water vapor permeability was investigated for all formulations at 25oC and 75% relative humidity. In addition, the in vitro nematicide action was evaluated using the nematode Panagrellus redivivus. The results indicate that the films have good water vapor barrier properties and effective nematicidal action, making it possible to develop applications for seed coating.

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Feasibility of application of metal oxide nanoparticles in Oriented Strand Board (OSB) panels

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The utilization of nanotechnology in Oriented Strand Board (OSB) panels has been recently studied to enhance the physical-mechanical properties of the panels, as well as to favor the polymerization process of the resin used in their production [1]. In this regard, the addition of aluminum oxide nanoparticles emerges as a procedure with potential application in wood-based OSB panels [2], aiming to add value to the material and tailor it to different proposed applications. The study aimed to evaluate medium-density panels (650 kg/m^3) produced with residual reforestation wood containing 13% polyurethane resin based on castor oil and 1% aluminum oxide nanoparticles by applying a pressure of 5 MPa, temperature of 100 ºC and pressing time of 10 minutes. The results were compared according to the values contained in the EN 300:2006 standard, recommended for the use of panels in dry conditions. The addition of aluminum oxide nanoparticles promoted an increase in the internal bond parameter of the wood particles, indicating improved heat conduction provided by the addition of nanoparticles and contributing to better agglomeration of the wood particles, resulting in OSB panels with a compression ratio close to 4.

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Fixed-bed adsorption studies for drug removal onto an eco-friendly low-silica nanozeolite

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The discharge of drugs generated environmental concerns, since they are toxic, chemically stable, poorly biodegradable, and difficult to remove from conventional wastewater treatments [1]. The present study aims to evaluate the adsorption capacity of an eco-friendly nanozeolite (nSOD) in the removal of the escitalopram oxalate drug through fixed-bed adsorption. nSOD was hydrothermally synthed (180 °C / 6 hours) from alum sludge and rice husk, being then characterized by XRD, ATR-FTIR, N2 porosimetry; ZP, pH_{ZCP}, EDX, and TGA. Adsorption was carried out on a system operating at 40 mL min^{-1}, pH 6.97, and bed mass 0.8 g [3]. The data were fitted to the Yoon-Nelson, Adams-Bohart, and Clark models. XRD diffractograms identified sodalite/analcime phases. ATR-FTIR spectrum showed (a)symmetric stretching/bonding vibrations of zeolitic frameworks from 1200-450 cm^{-1}. Moreover, nSOD showed good physio-chemical stability (-29.2 ± 1.4 mV), textural properties (SBET = 16 ± 1.0 m^2 g^{-1}, Vp = 12.9 ± 0.7 cm^3 g^{-1}, DP = 12.9 ± 1.0 nm), and pHZCP 8.30. EDX analysis reported Na (8.8 %), Al (11.1 %), Si (12.1 %), and O (60.4 %). TGA confirmed the thermal stability of nSOD, reporting weight loss of 5 % until 400 °C and no more after this. The overall drug removal was 60.4 % (5.4 L treated) after 180 min. The data were best fitted to Adam-Bohart model ($R^2 = 0.92$ / R^2_{adj} = 0. 91). Future studies intend to use nSOD at different values of pH (4- 9), flow rate (40-120 mL min^{-1}), and adsorbent mass (1-3 g). Therefore, eco-friendly nanozeolites can be successfully used for the adsorption of persistent drugs, being a suitable nanoadsorbent for large-scale processes.

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LANTHANUM: PREPARATION OF SPEC PURE STANDARD AND SYNTHESIS OF PEROXIDE

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Abstract

The following studies are presented: Preparation of lanthanum oxide for use as spec pure standard and synthesis and characterization of lanthanum peroxide. Using the fraction precipitation and cationic ion exchange techniques, with EDTA as eluent, it was possible to obtain pure lanthanum oxide ≥ 99.9%, whose Impurities were in the same level as in the imported standard. The yield for the combined techniques was reasonable high (≥ 80%). The raw material in the form of mixed rare earth carbonate (La2O3 45%) comes from by commercial rare earth concentrate. Emphasis was given to the analytical control to assure the purity of La2O2≥99.9% by spectrophotometry and mass spectrometry. A study was made for the optimization of dissolution lanthanum carbonate, from the lanthanum spec pure standard obtained here, as function of the concentration of ammonium carbonate and ammonium carbonate\ammonium hydroxide searching the maximum solubilization of the lanthanum carbonate. The lanthanum peroxide was prepared by the addition of hydrogen peroxide to the complexed soluble lanthanum carbonate. These studies included also the determination of active oxygen, the total lanthanum oxide by gravimetry and complexometry and the C, H, O contents by microanalysis. The peroxide was also investigated by infrared spectroscopy and thermal analysis. The analytical data collected allowed to conclude that the stoichiometric formula for the peroxide is La2O2(CO3)2 1.25H2O. References

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Synergistic effect of the addition of recycled carbon fibers and carbon nanotubes on the electromagnetic properties of composites with epoxy resin

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Carbon fiber reinforced polymer (CFRP) has been increasingly used in the automobile industry to reduce vehicle weight and improve performance. As a result, there is a significant increase in waste production from this material. Carbon fibers (CF) can be recovered by mechanical recycling and used to prepare other parts. In this work, hybrid epoxy resin matrix composites were developed with the addition of recycled CF and multi-walled carbon nanotubes (MWCNT) to obtain a material that can be used as a radar-absorbent material (RAM). Composites of epoxy resin with the addition of 20 wt% of CF and 0.5 and 1wt% of MWCNT (NC7000, Belgium) were prepared by mechanical mixing into the epoxy components, set in silicon molds, and then cured in an oven. After preparation, the samples were characterized by field emission gun scanning electron microscopy (FEG-SEM, TESCAN - MIRA3) and the electromagnetic interference shielding (EMI SE) in the X-band (8.2-12.4 GHz) was measured in a vector network analyzer (VNA, Agilent Technologies, model PNA-L N5235A) with a coupled waveguide (WR-90). Adding 1 wt% of MWCNT promotes a total attenuation (SET) of 2 dB. Adding 20 wt% of CF with 1 wt% of MWCNT in the epoxy resin composition promotes a synergistic effect, increasing the SET values by 25 dB. These hybrid composites are a promising material for future EMI SE applications, offering substantial attenuation.

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The influence of load and speed on the coefficient of kinetic friction and temperature in a polyamide 6 slide bearing

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Engineering polymers how polyamide 6 (PA6) have been used in the manufacture of various types of components, mainly where chemical inertia, noise reduction and low weight are necessary. In this study, to understanding the effects of load (F) and speed (V) on the coefficient of kinetic friction and temperature of PA6 sliding bearings, assemblies composed by a PA6 slide bearings and carbon steel shafts both manufactured by machining, operating without lubrication was tested. A factorial planning 2^2 with a central point was used, as inputs to perform the tests the load (60, 75 and 90 N) and speed (0.48, 0.60 and 0.72 m.s-1) ranges, were variated and the total time for each test was 120 minutes. Based in these conditions the friction coefficients ranges between 0.2 (75 N at 0.6 m.s-1) and 0.31 (60 N at 0.72 m.s-1) and temperatures ranges between 30.8 °C (90 N at 0.48 m.s-1) and 36.7 °C (60 N to 0.72 m.s-1) were obtained. For the friction coefficient, the load is the factor of greatest influence, decreasing the friction. While the sliding speed is the factor of greatest contribution to the increase in temperature over time. The morphological analysis of the polymer-metal contact interface was performed by SEM, and reveals that with the increase in the severity of the test there was a greater removal of material, resulting in the bearing surface flatter polymer, greater clearance of the tribological shaft-bearing pair and consequently decrease in the coefficient of friction over time.

The potential use of waste plastic (HDPE) from recycling company as a raw material in the production of medium-density particleboards

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The use of industrial and agroforestry waste and/or by-products as raw material for the production of more sustainable materials has been widely studied in recent years. Within this context, the use of lignocellulosic waste to manufacture particleboards stands out for presenting research that indicates its feasibility of use and performance favorable to the regulations established for these composites, such as the use of sugarcane bagasse [1]. New studies are being developed for this type of material, evaluating the introduction of non-lignocellulosic raw materials in the production of hybrid panels, such as waste plastics. When subjected to higher pressing temperatures, these panels show performance improvements due to the melting of the plastic, which contributes to better particle agglomeration and a reduction in voids [2]. This study aims to evaluate the physical and mechanical performance of hybrid panels, using waste plastic (high-density polyethylene) from a recycling factory, in consortium with sugarcane bagasse particles. Panels were produced with an average density of 750 kg/m³, using a proportion of 80% by mass of bagasse particles and 20% of residual plastic, with the particles being agglomerated with PU resin based on castor oil (12% content). As production parameters, a pressure of 5 MPa and a pressing temperature of 200 °C were applied for a period of 10 minutes. Through physical and mechanical tests, it was possible to observe the contribution of melted plastic to the performance of these panels, complying with the ISO-16893 (2016) standard for structural use in dry conditions.

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BS01-Pioneering Materials Solutions for Health Challenges

Advancements in Tissue Engineering: The Role of 3D Printing of Biomaterials

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Tissue engineering has advanced significantly with the use of 3D printing of biomaterials, enabling the creation of personalized structures for cell regeneration. This technology facilitates the precise reproduction of biological tissues, promoting better integration with the body. The combination of natural and synthetic polymers in 3D printing offers new possibilities for the development of functional and bioactive scaffolds. These advancements have the potential to revolutionize regenerative medicine, creating more efficient and accessible solutions. The future of the field promises personalized treatments and greater success in repair therapies.

Different food-grade bigel systems as carriers for bioactive compounds

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<div>Bigel systems are new two-phase gels characterized by two gelled phases of different polarity, generally the aqueous phase (hydrogel) and the oil phase (oleogel), with three-dimensional semi-solid structures. Similar to emulsions, bigels can be presented as oleogel-in-hydrogel systems and hydrogel-in-oleogel systems. The properties of bigels are highly dependent on the structures of the hydrogels and oleogels and the hydrogel/oleogel ratios. Various biopolymers for the formulation of hydrogels and oleogels have been tested for the formulation of these matrices. Recently, food-grade bigels formulated with hydrogels based on agar and xanthan gum, or gelatin and xanthan gum, and sunflower oil oleogels structured with beeswax have demonstrated good stability and promising properties for food formulations. Bigels have been widely investigated over the past decade, especially for pharmaceutical and cosmetic purposes and very minor application is found in the food area, however, a field with potential for increasing expansion. In this area, most of the work developed has been limited and restricted mainly to bigels as substitutes for saturated and trans fats in food formulations. However, more recently, efforts are being made to advance knowledge about bigels as delivery and distribution systems for food bioactive compounds. Compared to other emulsion systems, oleogels, and hydrogels, bigels have demonstrated great advantages as stable carriers of bioactive compounds. Part of its successful application is justified by the fact that its constituents, i.e., oleogels and hydrogels, are sound delivery systems for bioactive compounds with different polarities, with the potential to deliver lipophilic and hydrophilic ingredients individually and simultaneously. As strongly evidenced, the applicability of bioactive compounds in bigels goes beyond improving their availability or transport. These systems are also capable of providing better protection to these labile compounds.

Inorganic semiconductors- based materials for health applications: progress, challenges, and prospects

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The spreading and adhesion of pathogens (bacteria, virus, fungus) are a major cause of nosocomial or health care associated infections. Developing safe and effective approaches to combat infections caused by bacteria and biofilms has become an urgent clinical problem. Nanomaterials of inorganic semiconductors exhibit antibacterial activities under ambient illumination that result in cell membrane permeability and disorganization, representing an important opportunity for health-related applications. Thus, to broaden this area, this talk first discusses the essential characteristics, potential mechanisms, and structure–function relationship between inorganic semiconductors and pathogen adsorption and chemical reactivity based on the structure and properties of the exposed surfaces at the morphology, metal center, and ligand functionalization. Moreover, the stability, utilization safety, and compatibility of inorganic semiconductors are illustrated in selected examples investigated in our Labs. The current development and progress are also summarized to highlight their practicability by the joint use of advanced experimental techniques and first principles calculations. Finally, we propose future opportunities and challenges from materials design and manufacture to the computational prediction of inorganic semiconductors. It is anticipated that our work will expand the interest of researchers for more impact in this area.

Microalgae as new ingredient for biotechnological products, stretching the knowledge of material sciences

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Microalgae have emerged as a promising sustainable resource for the development of innovative biotechnological products, offering a diverse array of bioactive compounds and materials with unique properties. The aim of this work is explore the potential of microalgae as new ingredients in various industrial applications, emphasizing their role in enhancing material sciences. We will delve into the biochemical pathways of microalgae that allow for the extraction of valuable compounds, which can be utilized in the food, pharmaceutical, and cosmetic industries. Additionally, we will discuss the advancements in bioprocessing techniques, including cultivation, extraction, and modification of microalgal biomass, which have led to the creation of novel biotechnological products. By investigating the synergy between microalgae and materials science, this presentation aims to highlight the transformative potential of these organisms in developing eco-friendly solutions that address contemporary challenges in sustainability and resource efficiency.

Biomimetic hydrogels for 3D bioprinting cardiac patches

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The urgent need for solutions in cardiac regeneration post-myocardial infarction underscores the critical importance of innovative approaches to restore heart function and improve patient outcomes. The aim of this study was to combine bioactive materials and cells with 3D bioprinting technology to fabricate cardiac patches capable of repairing injured cardiac tissue. Methacrylated gelatin (GelMA), derived from denatured collagen, forms a hydrogel that is biocompatible, photo-crosslinkable, and enzymatically degradable, providing an environment where cells can adhere and proliferate. Various compositions of GelMA-based bioinks have been explored, with additional incorporation of bioactive compounds such as platelet-rich plasma (PRP), fibronectin/elastin/laminin (FEL), and decellularized extracellular matrix (ECM) to promote cellular functions. Rheological tests demonstrated that GelMA and its blends exhibited favorable shear-thinning behavior, predicting their printability through material-extrusion technology. Scanning electron microscopy (SEM) images revealed the microporous structure of the hydrogels, which provides a suitable environment for cell adhesion and proliferation. The elastic modulus of the materials was obtained by compression testing and displayed similar values to native myocardial tissue. For biocompatibility assessment, mesenchymal stem cells and endothelial cells were included into the hydrogels (10,000 cells/50 µL) and after crosslinking with UV light they were maintained for 1 and 7 days in culture. Cell morphology was analyzed by fluorescence microscopy while cell viability was verified by ATP quantification and live/dead assay. The incorporation of ECM, FEL and PRP enhanced cell proliferation, compared to pure GelMA hydrogel. The bioinks were used to print a 3-layered patch with hexagonal porous and 1 cm2 , and in vitro cytotoxicity assays revealed the viability of the cells.

Comprehensive Physico-Chemical Analysis of Poly (N-vinyl caprolactam): A Thermoresponsive Polymer with Promising Applications as a Drug Delivery System in Cancer

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Poly (N-vinyl caprolactam) (PNVCL) is a biocompatible polymer synthed via radical polymerization of N-vinyl caprolactam monomer, exhibiting notable properties for biomedical applications such as bony regeneration and drug delivery. PNVCL's thermoresponsive behavior, attributed to its lower critical solution temperature (LCST), enables a sol-gel transition in aqueous mediums, facilitating the encapsulation of molecules during phase transition, thus serving as a drug delivery system (DDS). The LCST of PNVCL decreases with increasing molecular weight and solution concentration, impacting its phase transition temperature. Synthesis of PNVCL involves radical polymerization under controlled conditions, followed by purification. Characterization techniques such as FTIR and NMR confirm the conversion of monomer to polymer. Uv/Vis spectroscopy under temperature control demonstrates the LCST of PNVCL and PNVCL-SiO2, with the latter showing altered transmittance due to the presence of silica nanoparticles. Additionally, the concentration of PNVCL influences its thermoresponsive behavior, with lower concentrations requiring higher energy for phase transition. Understanding these properties provides insights for tailoring PNVCL for diverse biomedical applications. Concerning the promising physicochemical properties for a biomedical application, the next steps are the evaluation of biological assays of these materials for breast cancer.

Cytotoxicity and modulation of cell death in fibroblasts caused by Ag_2WO_4 dose and morphology-dependent

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The environmental impact of new materials must be taken into consideration in the development of emerging technologies, especially in the realm of healthcare material innovation, where the morphology/ relationship is essential. Analyzing this relationship enhances material properties and their interactions with dynamic biological systems. [1] In this study, orthorhombic α-Ag2WO4 particles were synthed by three different routes, resulting in distinct morphologies: cuboidal, hexagonal rod-like and nanometric rod-like. Possible cytotoxic mechanisms such as internalization, electrostatic interaction, ion release and ROS production were examined. Uptake tests demonstrated that the first proposed mechanism was not possible due to their negative surface charge. AW-NR exhibited autophagy in the absence of light and during photoactivation, primarily attributed to its ability to generate singlet oxygen. The cytotoxic effects of these materials were evaluated in NIH/3T3 murine fibroblast cell lines. This analysis was conducted both in the absence and presence of light. To achieve this, after material synthesis and characterization, cell viability assessments were performed using MTT salt and neutral red dye methods. Furthermore, alterations in cell morphology, nitric oxide and ROS production, cell death markers, and flow cytometry were examined after 24 hours of exposure. All samples (7.8 µg/mL) generated cytotoxic effects on 3T3 fibroblasts, such as decreased viability, changes in cell morphology, activation of oxidative stress through increased production of NO and ROS, and activation of cell death pathways (apoptosis and necrosis). White light has enhanced this effect. The nanometric rod-like morphology showed the most damage to the cells, through photo-generated hydroxyl radicals, followed by the cuboidal and hexagonal rod-like morphology.

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Development of polypyrrole (nano)structures decorated with gold nanoparticles toward immunosensing for Congenital Adrenal Hyperplasia serological diagnosis

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The National Newborn Screening Program (NNSP) is a set of preventive actions aimed at identifying disorders and diseases in neonates in a timely manner for appropriate intervention. Although essential and mandatory, the NNSP does not cover the entire national territory and thousands of newborns are not screened in time. In this context, electrochemical biosensors based on modified printed electrodes with nanostructures of conductive polymers show promise. These biosensors possess various structural characteristics that make them portable, cost-effective, highly sensitive, and compatible with modern microfabrication technologies. Congenital Adrenal Hyperplasia (CAH) is one of the diseases included in the NNSP and results from inborn errors in adrenal steroid metabolism. The most prevalent form of CAH is 21-hydroxylase deficiency, which leads to excess secretion of 17-hydroxyprogesterone (17-OHP). This biomarker is used in the initial diagnosis. In our work, polypyrrole nanotubes decorated with gold nanoparticles were electro-synthed on a school graphite substrate and screen-printed electrode (SPE) [1]. This was followed by the attachment of a self-assembled monolayer (SAM) of 3-mercaptopropionic acid and covalently linked 17-OHP antibodies. The modified substrate was applied in the development of impedimetric immunosensors as an alternative method for neonatal CAH screening at the point of care. The modified electrodes were characterized using microscopic, spectroscopic, and electrochemical techniques. The results demonstrate successful electropolymerization and deposition of the hybrid nanostructured material, enabling the SAM anchoring and subsequent covalent binding of the 17-OHP antibody. The sensor has shown potential application for the detection of 17-OHP and may be a viable alternative to the conventional methods used in NNSP.

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Development of Silver Selenite-based Semiconductors Towards Rhodamine B degradation and Antimicrobial Activity

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In the last decades, the volume of dyes manufactured – for the most diverse applications (e.g., clothing, food, pharmaceuticals, etc.) has largely increased, of which ~15% reach water bodies. This practice raises significant concerns regarding both environmental integrity and public health, causing diverse detrimental effects, including waterborne illnesses such as nausea, hemorrhaging, skin and mucous membrane ulceration, dermatitis, nasal septum perforation, severe respiratory tract irritation, and even cancer. In addition, the emergence of resistant, highly adaptable, pathogens render conventional treatments ineffective. The high risk of rapid contamination poses a threat to mankind, and has made it necessary to develop novel, economically viable, more efficient antimicrobial technologies. This study focused on the synthesis of Cu-doped silver selenites via the sonochemical method with the objective of enhancing their photocatalityc and antimicrobial properties. Characterization of the synthed materials involved X-ray diffraction, Raman spectroscopy and scanning electron microscopy. Its efficiency towards the degradation of RhB dye was assessed. Furthermore, evaluation of antimicrobial efficacy was performed against the gram-positive bacterium S. aureus and E. Coli. The antimicrobial mechanism of these materials is attributed to the generation of reactive oxygen species and the release of Ag^+ ions, which may be enhanced with the incorporation of Cu^{2+} ions. The findings of this study may have implications for the development of powerful antimicrobial materials aimed at combatting targeted pathogens, thereby contributing to advancements in microbial control strategies.

In Vitro tumor-immune system microenvironment model using 3D printed device for personalized medicine application in lung cancer

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Lung cancer is the second most common cancer and one of the leading causes of mortality, with 1,8 million deaths in 2020. The therapeutic costs for cancer treatment have surged by 402% in the last 4 years, reflecting the increasing complexity of care (WHO). Despite these escalating expenses, treatment effectiveness can vary significantly among patients. Recent studies suggest that the interaction between the immune system and cancer plays a crucial role in determining the prognosis of patients with various types of cancers (1). However, studying this interaction presents challenges, particularly in models such as immunocompromised mice.

This research project aims to develop a device for optimizing oncological treatment protocols, personalized to the patient, focused on in vitro simulation of the tumor environment and alternative to animal use. The technology, based on 3D spheroids of tumor and immunological cells, is developed in a microfluidic chip 3D printed in a biocompatible and autoclavable resin material. The device was modeled using Autodesk Fusion 360 software with a prototype of single holes for cancer spheroid and one channel to circulate monocyte into the system. Preliminary results show the success of 3D modeling and 3D printing production of device model prototypes, using different types of materials, including transparent water-washable resins and biocompatible autoclavable resins, achieving channels of up to 300 µm in diameter, 10 µm Z-axis pixel resolution, and 50 µm layers. THP1 monocyte cell were cultured and successfully circulated in the device using a peristaltic bomb. Lung cancer spheroids were also generated using the protocol described by DE SOUZA CASTRO et al (2023) (2).

The development of the system, at TRL4, has shown promising results for possible future customization and application in SUS for drug screening and/or personalized alternative treatments in in vitro reproduction of patient disease from biopsy and blood circulating cells.

Marine collagen skin dressing as an alternative to accelerate the healing of wounds

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Skin wounds could be caused by several situations and compromise patient life, leading to death in severe cases. There is a growing need for efficient skin dressing (SD) that could be effective and reduce the treatment period. Collagen (Col) is the most used biomaterial in SD, and marine sponges have been considered a potential source through studies demonstrating their benefits [1]. The hypothesis was that SD manufactured with Col from marine sponges could help the healing process of skin wounds. The aim of this project was to produce a SD made of marine Col and evaluate its biological performance in vivo. Col was extracted from Chondrilla caribensis [2], a hydrogel of Col and sodium alginate was prepared in a ratio of 50:50 and SD were obtained through casting. SDs were sterilized for 24 hours in UV light before being placed in animals. A 15mm full-thickness wound was performed in the backs of animals and they were divided into Control (CG - just injury) and Treated (SD placed for 10 days). The histological results demonstrate that after 10 days, CG had an incomplete, thick epidermis on the edge of injury, while in the reticular dermis there was a transition between granulation tissue and Col fibers. Only granulation tissue was observed in the papillary dermis. Otherwise, the treated group had a complete reepithelization process at the injury site, with a reticular dermis, an arrangement of Col fibers, and numerous sebaceous glands associated with hair follicles. It was possible to conclude that SD manufactured with marine Col had a positive effect on the wound healing process.

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Non-inferiority in vivo study of a polymer coating on CoCr stent

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Polymer coatings can be applied to medical devices, such as CoCr stents, to improve their performance against vascular complications, promote endothelial healing, and minimize the body's inflammatory response, providing greater comfort to the patient. The proposed objective of the study was to evaluate the non-inferiority of a polyurethane-based polymer as a coating for CoCr stents compared to the Bare Metal Stent, without coating, through initial visual qualitative analysis of early endothelialization up to 28 days. In this context, an experimental study was conducted in an animal model using a polyurethane-based polymer coating and Sirolimus drug, so that adjusting the concentration of these two formulations consisted of maintaining a similar viscosity so that the film would cover the entire stent delivery system. The coating was done through the immersion methodology with 3 layers of coatings interspersed with 1-hour drying for each layer. The in vivo study was conducted with 3 Moura pigs weighing between 19.0 and 22.5 kg. According to the experimental protocol, 8 stents were implanted in the carotid artery of the pigs, with 3 stents coated with polymer, 3 with polymer and sirolimus on the luminal (inner surface of the carotid artery) and abluminal (outer surface of the carotid artery) and 2 uncoated stents (BMS). After 28 days, euthanasia was performed, followed by removal of the stents. The animals with implanted stents underwent ultrasound techniques (echodoppler, IVUS, and angiography), where it was observed that the stents showed good integration with the artery wall and coverage by scar tissue. SEM analysis of the removed stents showed a good coating of the stent struts in relation to the porcine endothelium, leading to the endothelialization process. The polymeric coating used on the CoCr stent demonstrated a result of non-inferiority, but additional studies are needed to evaluate its biofunctionality.Reference:[1] UDRIȘTE, Alexandru Scafa et al. (2024),

Optimized Synthesis and Characterization of PNVCL Composite Electrospun Fibers for Biomedical Applications

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Nanocomposites is a midst to integrate properties of different components, resulting in superior hybrid materials. Harnessing the adaptability of nanomaterials, coupled with precise control over their morphology and dimensions, alongside the prospect of surface modification and functionality, captivates the attention of researchers worldwide. This convergence facilitates the creation of materials endowed with an unprecedented array of attributes. Augmented by novel processing techniques and treatments, this endeavor unlocks avenues for crafting materials with hitherto unseen physical, chemical, mechanical, and biological traits, thus aligning with the contemporary demand for innovation. Within this framework, Poly(N-vinylcaprolactam) (PNVCL) emerges as a main role a biocompatible and thermoresponsive polymer, complemented by the attributes of TiO_2 nanoparticles, is used for their chemical erosion resistance and non-toxic properties. Thus, in this work, electrotrophied mats of Poly(N-vinylcaprolactam) with TiO_2 nanoparticles were prepared in order to obtain biocompatible materials with potential biological application and drug-controlled release. PNVCL was synthed in solution by radical polymerization technique using azobisisobutyronitrile (AIBN) as initiator and TiO_2 nanoparticles were synthed by the hydrothermal method. Polymer/nanoparticle composites were prepared by simple mixing and were found to cause an increase in the lower critical temperature of solubility with respect to the polymer. The composites electrotrospun mats showed photoprotective activity, not degrading under ultraviolet radiation and its antibacterial efficacy was assessed across various bacterial strains.

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Theoretical Approach for the Development of Graphite-Based Medical Sensors

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Currently, there is a growing demand for non-invasive techniques that can identify metabolic changes and the presence of pollutants. In this context, highly sensitive sensors play a crucial role in the screening and early diagnosis of diseases, as well as in the detection of environmental pollutants. This study focuses on the utilization of graphite surface, a sp2 carbon-based nanostructured material, as a sensor to investigate its interaction with organic gases, including acetone, ethanol, and methanol [1,2]. For theoretical simulations, we employed Density Functional Theory (DFT) implemented in the CRYSTAL17 program [3]. We conducted mechanical calculations, including the optimization of graphite bulk, plane surface (001), and molecules, aiming to analyze the adsorption reaction. Our analyses revealed that the adsorption of organic molecules transforms graphite into a semiconductor material. We also observed that this transformation is enhanced when the graphite surface is doped with oxygen atoms. These results indicate that doping significantly contributes to the semiconductor character of graphite, making it highly promising for the development of highly sensitive sensors. These findings underscore the potential of graphite as a versatile and effective material for detecting organic gases, providing a solid foundation for future research aimed at creating innovative and highly accurate sensors for healthcare applications.

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Analysis of 3D Printed Biosilica and Spongin Scaffolds for Bone Tissue Repair

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Biosilica (BS) and spongin (SPG) derived from marine sponges have have sparked interest for their potential in promoting bone regeneration. Additionally, additive manufacturing, particularly 3D printing, has emerged as a promising technology for fabricating bone grafts with finely tuned interconnected porous structures, facilitating enhanced cell attachment, proliferation, and differentiation. Consequently, this study aimed to characterize the BS and BS/SPG 3D printed scaffolds and evaluate their biological effects in vitro. Physicochemical attributes of the BS, SPG and also3D printed scaffolds were analyzed through SEM, EDS and FTIR. In vitro analysis assessing the cellular viability of the MC3T3-E1 cell lineage via phalloidin/DAPI staining, alongside genotoxicity evaluation through the micronucleus assay. SEM examination unveiled distinct characteristics, including the presence of spicules in BS and the fibrillar structure of SPG. FTIR spectra indicated peaks corresponding to silicon oxide in BS samples and carbon oxide and amine in SPG samples. In vitro studies affirmed the biocompatibility and non-cytotoxicity of scaffold. The micronucleus test further substantiated the absence of genotoxicity in the samples. These findings collectively suggest that 3D printed BS and BS/SPG scaffolds may possess favorable morphological and physicochemical properties, indicative of in vitro biocompatibility.

Analysis of chitosan hydrogel as an alternative in the treatment of osteoarthritis

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Osteoarthritis presents significant clinical challenges, leading to the exploration of hydrophilic polymer hydrogels as a therapeutic avenue. Chitosan, which resembles cartilage components, was used to create hydrogels for the treatment of osteoarthritis. The study focused on characterizing these hydrogels. Chitosan was dissolved in HCl and urease was added at concentrations of 25 U/ml or 50 U/ml and 7.5 or 10 M urea. The results showed that the chitosan hydrogels from the groups with 50U/ml urease exhibited a shorter gelation time compared to the groups with 25U/ml urease, with times of 15 and 30 minutes, respectively. In addition, an increase in pH over time was observed in all groups, with the 50U/ml urease and 10 M urea group showing a faster increase in pH than the others. These findings corroborate the study by Chenite et al. which reveals that chitosan hydrogels form gels as their pH transitions from acidic to neutral, and shorter reaction times are associated with higher concentrations of urease [1]. In the degradation test, all groups experienced a decrease in mass at all times. The 50U/ml urease group exhibited a lower degradation rate compared to the 25U/ml urease group. In the drug release test, all groups showed a rapid release profile. Finally, none of the groups showed cytotoxicity. The results suggest that the chitosan hydrogel with 50 U/ml urease and 10 M urea is the best candidate for further studies, as it showed a safe gelation time and pH stability for in vivo applications, in addition to its slower degradation which allows for longer-lasting effects on the osteoarthritic joint.

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A new biomaterial developed from a marine compound for use in bone tissue engineering

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Due to the growing number of bone fractures and the difficulty in treating critical defects in bones, tissue engineering is always looking for new biomaterials with therapeutic applications [1]. This work aimed to develop a new biomaterial of marine origin, called Biomaterial M (BM) for use in bone tissue engineering. Bioglass45S5® (named Traditional Biomaterial (BT)) was used as a control group because it is a widely known biomaterial and is considered the gold standard in bone tissue repair. Through the alamarBlue®, DNA Quantification and Trypan Blue Viability tests, it was possible to verify that the BM showed no cytotoxicity, and was also able to induce proliferation and reduce cell mortality. The flow cytometry test showed that there were no apoptotic cells in the groups treated with BM. In addition, the cells treated with BM were also able to increase the activity of the LDH enzyme. In terms of oxygen consumption, there were no differences when compared to control, but both the BT and BM groups were able to reduce the amount of reactive oxygen species present in the exposed cells. FTIR analysis showed that both groups have an amorphous pattern. Calcium assays showed that BM is capable of releasing more calcium into the extracellular medium in the initial incubation periods when compared to BT. In summary, no level of cytotoxicity of the new biomaterial (BM) was detected, indicating that BM is a promising biomaterial for use in bone tissue engineering.

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Antibacterial effect of alpha-tungstate silver microcrystals against *Staphylococcus aureus*

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Staphylococcus aureus is a Gram-positive bacterium, associated with skin, cardiovascular, pulmonary infections, and is responsible for 80% of hospital-acquired infections [1]. With the excessive use of antibiotics, the occurrence of microorganisms resistant and multidrug-resistant to conventional antimicrobials have become increasingly common. Therefore, the development of new antimicrobial agents is necessary. Alpha - silver tungstate (α-Ag_2WO_4) is a material that has established antimicrobial properties. The use of different solvents in the synthesis can change its morphology and consequently, its antimicrobial activity [2]. Thus, the aim of this study was to evaluate the antimicrobial activity of α-Ag_2WO_4 microcrystals in rod and cube morphology against suspensions of *S. aureus* (ATCC 25923). Microcrystals were synthed by the controlled co-precipitation method using water as solvent (rod morphology) or sodium dodecyl sulfate (cube morphology). Antibacterial activity was evaluated by the microdilution method in Mueller Hinton broth. The minimum inhibitory concentration (MIC) was evaluated by reading absorbance (595 nm) and the minimum bactericidal concentration (MBC) was evaluated by quantifying colony-forming units per milliliter. Data were analyzed using one-way analysis of variance (one-way ANOVA) followed by Tukey's post-test (α= 0.05), or Kruskal-Wallis test, followed by the Dunn's post-test. MIC and MBC concentrations determined were 62.50 µg/mL for microcrystals in rod morphology and 125 µg/mL for microcrystals in cube morphology. In conclusion, a lower concentration of the α-Ag_2WO_4 microcrystal in the rod morphology is capable of inhibiting *S. aureus* compared to the microcrystal in the cube morphology.

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Antibacterial effect of titanium discs coated with alpha - silver tungstate microcrystal irradiated with electron beam

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Coating titanium with antimicrobial materials is a promising strategy to inhibition of biofilms formation on dental implant surface [1]. Alpha - silver tungstate (α-Ag_2WO_4) is a material known for its antimicrobial activity, which can be enhanced with electron beam irradiation, leading to the formation of metallic silver nanoparticles on its surface [2]. Thus, the aim of the study was to evaluate the antimicrobial activity of titanium discs coated with α-Ag_2WO_4 microcrystals irradiated with electron beam against *Streptococcus sanguis* biofilms, one of the initial colonizers of dental implant structures. The microcrystals were synthed using the co-precipitation method and grade 2 titanium alloy discs measuring 11 mm in diameter and 3 mm in thickness were used. Deposition on the discs was carried out using the spin-coating method. Part of discs were irradiated for 5 minutes using a portable irradiation equipment (40 kV acceleration, 15 mA current). To evaluate the antibacterial effect of discs coated with α-Ag_2WO_4, a standard strain of *S. sanguis* (ATCC 10556) was used, and mature biofilms (48 hours) were formed on discs without coating (control), irradiated discs, coated discs, and irradiated coated discs. Antimicrobial activity was assessed by counting colony-forming units per milliliter (CFU/mL). Data were analyzed using Kruskal-Wallis analysis, followed by Dunn's post-test. Coated discs and irradiated coated discs showed a reduction of 3.46 and 3.31 $\log_{10}$, respectively ($p < 0.0001$). Irradiated titanium discs did not show significant reduction. In conclusion, titanium discs coated with and without irradiation have a significant effect on control *S. sanguis* biofilm formation.

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Antimicrobial activity of printed resin discs functionalized with alpha - silver tungstate against *Candida albicans*

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The formation of microbial biofilms on the surface of implant-supported or conventional prostheses is frequently observed, compromising the success of rehabilitative treatment and the patient's systemic health [1]. Therefore, the functionalization of denture base resins with antimicrobial agents is a promising approach for controlling biofilm formation [2]. In this context, the aim of the study was to evaluate the effect of resins functionalized with alpha-silver tungstate (α-Ag_2WO_4), a material known for its antimicrobial properties, against mature biofilms of *Candida albicans*. The microcrystals were synthed by the controlled co-precipitation method, and the discs were obtained by printing in three-dimensions (3D), using stereolithography, in the dimensions of 10 mm in diameter by 2 mm in thickness. To evaluate the antimicrobial effect of the functionalized material, the standard strain of *Candida albicans* (American Type Culture Collection - ATCC 90028) was used and mature biofilms (48 hours) were formed on resin discs without microcrystals (control) and discs containing 0.2 and 0.3 % (by weight) of α-Ag_2WO_4. Antimicrobial activity was assessed by counting colony-forming units per milliliter (CFU/mL). From the results, it was observed that the resins containing α-Ag_2WO_4 in percentages of 0.2 and 0.3% showed reductions of 3.7 ± 0.4 and 4.5 ± 0.7 $\log_{10}$, respectively. Therefore, it is concluded that the functionalized resins demonstrated an antifungal effect against mature biofilms of *C. albicans* in vitro.

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Antimicrobial Applications of Alginate Films Loaded with $Cu_3Mo_2O_9$ Nanoparticles

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Alginate emerges as a promising candidate in biopolymeric technology development. Derived from seaweed, it's a cost-effective biopolymer known for its biodegradability, leading to widespread use. Yet, challenges like susceptibility to hydrolysis and mechanical limitations hinder its application. Nanotechnology offers a promising solution to these hurdles. Nanostructured materials are increasingly explored for their unique and superior properties. Copper molybdate, with its various compositions and applications ranging from supercapacitors to catalysts, stands out. Particularly, $CuMoO_4$ is extensively studied for its multifaceted applications, including antitumor activity. In this study, we focused on a less explored polymorph, $Cu_3Mo_2O_9$, renowned for catalyst development and energy storage devices. Nanoparticles of $Cu_3Mo_2O_9$ were incorporated into alginate films crosslinked with Ca^{2+} to assess antimicrobial efficacy. Films with 5% and 10% $Cu_3Mo_2O_9$ relative to the polymer mass were prepared and characterized using physical-chemical techniques. Antimicrobial activity was evaluated against methicillin-resistant *Staphylococcus aureus*, *Pseudomonas aeruginosa*, *Mycobacterium smegmatis*, and bacteriophages Φ6 and MS2. This study opens avenues for developing cost-effective, eco-friendly antimicrobial composites with practical applications.

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Anti-SARS-CoV-2 evaluation of different forms of silver tungstates (α-Ag2WO4)

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Many efforts have been directed towards the search for materials with virucidal activity to control the viruses spread with a major impact on public health, such as SARS-CoV-2. Studies in the area indicate that silver-based materials have been widely used in different industrial applications, due to their physicochemical and biological properties, such as antifungal, antibacterial, and antiviral. Silver tungstate (α-Ag2WO4) has proven antimicrobial activity, and the impregnation of this material in different polymeric matrices, such as non-woven fabric (TNT), polypropylene (PP) and thermoplastic polyurethane (TPU), appears as a promising alternative for pathogens elimination. In this way, we evaluate new approaches for the manufacture of biocidal materials, which can be used in the development of Personal Protective Equipment (PPE), which have the capacity to contain the transmission of pathogens (viruses, bacteria, and fungi). Therefore, we investigated whether silver tungstate microcrystals (α-Ag2WO4) in different forms (cube, rod and nano), encapsulated or not in a chitosan matrix, would present anti-SARS-CoV-2 activity.

Assemble of lanthanides complexes with chalcone and avobenzone to investigate antimicrobial activities and photostability increasing

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The biological properties of chalcones, characterized by α,β unsaturated carbonyl group linking two aromatic rings, attract in health fields, and heteroaryl amino chalcones, like the 3-(4’-dimethylaminophenyl)-1-(2-furanyl)prop-2-en-1-one (DMAFP), can show anticancer and antimicrobial activity [1]. Combining chalcones and lanthanide (Ln) β-diketonate complexes can lead to activities such as DNA photocleavage [2]. No studies was found regarding Ln complexes with chalcones and avobenzone (4-tert-butyl-4'-methoxydibenzoylmethane; bmdm), a UVA-absorbing β-diketone found in commercial sunscreens. Thus this work aims to synthe and characterize Lnbmdm-DMAFP complexes to explore their biological activities and enhance bmdm photostability, once keto-enol tautomerism makes it photounstable [3]. DMAFP synthesis involved adding 4-(dimethylamino)benzaldehyde ethanolic solution to a 2-acetylfuran cold aqueous solution, followed by NaOH, resulting in a red solid, characterized by NMR spectroscopy. Ln(bmdm)3(H2O)2 (Ln = Gd or Eu) was obtained by adding LnCl3 aqueous solution to unprotonated BMDM ethanolic solution, yielding a yellow powder characterized by FT-IR. LnBMDM-DMAFP was formed by transferring DMAFP to Ln(bmdm)3(H2O)2 in THF, stirring at ambient temperature for 12 h, yielding a yellow solid precipitate with hexane. Lnbmdm-DMAFP remained visually unchanged until 250°C in a digital melting point device. FT-IR spectra exhibit ~32 cm-1 frequency shift from DMAFP C=O stretching to the Lnbmdm-DMAFP, indicating coordination. Future steps include Ln3+ complexometric titration, CHN analysis, thermogravimetric analysis, photostability and antimicrobial activity tests.

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Assembly of an electrochemical biosensor for the non-invasive detection of a lung cancer biomarker

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Lung cancer is considered one of the most common and remains the leading cause of cancer-related death. More than 75% of cases are only identified in the advanced stage due to poor prediction in the early stage. There are many traditional methods used to diagnose lung cancer, however, they are not very accurate in predicting lung cancer at an early stage and are very expensive. Therefore, the development of a more accurate, low-cost and rapid method is crucial for the early detection of lung cancer. Biosensors are developed using modern and advanced technologies and nanomaterials, are low cost and take less time to analyze samples. Furthermore, it can be handled by untrained people. The present work brings an innovative approach to monitoring the EGF protein that can identify a possible biomarker for this cancer using screen-printed carbon electrodes. The biosensor platform was developed using polypyrrole nanotubes and Ni(OH)2. The electrode was characterized by FTIR and SEM spectroscopy, where the deposition of Ni(OH)2 on the PPyNTs was observed. The materials were also characterized by cyclic voltammetry (CV). Both materials presented a CV profile with broad redox peaks and large capacitive current, characteristics of PPyNTs, while in the presence of Ni(OH)2 a small decrease in current was noted. The materials were characterized by EIS to better understand this behavior. The biosensor was prepared with antibodies against the ESF protein, followed by blocking with BSA. The biosensor successfully detected proteins at such low concentrations, showing potential for early diagnosis of lung cancer biomarkers.

A versatile bio-packing based on copaiba oil incorporated into carboxymethyl cellulose hydrogel

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Essential oils are aromatic, volatile compounds that can be extracted from roots, stems, leaves, flowers or all other parts of certain plants. Typically, these oils are normally extracted by steam distillation. These substances have different chemical groups such as carboxylic acids, alcohols, aldehydes, ketones, esters and hydrocarbons, each with its aromatic characteristic and biochemical action[1]. The properties of essential oils, such as antimicrobial and antioxidant properties, increase the possibilities of applying these compounds in active packaging. Therefore, the use of essential oils encompasses several areas, enabling their exploration in different sectors and favoring technological development in an ecological way through the use of waste [2]. In this context, this research proposes using Copaiba essential oil incorporated in carboxymethyl cellulose hydrogels as bio-packing as a sustainable alternative. This bio-packing is eco-friendly, low-cost, widely available, and quickly produced. The antimicrobial activity was evaluated. Additionally, the bio-packing was characterized by Raman, XRD and SEM analyses. In addition, the antimicrobial activity using Escherichia coli (ATCC 1597) was performed. The results indicated the link among essential oil with chemical groups in the carboxymethyl cellulose. Furthermore, the bio-packing demonstrated antibacterial activity against Escherichia coli. Thus, for the first time, this bio-packing using Copaiba essential oil loaded into hydrogel matrix presented a great future for applications as a versatile action for bio-packings applications.

Characterization of the antibacterial activity of $NiWO_4$ and $NiWO_4$:Ag nanoparticles encapsulated in chitosan biofilm

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Antimicrobial resistance poses a global threat to the effectiveness of modern medicine, driven by the improper use of antimicrobial treatments. Countries across all income levels face concerning rates of resistance, with up to 90% in low and middle-income nations [1]. The importance of responsible antibiotic use is emphad, along with the need to identify new treatments. Considering this, semiconductors materials such as SiO2-Ag have been explored for their antimicrobial capacity, especially against pathogens like SARS-CoV-2[2], with the integration of silver nanoparticles into semiconductors showing a synergistic effect on biocidal activity. The encapsulation of nanoparticles in chitosan forms biocomposites with a broad spectrum of antimicrobial activity, offering a favorable alternative due to its biopolymeric nature and lower environmental impact.

In the present study, $NiWO_4$ and Ag doped $NiWO_4$ based materials encapsulated in chitosan were investigated for their antimicrobial activity against gram-negative bacteria such as Escherichia coli and Klebsiella pneumoniae. $NiWO_4$:Ag materials underwent morphological changes during the process. Tests consisted of antibiogram analysis and characterization of films before and after the process using techniques such as infrared spectroscopy, X-ray diffraction, SEM coupled with EDS mapping. As next steps, the project aims to test gram-positive bacteria and resistant bacteria, aiming to expand the antibacterial activity of the analyzed material.

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Clay minerals as Potential Photoprotection Agents for Oxytetracycline

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Oxytetracycline (OTC) is an antibiotic of the tetracycline class, widely used in veterinary and human medicine due to its efficacy against a wide range of bacteria. However, when exposed to light, OTC undergoes photodegradation, which can cause its efficacy to be lost or reduced. Among the strategies to mitigate this problem is the formation of hybrids. This study aimed to investigate the photostability of drug/clay hybrids (OTC/VEEGUM and OTC/PAL). Adsorption was done using 2g of clay in 2gL-1 of the drug under stirring for one hour of reaction. The light stability tests were carried out in a radiation box with a solar spectral lamp and characterized by XRD and TG. The XRD patterns for Veegum clay are consistent with a 2:1 phyllosilicate structure [1]. The changes observed between the diffractograms of the raw clay and the hybrids suggested a high interaction between the organic molecule and the inorganic structure. For the systems with clay minerals of fibrous morphology, there were no significant changes in the structure after adsorption or even exposure to radiation for 200 hours. This result suggests that the drug was taken up on the external surface, which agrees with previous studies [2]. The results obtained in this study showed that there was intercalation of the drug, and TG revealed that the incorporation of the drug into the clay has the potential to improve the photostability of the drug; this effect can be attributed mainly to the lamellar nature of the clay which makes the exposed material a promising excipient for increasing the photostability of the drug.

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Cobalt sulphide Quantum dots (CoSQD) synthed by a green chemical route for potential biomedical applications.

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Climate change and all environmental advances have caused many worries in society. Then, the development of sustainable materials using materials by a green chemical route is a great challenge. In this sense, various sources have been implemented for biomedical applications, like bioimage analysis, using a diversity of materials, including nanoparticles by semiconductor metals. Therefore, most of metals used are toxical or presented highly difficult in their syntheses. In this sense, present research has evaluated producing a new Quantum dots based on cobalt sulphide, a potential semiconductor that not only provided the possibility of bioimage, but showed a high biological potential for improving tissue regeneration and applying in magnetic treatments in human body, using carboxymethyl cellulose as stabilizer. Thus, Spectroscopy analysis (FTIR, UV Vis), X-ray diffraction, and morphological analysis (TEM, ZP) were used to characterize this nanomaterial. The results showed that the CoS presented a of 3 nm with good photoluminescence and magnetic potential, demonstrating a low-cost and environmentally friendly chemical route. In addition, the chemical groups that stabilized the CoS QD were the carboxylates. Furthermore, quantum dot production provided a potential application of these nanomaterials to biomedical applications. Agradecimento:BIOSEM-LESMA/UFVJM, FAPEMIG (APQ-02565-21), FINEP/MCTI (01 22 0528 00), CNPq and CAPES.

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Degradation of Sulfamethoxazole Employing Zn2GeO4 as a Emerged photocatalyst

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The generation of antibiotic-resistant bacteria is trigged by the widespread disposal of antibiotic pollutants into water environment. This problem creates a threat to human health and ecological systems. However, it is known that conventional treatments are not capable of eradicate these pollutants compounds. Recently, photocatalysis has received much attention due to its low cost, efficiency in degrading antibiotics under sunlight and ambient conditions, as well as environmental friendliness. [1] Therefore, the design of nanomaterials with highly selective and photocatalytic activities are urgently needed. [2,3] In this scenario, nanoparticles of Zn2GeO4 synthesised by two routes, microwave-assisted hydrothermal method, and co-precipitation. The structural characterization of the semiconductors was conducted using X-ray Diffraction, Raman Spectroscopy, and UV-Vis Spectrophotometry, while morphological analyses was determined through Scanning Electron Microscopy. Afterwards, all samples were evaluated for degradation of a model antibiotic molecule, sulfamethoxazole (SMZ).

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Development of a biosensor for detection of Helicobacter pylori

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population, poses significant health risks, including serious and potentially fatal complications such as cancer. Detection of H. pylori typically relies on direct methods such as culture, polymerase chain reaction tests, enzyme-linked immunosorbent assays, optical sensors, and next-generation sequencing (NGS). These methods target bacteria, making them suitable for analyzing water samples. However, these approaches are often time-consuming, complex, labor-intensive, require specialized personnel, and suffer from limited specificity. Notably, there is a paucity of biosensors for H. pylori detection, highlighting the need for a simple and accurate method to detect H. pylori at low concentrations in environmental samples. In this work, the objective is to develop a sensitive impedimetric biosensor for detecting H. pylori at low concentrations using screen-printed carbon electrodes. The working electrode was modified with PPyNTs and carboxylated multi-walled carbon nanotubes (MWCTN). The electrode was characterized using FTIR spectroscopy and MEV, where the deposition of carbon nanotubes on the PPyNTs was observed. The materials were also characterized by cyclic voltammetry (CV). Both materials presented a CV profile with broad redox peaks and large capacitive current, characteristics of PPyNTs. In the presence of MWCNT, a slight decrease in current was observed, indicating that the electrode/electrolyte interface became less electroactive and with a slightly smaller interface area. The materials were characterized by EIS to better understand this behavior. Antibodies against HopQ protein, an outer membrane protein of H. pylori, were covalently linked to the electrode surface through EDC/NHS coupling, followed by blockage with BSA. The biosensor successfully detected HopQ protein in concentrations as low, showing potential for early diagnosis of H. pylori infections.

Development of a photoelectrochemical sensor for determining creatinine based on molecularly imprinted polymer and tungsten trioxide chemically imprinted

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In recent years, the development of photoelectrochemical sensors, also known as PEC (photoelectrochemical) sensors, has been increasing, as they can offer increased sensitivity compared to electrochemical sensors, in addition to low cost and fast measurements. However, when applied to complex real samples, such as biological matrices, these sensors face problems due to their lack of selectivity. Furthermore, the use of chemical printing technology in the manufacture of photoelectrochemical sensors is still considered incipient [1, 2]. Therefore, this work produced a photoelectrochemical sensor containing WO_3 and a molecularly printed polymer for the determination of creatinine in biological fluids. The electroanalytical determination of creatinine is not simple, as it is a molecule with little electroactivity at the potentials studied by electroanalytical techniques. Printed WO_3 was obtained from a simple synthesis involving Na_2WO_3, ethanol, HCl and creatinine, while MIP was obtained from an iniferter reaction anchored in graphene oxide. As a source of radiation, a point laser with a maximum wavelength of 532 nm was used. The work is still in progress, but chronoamperometric photocurrent measurements indicated promising results for the determination of creatinine. The parameters of pH, supporting electrolyte, supporting electrolyte concentration and oxidation potential were optimized and allowed the quantification of creatinine at low concentrations (0.6 µmol L-1). A better characterization of materials, selectivity study and determination of figures of merit are among the future stages of the study in question, as well as the application of the analytical method to biological fluid samples.

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Development of electrospun fibers of PLA/PBAT with Ag_2WO_4 for obtaining antimicrobial membranes

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Antimicrobial membranes play a fundamental role in various applications, where the prevention of bacterial infections is crucial. In wound dressings, for example, these membranes assist in protecting the affected area, preventing the proliferation of pathogenic microorganisms, and promoting an environment conducive to rapid and safe healing. Additionally, in the medical industry, especially in implantable devices such as catheters and prostheses, antimicrobial membranes are essential for reducing the risk of hospital-acquired infections and ensuring the integrity of the surgical site. In food and water processing environments, these membranes play a crucial role in purification and disinfection, ensuring the safety and quality of consumable products. In this study, membranes of PLA/PBAT, a compostable polymer, were developed with silver tungstate particles, aiming to obtain compostable and antimicrobial membranes. An interaction between the particles and the polymeric matrix was observed, improving the thermal and mechanical properties. Furthermore, due to the controlled release of Ag+ ions and the production of reactive oxygen species, this material was capable of inhibiting gram-positive bacteria (methicillin-resistant Staphylococcus aureus), gram-negative bacteria (Pseudomonas aeruginosa), and fungi (Candida albicans). This technological development may aid in the advancement of antimicrobial membranes, especially for air filtration and wound dressings.

Development of New Materials Based on Silver Silicates and Evaluation of Antimicrobial Activity

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Emerging pathogens pose a serious threat to human health as they can adapt to the host, developing effective strategies against conventional treatments. They are easily transmitted through human bodily fluids, airborne contagion, or contaminated surfaces. Transmission from contaminated surfaces accounts for a significant portion of new infections, making the development of new antimicrobial technologies crucial in the current context. To make these technologies economically viable, it is necessary to increase antimicrobial activity to minimize the amount of material applied. In this study, silver silicates were synthed using the microwave hydrothermal method, aiming to optimize their antimicrobial properties. To characterize the obtained materials, X-ray diffraction, Raman spectroscopy, infrared spectroscopy, scanning electron microscopy, and transmission electron microscopy were conducted. The antimicrobial activity of the samples was tested against the gram-positive bacterium Staphylococcus aureus, and a dependency of antimicrobial activity on the synthesis method was observed. The antimicrobial mechanism of these materials is due to the production of reactive oxygen species and the release of Ag^+ ions. This work may contribute to the development of new efficient microbial agents for the elimination of pathogens of interest.

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Development of poly lactic acid / polypyrrole blends for antibacterial applications

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Bacterial contamination is driving studies to develop new polymeric materials with antibacterial activity, in accordance with [1]. This study discusses the synthesis of polypyrrole (PPy), according [2], and its later combination with poly (lactic acid) (PLA) to obtain blends obtained through extrusion and injection techniques. In turn, the blends were characterized by Fourier Transform Infrared Spectroscopy (FTIR), Scanning Electron Microscopy (SEM), Impedance Spectroscopy (IS) and Dynamic-Mechanical Analysis (DMA). FTIR measurements confirmed that the blends were obtained in conductive form. SEM images of the blends show a homogeneous surface with the presence of small cracks. Evaluation using impedance spectroscopy (IS) revealed that the blends with 50% PPy showed higher conductivity compared to the lower levels of conductive polymer. Finally, dynamic-mechanical evaluation (DMA) showed that the blend with 50% PPy showed superior resistance. The antibacterial activity of the blends was evaluated using the inhibition halo method against Staphylococcus Aureus and Escherichia Coli. The injected blends showed no halo of inhibition against Escherichia Coli, while pure PPy showed inhibition. For Staphylococcus Aureus, the blends with 50% PPy and pure PPy showed inhibition halos. This study shows a new perspective on obtaining blends based on conductive polymers using conventional processing techniques.

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Eco-friendly synthesis of zinc oxide nanoparticles for wastewater treatment

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Inequality concerning access to drinking water affects around 32 million Brazilians. In addition, approximately 90 million do not have access to sewage collection, which shows the need to apply new wastewater treatment technologies [1]. Zinc oxide nanoparticles have a wide range of uses, from treatment to disease prevention, due to their biocompatibility and antibacterial properties. This work proposes a sustainable and economically viable synthesis route for zinc oxide nanoparticles aimed at wastewater treatment [2][3]. This green synthesis of zinc oxide nanoparticles uses fresh Arabica coffee in natural extract due to its antioxidant properties. The presence of phenolic compounds and other coffee metabolites creates a reducing environment in which a metal salt, zinc acetate, can be added as a zinc ion precursor. Under stirring and heating conditions, the nanoparticles can nucleate and stabilize. A comparison of routes using different extract concentrations and varying the pH of the reaction was defined to determine the influence of these factors on the stability and final of the nanoparticles. After drying and calcination, UV-Vis spectroscopy preliminary identifies the formation of nanoparticles. Moreover, scanning electron microscopy (SEM) and dynamic light scattering (DLS) perform morphological characterization, followed by antimicrobial activity tests.

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Efficient synthesis method for a promising photocatalytic BiVO4 material

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In this work, the synthesis of promising photocatalyst material was carried out using the urea combustion method, i.e., bismuth vanadate in monoclinic-phase BiVO4 [1]. To obtain this compound, raw materials were used: bismuth oxide (Bi2O3) and vanadium pentoxide (V2O5), subjected to temperatures between 600-700 °C for two hours, in the presence of stoichiometric and in excess urea (CO(NH2)2). This combustion process is a promising technique for the synthesis of materials because it efficiently converts precursors into final products of high purity and homogeneity [2]. The samples were characterized structurally and morphologically by X-ray diffractometry, Infrared Spectroscopy, Raman Spectroscopy and Scanning Electron Microscopy. The results indicated the presence of the monoclinic main phase BiVO4 in the BV4-600 and BV4-700 compositions. Infrared spectroscopy showed the presence of metal oxygen V-O and Bi-O bonds in all compositions, which is consistent with the expected structure of the materials. Raman Spectroscopy measurements revealed typical BiVO4 modes. The microstructural characterization showed the presence of nanometric particles with characteristic morphology. This indicates that the urea amount is essential to obtain materials with specific structure and, possibly, the material synthesized in this study presents photocatalytic effect.

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ESI(MS)-NMR Combined Study of Benzoylguanidines with Potential Biological Activity

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Guanidines are important molecules in biological research [1]. Guanidinium group has chemical properties such as ability to form H-bonds, charge pairing and cation-π interactions which allows molecular recognition. Benzoylguanidines display therefore potential use as strong and selective Na^+/H^+ exchangers inhibitors. The inhibition of the Na^+/H^+ exchanger during cardiac ischemia and reperfusion has been shown to be beneficial for the preservation of the cellular integrity and functional performance. Benzoylguanidines that are targeted specifically against NHE-1, increases the potential for the treatment of patients with heart disease. In this sense, this work aims to describe the synthesis and characterization of this benzoylguanidines and bis-benzoylguanidines with potential pharmacological activity as selective inhibitors of NHE. The synthesis method used is based on the reaction between a benzoylthiourea and an amine, catalyzed by $Bi(NO_3)_3.5H_2O$, at 120°C for 24 hours. ^1H NMR of guanidines showed the chemical shift of the NH protons around 4 and 12 ppm. The signal in the region of 12 ppm was attributed to amide NH proton, this was supported for the formation of a pseudo six-member ring. ^{13}C NMR data confirmed the structures of guanidines. Both, guanidinic and carbonyl (amide) carbon atoms, when observed, were identified for their respective resonances around 158 and 177 ppm. In the ESI(+)-MS, all the guanidines were identified. Therefore, the successful synthesis and full spectroscopic and spectrometric characterization of this molecules has been described.

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Graphene oxide/CoFe2O4@γ-Fe2O3 proton conductor for impedimetric olfaction of clinical relevante VOCs.

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Electronic nose devices operating in high humidity, at room temperature, are of great interest for non-invasive clinical diagnosis. In this investigation, we explored the potential of an electronic nose device using an array of 7 affordable graphene oxide/CoFe2O4@γ-Fe2O3 nanocomposite sensors for non-invasive clinical diagnosis at room temperature and high humidity (80% RH). The study successfully discriminated several clinically relevant volatile organic compounds (VOCs), including ethanol and acetone, at various concentrations using linear discriminant analysis (LDA). The nano-composites were characterized by thermal analyses (TG), FTIR spectroscopy, X-ray diffractometry (XRD), scanning electronic microscopy (SEM), transmission electronic microscopy (TEM), impedance spectroscopy (EIS), Raman spectroscopy, and X-ray photon spectroscopy (XPS) and confirmed the properties of the nanocomposites and suggested proton conduction as the primary detection mechanism.

Kinetic study of water absorption in sodium alginate filaments obtained by the wet spinning technique

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Polymer fibers are used in a wide variety of applications ranging from scaffolding biomaterials, drug release and sensors to health industry [1-3]. There are several methods for obtaining polymeric fibers, among which wet-spinning stands out. The wet-spinning process begins with extruding suspension through a nozzle of the desired diameter into a coagulation or precipitation bath to form filaments [3]. The aim of this study was to assess how the incorporation of *Aloe vera* in different proportions affects the structure and properties of alginate filaments obtained by wet spinning technique. This study was based on the degree of swelling of the samples obtained at different pH values. To produce filaments of this polymer, a 3% (w/v) solution of sodium alginate was prepared in deionized water under agitation. The wet spinning technique was then used with a calcium chloride coagulation bath at concentrations of 50, 100 and 150 mmol/L. *Aloe vera* was incorporated to the alginate solution in proportions of 0, 10, 20 and 30% (w/w) in relation to the mass of alginate. Twelve samples were obtained. The degree of swelling was calculated according to the temperature and pH of the aqueous solution in which the filaments were immersed. The test was carried out at 27°C and three different pH values (5.5, 7.0 and 8.5). The experiments were carried out in triplicate. The results indicate that the alginate filaments have good sweeling properties, making it possible to develop applications for active bioabsorbable suture.

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Mineralization and Reduction of Toxicity in Real Textile Effluents through Photocatalysis Employing g-C_3N_4/$CoMoO_4$- Based Heterostructures

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There are multiple sources of water pollution, and among them, azo dye-based residues from textile, paper, and dye industries stand out as one of the most significant pollutants. In this context, the study focused on evaluating the phytotoxicity of these pollutants and seeking effective solutions for their degradation. Nanocomposites of g-C_3N_4/$CoMoO_4$ were developed using the hydrothermal microwave-assisted method followed by mechanical mixing to be applied as photocatalysts for the degradation of both rhodamine B and real effluent from a textile company. Structural characterization of the materials was conducted using techniques such as Xray diffraction (XRD) and Raman spectroscopy, while morphology was analyzed by scanning electron microscopy. Electronic properties were evaluated using diffuse reflectance spectroscopy (DRS). It was observed that varying the concentration of g-C_3N_4 resulted in an improvement in the photocatalytic activity of $CoMoO_4$, however, although g-C_3N_4 demonstrated superior photocatalytic activity compared to heterojunction with $CoMoO_4$, its ability to mineralize the actual effluent was lower compared to heterojunction. The phytotoxicity using L. sativa showed that as the photocatalysis time increases, the toxicity decreases, demonstrating that the heterojunction is effective in mineralizing and reducing the hazardous nature of the residue. Thus, the heterojunction proved to be more effective than g-C_3N_4 in degrading real effluent from the textile industry.

NMR and XRD Conformational Study of Brominated Guanidines

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Brominated guanidine compounds have been studied for a possible drug for Leishmaniasis [1]. Leishmaniasis is a neglected disease that affects more than 12 million people in various countries, such as Brazil. The results against different strains of leishmaniasis are promisor, being more effective and safer than current medications. In this sense, this work describes the conformational study of some brominated guanidine molecules with potential antileishmanial activity using Nuclear Magnetic Resonance (NMR) and X-ray diffraction (XRD) techniques. The monobrominated molecules in this series had their *E/Z* isomerism studied by NMR, proving a predominance of the *Z* isomer [1]. Different from this, the new tribrominated molecule in this work showed a predominance of the E isomer. ^{1}H, ^{13}C and 2D NMR spectra were acquired. The ^{1}H NMR spectra of monobrominated compound have their NH signals around 5 and 12 ppm, proved the Z isomer. In contrast, tribrominated molecule showed the signals at 8.61 and 9.64 ppm attributed to NH1' and NH2' with high intensity, that were associated to both *E* and *Z* isomers in solution. The XRD study characterize the monobrominated compound as a non-centrosymmetric trigonal space group $P3_2$ and, as indicated by the NMR analyses, with *Z* conformation. On the other hand, tribrominated compound crystallized in the monoclinic space group $P2_{1/c}$, presenting an *E* conformation. The *Z/E* conformational ratio is directly related to the position of the double bond of guanidine nucleus. NMR and XRD analysis provide the complete conformation study of brominated guanidine compounds with potential activity against leishmaniasis.

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Optimization of chlorhexidine chemical bonding conditions on Kraft lignin

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The COVID-19 pandemic shed some light on the importance of fast response against pathogenic agents which are both efficient and safe for human beings and the environment. Chlorhexidine (CHX) is an active substance mostly used in commercial mouthwash formulations which was reported as being capable of inactivating different types of pathogens [1,2]. Chen et al. [1] mention that when combining CHX with polymers, it is normally incorporated into the polymeric substrate without any chemical attachment, accelerating expiration due to rapid release. In this context, this work aims to study optimal conditions to link chlorhexidine digluconate with Kraft lignin (KL), with the aid of a crosslinker to produce a long-lasting pathogen-inactivating material (KL-CHX). Kraft lignin is a material of natural origin mostly comprised of phenolic units, which not only provide different properties but also allow many sorts of modifications [3]. A factorial experimental design 22+1 was applied to optimize reaction conditions, where the chosen factors were reaction temperature and proportions of CHX relative to KL. The materials were evaluated regarding phenolic hydroxyl group concentration via UV photometry, solubility, thermogravimetric analysis, Fourier-transformed infrared spectroscopy. Results like the decrease in the phenolic OH concentration and solubility indicate that the reticulation occurs successfully. Potentially, this material can be applied as personal protective equipment for medical use.

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Photocatalytic Activity and Toxicity of Ag_3PO_4:La-Based Materials

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This study investigates the enhancement of photocatalytic efficiency achieved by incorporating La^{3+} into Ag_3PO_4 for the photodegradation of Ciprofloxacin (CIP) under visible light irradiation. The sample incorporated with 2% La^{3+} (APL2) achieved a 32.6% mineralization of CIP, nearly three times higher than pure Ag_3PO_4. Toxicological analysis of the residue from CIP photodegradation using the microalga Raphidocelis subcapitata revealed high toxicity due to the leaching of Ag^+ ions from the catalyst. This highlights the need for careful disposal of wastewater after using the photocatalyst. The toxicity of the APL2 photocatalysts was thoroughly assessed through comprehensive toxicological tests involving embryo development in Danio rerio, revealing their potential to induce death and malformations in zebrafish embryos, even at low concentrations. This emphas the importance of meticulous waste management, as well as a balance in the development of new photocatalytic materials considering both efficiency and toxicity.

Reduced graphene oxide electrical devices for the differentiating the blood coagulation

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Blood coagulation is a complex biochemical reaction sequence in the hemostasis process. Coagulation tests are performed using relatively costly methods, such as laboratory tests or portable coagulometers [1]. Despite its portability, the cost of a test strip (~ US$ 5) of a typical coagulometer is relatively high for routine use in hospitals or for patient self-testing [1]. This study presents sensors based on rGO deposited on interdigitated electrodes to determine blood coagulation time through electrical measurements. Electrical sensors were manufactured by depositing graphene oxide (GO) onto interdigitated electrodes, resulting in subsequent electrochemical reduction. Initial tests were conducted to determine the change in impedance or resistance of the devices of animal blood samples containing CaCl2, which is responsible for accelerating the coagulation process [2]. The use of the electrochemical reduction method of GO for rGO production proved advantageous, as it does not involve toxic reagents and by-products. In blood coagulation tests, a significant variation in resistance was observed in the sensors utilizing samples containing CaCl2, compared to the sensor containing only blood and water or NaCl. Additionally, in AC measurements, an increase in impedance proportional to the blood coagulation time was noted when analyzing blood with the CaCl2 solution. The devices proved reproducible and feasible for application in the differentiation of blood samples with distinct coagulation times at a low production cost, with good sensitivity and adequate analysis time (1000 s) compared to conventional tests. Additional tests varying the CaCl2 concentration (50 to 500 mM) to simulate different clotting times are in progress.

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Revolutionizing Materials: Crafting Propolis Extract Composites through Electrospinning

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The search for active principles (AP) for application in pharmaceuticals, cosmetics, and food industries is extremely valuable. Bee propolis is one of the best-known, described, and used for therapeutic and functional purposes. It is mainly used due to its antifungal, antioxidant, and anti-inflammatory activities. However, propolis usage has some obstacles, such as its low bioavailability and rapid degradation in the gastrointestinal tract. The advent of the production of composites as nanofibers (NFs) by electrospinning has the potential to mitigate such limitations, making it possible to produce composites containing these products, transforming them into more thermostable, bioavailable, and consequently improving release and biotransformation aspects of these AP. Therefore, this work aimed to produce NFs using polymeric solutions added to propolis, as well as to characterize these structures and evaluate the antioxidant activity of the selected raw material and the composites formed. As obtained results, composites of propolis extract were produced, obtaining solids of fibrous appearance, not unidirectional, and slightly heterogeneous, when observed by the images obtained from the analysis of scanning electron microscopy (SEM) and energy dispersive X-ray spectroscopy (EDS), Fourier transform infrared spectroscopy (FTIR), the presence of the active ingredient, propolis extract, and the other components zein and polyethylene oxide (PEO) was verified. In thermogravimetric analyses, the bioactive compounds of propolis were found to be stable at room temperature but still thermosensitive at high temperatures. Finally, it is possible to manufacture nanofibers by electrospinning using zein, PEO, and propolis extract, which are releasable, and their antioxidant activity is maintained adequately.

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Safety of a hydrogel enriched with natural marine products

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Hydrogels (Hyd) represent a class of materials composed of a three-dimensional, hydrophilic polymeric network capable of absorbing high quantities of water or biological fluids [1]. The use of these materials for drug delivery has been increasingly studied, as they can be manufactured to provide controlled delivery of drugs with a localized effect in the region where they are administered. The aim of this study was to identify whether the PNM-enriched hydrogel has genotoxic effects. To this aim, the micronucleus test (MN) [2] was carried out using the indirect contact technique, in which the culture medium was initially conditioned for 24 hours with a Hyd manufactured with alginate (ALG) and calcium carbonate CaCO3 at 1.5% and GDL in a 4:1 ratio in relation to the volume of the ALG:CaCO3 solution. The groups evaluated were:
CG = cells that were exposed to normal culture medium
HG = cells that were exposed to culture medium conditioned with hydrogel
1PNMG = cells that were exposed to hydrogel-conditioned culture medium enriched with compounds extracted from the marine sponge Dysidea robusta, hexane partition phase 4 (DRMH4) at a concentration of 125 ug/mL.
2PNMG = cells that were exposed to culture medium conditioned with hydrogel enriched with DRMH4 compounds at a concentration of 250 ug/mL.
This study showed no difference in MN formation between the control group and the other tested groups ($p = 0.5625$). It can be concluded that the hydrogel, whether enriched or not with DRMH4 as manufactured in this study, is safe and has no genotoxic effect."

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Spicing Up with Antioxidant Action: Spirulina Biopolymeric Films

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Society's increased concern for the environment regarding sustainable and more ecological options has contributed to increased research into the production of biodegradable packaging. Food packaging is used to protect the product and, depending on its functional characteristics, extend its useful life. The production of biopolymeric films that perform some functions is increasing, and microalgae and cyanobacteria are gaining visibility due to their availability and biological properties, which provide important active properties to the films. In this context, this work aimed to screen films formulated with different biopolymers incorporated with different concentrations of Spirulina and select the best films obtained according to their physical and visual characteristics for subsequent characterization. Filmogenic formulations were prepared using casting methods and subjected to analyses to evaluate the physicochemical, optical, mechanical, thermal, barrier, surface properties, functional groups, and antioxidant activity. Significant differences related to antioxidant activity were evident between the concentrations of internal biomass, with the highest averages being found at concentrations of 5%, 320.08 ± 35.7 µmol of TE/g of film. The production of the films was carried out successfully, and the films obtained promising results in terms of mechanical, thermal, barrier, and antioxidant properties for the food packaging area. They can be applied to foods sensitive to light and susceptible to oxidation. Adding whole Spirulina biomass to these films provided better barrier properties and greater antioxidant activity.

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Study of the effect of electron-beam irradiation on the bactericidal properties of AgI

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Electron-beam irradiated silver-based materials show strong bactericidal activity due to surface metallic silver, which triggers a plasmonic effect. This study investigated the minimum inhibitory concentration (MIC) of electron-beam irradiated AgI towards gram positive and negative bacteria. A two-step synthesis was employed to prepare the samples. First, via co-precipitation, a solution was prepared by mixing two aqueous solutions of 0.04M of KI and $AgNO_3$. Then, this mixture was transferred to a Teflon autoclave, and the AgI powder was synthed via the microwave-assisted hydrothermal method at 110°C for 15 minutes. The samples were irradiated with 40, 60 and 80 kV for 2 minutes [1]. X-ray diffraction revealed the formation of β,γ-AgI phases. Raman analysis suggested the formation of metallic silver nanoparticles after irradiation. The estimated bandgap values slightly increased for irradiated samples. The experiments were carried out to determine the MIC for two types of bacteria, *S. aureus* (a gram-positive spherical bacterium) and *E. coli* (a gram-negative bacillus bacterium), with concentrations ranging from 250 to 1000 µg/mL. The AT-40kV sample inhibited the bacterial growth of *E. coli and S. aureus* at the minimum inhibitory concentration of 500 µg/mL and 250 µg/mL for the AT-40kV and AT-60kV samples, respectively. And the results of AT(Non-irradiated) and AT-80kV samples showed MIC between 500-1000 µg/mL. Thus, we obtained results that clearly demonstrate that electron-beam irradiated AgI is a promising biocidal agent for several emerging microorganisms.

Synthesis and Characterization of Antimicrobial Properties in Chitosan Scaffolds Crosslinked with Ag_3PO_4

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Scaffold utilization is expanding significantly, particularly within the biomedical realm. Within tissue engineering and regenerative medicine, scaffolds are pivotal, regulating the local microenvironment and offering benefits such as enhanced cellular anchoring, colonization, and metabolic activity. Chitosan scaffolds, formed initially as a gel and then lyophilized to create a porous three-dimensional structure resembling native tissue properties, provide structural support while facilitating nutrient, growth factor, and cell diffusion. In this work, chitosan scaffolds were developed using Ag_3PO_4 particles obtained via the coprecipitation method as a cross-linking agent. The concentrations of Ag_3PO_4 necessary for chitosan's spontaneous gelation were varied from 0.5% to 8.0% (wt), followed by comprehensive physical-chemical characterizations. Additionally, computational simulations were conducted to elucidate the mechanism behind spontaneous cross-linking, focusing on the interaction between chitosan monomers and the low-index surfaces (100), (110), and (111) of Ag_3PO_4. Furthermore, the antimicrobial efficacy of lyophilized scaffolds was assessed against methicillin-resistant *S. aureus* (MRSA) and *P. aeruginosa*, and the cytotoxicity was evaluated using the *in vivo* model *C. elegans*.

Acknowledgments

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Synthesis and evaluation of chitosan/FeWO4 films as potential antimicrobial material

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Therapeutic strategies based on nanotechnology offers a promising approach to overcome limitations in prevention, diagnosis, and therapies against opportunistic pathogens. Nanomaterials with biocidal properties can be utilized in personal protective equipment and disinfection protocols to prevent SARS-CoV-2 contamination, as well as in vaccines or immunomodulators. [1,2] On that matter, the semiconductor FeWO4 was synthesised by microwave-assisted hydrothermal method and thermically threated. The obtained powered was structural characterized through X-ray Diffraction, Raman Spectroscopy, and UV-Vis Spectroscopy, while morphological aspects were analysed through scanning electron microscopy. To evaluate the biocide potential, tests minimum inhibitory concentration (MIC) was taken against Gram positive and Gram negative bacterias, such as S. Aureas and E. Coli, respectively. Additionally, the sample was analysed against a very common fungus, Candida Albicans. At the end, it is pretended to evaluate the effects against Sars-CoV-2 and support this semiconductor on versatile matrix.

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Synthesis and nanoparticles preparation of cationic amphiphilic PULL-DEAE with different degrees of substitution.

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Cationic polysaccharides have been increasingly searched for biomedical applications, due to their relevant properties, such as electrostatic conjugation with anionic biomolecules, such as nucleic acids and proteins, mucoadhesive interaction, pH responsiveness, and other [1]. Pullulan is a polysaccharide produced by the fungus Aureobasidium pullulans, which presents relevants properties in the biomedical application, such as biocompatibility, non-toxicity, and hydrophilicity, besides presenting several hydroxyl groups in the backbone which makes possible to chemically modify [2]. However, due to the high hydrophilicity, pullulan is not capable of self-aggregation, to apply for nanoparticles formulation [2]. Therefore, in this work, pullulan was chemically modified with different 2-chloro-N,N-diethylethylamine (DEAD) (6,641%, 13,283 % and 19,925% w/w), resulting in a cationic pullulan (PULL-DEAE) with different capacity of self-aggregation. Following the synthesis, the nanoparticles based on PULL-DEAE was prepared by nanoprecipitation method. For the characterization, the chemical modification was successful confirmed by 1H NMR, and FTIR, besides, Critical Aggregation Concentration (CAC) confirmed the amphiphilic of PULL-DEAE. The nanoparticles were characterized in terms of and zeta potential, observing an increase in pH sensitivity with higher amounts of DEAE. Therefore, the material presents a potential polysaccharide to be applied in drug carrier and gene delivery.

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BS02-Intelligent self-assembled and supramolecular nanomaterials for health and energy applications

Dynamic Redox Switching – From Sensors to Molecular Machines

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Molecular switches are highly sought after to enable the reversible modulation of various molecular properties such as electronic structure, charge or conformation, which facilitates numerous applications in sensing, (opto)electronics, energy storage or molecular machines. Herein, a range of dynamic redox switches, which undergo a secondary switching process following a redox event, will be discussed. This includes redox-active supramolecular hosts in which various non-covalent interactions, such as hydrogen, halogen or chalcogen bonding can be judiciously turned ON or OFF. This enables the construction of redox-switchable anion receptors which also serve as powerful electrochemical sensors.[1] For example, their integration into self-assembled monolayers enables highly tunable, sensitive and continuous flow anion sensing.[2] Additionally, redox-driven conformational switches based on overcrowded alkenes, such as bisthioxanthylidenes, will be discussed. These systems undergo conformational changes following redox stimulation, enabling highly reversible multi-state switching of color, fluorescence, polarity, geometry and (anti)aromaticity.[3]

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Lanthanides(III) based compounds: different strategies for luminescent temperature sensing

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Nowadays, as traditional contact temperature reading methodology becomes inefficient, alternatives have been emerging, such as remote measurements, with emphasis on luminescence thermometry searching for highly sensitive and accurate thermometers [1]. In this scenario, the unique optical properties of a variety of lanthanide ions have proven to be attractive for composing the architecture of the most diverse types of luminescent temperature sensors [2]. Therefore, our research group and collaborators have been studying different strategies and architectures in the use of trivalent lanthanide ions to evaluate their viability as temperature sensors. The different approaches range from lanthanide ions as dopants in inorganic matrices, such as $LaAlO_3$, $LiYF_4$, SrY_2O_4, in hybrid or non-hybrid systems, to as metallic centers in complexes based on ligands that act as antennas. In this way, core@shell type up-converter nanoparticles containing Er^{3+} or Tm^{3+} and Yb^{3+} ions covered suitable layers, phosphor downshifting red emitters doped with Eu^{3+} and/or $Tb^{3+/4+}$ and also Eu^{3+} complex [3] supported in a polymeric film had their thermometric behavior monitored in the biological temperature interval as well as under higher and lower temperature range depending on the lanthanide ion involved and the type of excitation. In all systems the traditional ratiometric approach was applied and the main figures of merit were estimated and interpreted considering the likely dominant mechanisms in each case and their potential applications envisioned.

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Protein assembly in understanding Alzheimer's disease progression.

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Alzheimer's disease (AD) is a slow but relentlessly progressing neurocognitive disorders that affects memory and cognition in individuals. The two principal proteins implicated in the pathology of AD are amyloid-beta (Aβ) and tau isoforms whose total content can be quantified in cerebrospinal fluid (CSF) and blood using commercially available biochemical assays. In this talk, I will present results from a preclinical study conducted in collaboration with neurologists using atomic force microscopy (AFM) to resolve and quantify the morphology of protein aggregates at a single particle level adsorbed on red blood cells (RBCs) and those present in CSF from patients at various stages of decline in memory and cognition. The AFM measurements revealed patient age and stage of neurocognitive disorder-dependent differences in morphology of protein aggregates on RBCs, referred to as physical biomarkers. The prevalance of pathological fibrils on RBCs when correlated negatively with CSF- Aβ 42/40 ratio was observed to be significantly higher in Aβ-positive patients. Next, we detected direct evidence for protein fibril length to be correlated with AD severity from AFM mapping of CSF from AD patients. The findings highlight the diagnostic relevance of physical biomarkers obtained using nanoscale imaging under standard laboratory conditions.

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Protein Cages as Responsive Materials

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Hybrid materials between biological and synthetic macromolecules can have interesting properties, as these materials combine the function and precision of biomacromolecules with the versatility of their synthetic counterparts. In recent years we have studied the assembly of (virus capsid based) proteins on a variety of scaffolds with different shapes and functions, such as charged polymers, nanoparticles, and DNA origami[1].

Encapsulins are protein cages found in bacteria that have interesting properties with respect to (thermal) stability and cargo loading. In the past we and others have studied the application of encapsulins, but so far, their preparation, durability and functionalization are restricted to fundamental studies[2].

Recently, we reported the design of encapsulins with functional loops on its surface[3]. This allows for future site specific genetic or chemical modification. Both the genetic and chemical manipulation of the encapsulin based protein cages allows for the introduction of functional compounds, such as fluorescent proteins for recognition of enzymes for therapeutic applications. Exciting new developments are the introduction of moieties that respond to an external trigger, where promising results are obtained with - amongst others - light responsiveness.

In the present contribution, I will highlight our studies towards functional materials by combining synthetic compounds with plant virus-based proteins. Furthermore, the latest results on the modification of biomacromolecular cages based on Encapsulins with triggered responses will be discussed. The presented research paves the way for further design, engineering, and production of protein-polymer materials, for instance for drug delivery, vaccine development or other health applications.

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Active-Hinge Micro-Origami Tessellations for Reshapable Electronic Applications

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Choreographing the transformation of patterned surfaces into adaptable shapes, to exhibit designable mechanical interactions with their environment, is a complex challenge. We have introduced a new category of strain-engineered dynamic-shape materials that allow for diverse multi-dimensional shape modulation, leading to unprecedentedly adaptive microarchitectures.[1] Using micro-origami tessellation, we can create strategic creases in manifold materials that house actuator micro-hinges. These hinges autonomously reshape upon electrochemical cues. Examples of these novel 4-dimensional (4D) metamaterials include freestanding multifaceted folded structures, auxetic mesosurfaces, and dynamically morphing cages. Such 4D mesostructures are integrated into dual proof-of-concept demonstrations that pave the way for more intelligent shape-changing biomedical technologies, viz. a morphogenetic micro-supercapacitor for high-density energy conversion and storage applications, and a dynamic-shape microelectronic soft implant prototype.[1] These realizations lay the groundwork for designing comprehensive 4D metamaterials,[2] setting a vista to the tangible realization of electronic information-driven morphogenesis.[3]

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Electrically driven dynamic molecular switches that can learn

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There is strong drive to develop "intelligent" devices that mimic key aspects from living systems. This Nature inspired approach to develop device with life-like properties may lead to new ways of energy efficient computing (like our brains) or sensing. Switches constitute a fundamental component in any circuitry, therefore we are developping a new type of molecular switch that can learn, change and adapt. Normally molecular switches are static, meaning they can only switch between discrete on and off states irrespective of their past. We are developping dynamical switches that couple different processes with different time-constants leading to time-dependent, or dynamical, switching behavior. These switches can remember their past and change their switching probability depending on how often and how quickly they are switched. Their switching dynamics can also be influenced by their anvironment and show the ability to adapt their structure in response to applied voltage. This work demonstrates that dynamical molecular switches pave the way to complex molecular devices where multiple electronic functions are programmed within a single molecular layer.

Embedding electronic function in dynamic nanostructures

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Molecular electronics operates in the quantum realm of distances less than 100 nanometers. This provides new opportunities to complement and extend silicon-based technology for high-density, low-energy computing. In this talk I will describe the difficulties encountered in designing materials at the nanoscale, and present recent research in which massively parallel computer simulations are guiding experiments in the creation of novel materials for a broad range of device applications. I will describe our attempts to decipher design rules for the synthesis of organic thin films and molecular crystals that exhibit technologically useful switching and memory storage.

Enhanced Luminescence Lateral-flow Assay (ELLA) for Urinary Biomarker Monitoring

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Developing effective portable sensors for precise biomarker detection is vital in early disease diagnosis yet remains a formidable task. To tackle this challenge, we created the Enhanced Luminescence Lateral-Flow Assay (ELLA), harnessing highly luminescent upconverting nanoparticles (UCNPs) alongside a portable reader and smartphone App. Demonstrating the sensor's efficacy and adaptability, we conducted kidney health monitoring as a proof of concept. We designed Er^{3+}- and Tm^{3+}-doped UCNPs coated with multiple layers, including an undoped inert matrix shell, a mesoporous silica shell, and an outer layer of gold (UCNP@mSiO_2@Au). These coatings synergistically amplify emission by over 40-fold and facilitate biomolecule conjugation, making UCNP@mSiO_2@Au user-friendly and suitable for diverse bio applications. Employing these optimized nanoparticles in lateral flow assays, we successfully detected two acute kidney injury (AKI)-related biomarkers—kidney injury molecule-1 (KIM-1) and neutrophil gelatinase-associated lipocalin (NGAL)—in urine samples. Leveraging our sensor platform, KIM-1 and NGAL can be precisely detected and quantified within the range of 0.1 to 20 ng/mL, with low limits of detection at 0.28 ng/mL and 0.23 ng/mL, respectively. Validating our method, we analyzed clinical urine samples, obtaining biomarker concentrations closely correlated with ELISA results. Significantly, our system enables biomarker quantification in under 15 minutes, highlighting the efficacy of our novel UCNP-based approach and its potential as dependable, rapid, and user-friendly diagnostics.

Exploring Photoluminescent Self-Assembled Monolayers on Commercial Glass for Biomedical Detection: A Promising Approach

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Exhaled air, comprising gases, Volatile Organic Compounds (VOCs), and aqueous microdroplets, serves as a critical matrix for detecting lung diseases, including Covid-19. During the onset or resolution of a disease, biochemical processes in the body emit gases and VOCs, which can traverse from the bloodstream to the lung alveoli and subsequently be detected in exhaled air. Gas chromatography plays a pivotal role in this domain due to its capacity to identify, separate, and quantify trace-level gases. However, traditional gas chromatography systems are bulky, lack real-time detection capabilities, and are not easily adaptable to diverse environments.
Therefore, this project aims to develop an optical platform on glassy systems utilizing a strategy of chemical functionalization of Self-Assembled Monolayers (SAMs) for the immobilization of advanced photoluminescent materials such as Lanthanide Complexes and perovskites.
A wide array of techniques, including Single X-ray diffraction, powder X-ray diffraction, Raman Spectroscopy, Transmission Electron Microscopy, and Photoluminescence Spectroscopy, are employed to characterize the materials.
To assess the viability of the synthed materials for detecting VOCs, theoretical investigations and experimental photoluminescent analyses were conducted. The results suggest that the observed photoluminescent changes found in complexes and perovskite in the presence of VOCs are attributed to resonance between the density of states of the complex and the target, rather than a direct reactivity between them.
Finally, the functionalization on glass substrates of advanced photoluminescent materials demonstrated the formation of an Optical Platform with potential for Biomedical Compound Sensing. Moreover, there us the possibility of further enhancement of efficiency by incorporating ligands with energy levels resonant with biomarkers.

Intelligent Polymeric Nanocomposites: Modulating Mechanical Properties Through Magnetic Stimuli

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Intelligent or stimulus-responsive polymeric nanocomposites exhibit properties modulated by incorporated nanostructures in response to stimuli (temperature, light, magnetic fields, etc.). Although optimizing formulations necessitates studying parameters like dispersibility, matrix/nanoparticle compatibility, the mechanical property measurement under a magnetic field adds complexity to the investigation. In this study, we developed nanocomposites based on poly(butylene-adipate-co-terephthalate) (PBAT) and Fe3O4@poly(1,4-butanediol) nanoparticles (IONPs), exploring their mechanical behavior under a magnetic field. Nanocomposite films, produced via tape casting, demonstrated homogeneity and high transparency, indicating excellent IONPs dispersion. By varying the IONP/PBAT mass ratio, films exhibited magnetic properties that increased with NPs content. Thermal analysis (DSC and TGA) suggested that IONPs possess a polymeric molten shell, potentially indicating fluid iron-like behavior at room temperature, which could pave the way for magnetically-responsive materials. We anticipate confirming that the applied magnetic field altered Young's modulus, reflecting IONPs' orientation, and stiffening the material. These findings hold promise for modulating mechanical properties and expanding applications to devices, packaging, and smart textiles.

Urease Nanoflowers in Conjugated Polymers as thin films: an alternative approach for biosensor

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Enzymes are well-known for their catalytic efficiency and wide application, such as in biocatalysis and the development of biosensors [1]. Complementarily, nanoparticles (NP) present properties for developing devices employed in catalysis. In 2012, Zare et al. discovered a new class of nanoparticle: enzyme hybrid nanoflowers (EHN), which are nanostructures that combine enzymes and NP [2]. Despite the various reports about the synthesis and applications of EHNs, there are few studies about the immobilization of these nanostructures on solid supports. The present work brings a novel approach by immobilizing nanoflowers in thin films using a conjugated polymer (CP) matrix. Particularly, CPs present optoelectronic properties that can be combined with the improved catalytic activity of EHNs. The spin coating and casting techniques were used to form thin films of CP/urease EHN. The adsorption of the nanoflowers onto the polymer matrix was confirmed by UV-Vis and FTIR techniques. Subsequent studies using fluorescence spectroscopy enabled the observation of a quenching effect, suggesting interchain interactions between the film layers. The catalytic activity measurements for films with 1 to 3 layers indicated higher values for the 2-layer film, reinforcing the interactions suggested by the quenching effect, which may reduce the activity due to active site obstruction for the thicker film. Therefore, this work demonstrates a promising strategy for immobilizing urease-based EHN on solid supports with potential applications in biosensor development by leveraging the synergistic effects of material functionalities. Acknowledgments: INEO, Capes, and FAPESP (grant number 2020/04427-2, 2014/50869-6).

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Binary bile salts/nanocellulose aggregates for potential use as rheological modifiers and drug release

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Binary bile salt systems can be aggregated in different morphologies, that are altered by intermolecular interactions with other particles [1, 2], such as cellulose nanocrystals (CNCs) or nanofibrils (CNFs), interfering in the viscoelastic properties of the systems [3]. Here, aggregates of sodium deoxycholate (NaDC)/sodium taurodeoxycholate (NaTDC) formed by (i) 50/9.2, (ii) 100/9.2, (iii) 100/50, and (iv) 50/50 (mM/mM) mixed with 0.96, 2.40 or 4.80 g/L CNC or CNF were obtained. Dynamic Light Scattering showed medium-sized aggregates (101 – 650 nm), except for system (iii) with CNCs (< 100 nm). Zeta Potential indicated stable dispersions (values greater than |30| mV) and the system (iv) with CNFs is the most stable. Zero-shear viscosity increased with the increment of CNC or CNF for all systems. However, systems (i), (ii), and (iii) containing CNCs or CNFs exhibit low viscoelasticity, while system (iv) showed high viscoelastic properties. Small-angle X-ray Scattering curves showed the formation of elongated and cylindrical aggregates in system (iv) with CNF, explaining the high viscoelasticity and gel-like behavior for this system due to the entanglement among the aggregates. Supramolecular nanomaterials of binary bile salts with nanocellulose can be used as rheological modifiers and/or as a platform for the controlled release of specific substances.

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Development of luminescent nanoparticles based on Nd3+ and Yb3+ for use as nanothermometers in biological systems

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Lanthanide-doped luminescent nanoparticles (NPs) have recently gained interest due to their wide range of application possibilities. Since they have well-defined emission peaks, high photostability, low toxicity, easy color tunability, and low background noise, they have been used as promising candidates in biosensing. In this scenario, the neodymium in its trivalent state (Nd3+) stands out as a doping ion thanks to its excitation and emissions localized between the first and second biological windows in the near-infrared, which allow deep penetration in biological systems. In addition, co-doping with the trivalent ytterbium ion (Yb3+) enables a temperature-dependent phenomenon called phonon-assisted energy transfer. Thus, the combination of these two ions allows the exploration of optical nanothermometry in a wide variety of applications related to thermal monitoring. In this work, using the high-temperature co-precipitation method, we synthed core NaYF4 NPs doped with 10% Yb3+, followed by a 10% Nd3+ doped layer, and an inert undoped matrix shell. For further applications, the NPs were coated with a mesoporous silica (NP@mSiO2) layer or decorated with amino groups (NP-NH2) to facilitate conjugation to additional molecules. Structural characterizations confirmed the purity and the hexagonal crystalline structure of the sample. Additionally, the emission spectra of the produced particles displayed the characteristic emissions of Yb3+ and Nd3+ at 980 nm and 1059 nm relative to the transition 2F5/2 → 2F7/2, and 4F3/2 → 4I11/2, respectively. The optical thermometry tests showed a linear response with a thermometric parameter defined by Δ=I_1059/I_980 and relative thermal sensitivities of S_r= 0,34% K-1 for NP, S_r= 0,26% K-1 for NP@mSiO2 and S_r= 0,33% K-1 for NP-NH2. Due to their unique properties, the produced optimized nanoparticles present great potential to be used as nanothermometers in biological applications, especially when combined with photothermic agents.

Formation of bile salt-lecithin-carboxymethyl cellulose hydrogels: rheological and structural properties

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The self-aggregation of surfactant molecules has been widely investigated, for instance, bile salts and lecithin [1-3]. The great interest in these particular materials is due to their potential applications in the cosmetic, food, and pharmaceutical industries [1, 2]. Above the critical micellar concentration (cmc), lecithin and bile salts undergo self-aggregation, forming different morphologies such as spherical and cylindrical micelles [3]. The addition of carboxymethyl cellulose can modify the rheological and structural properties of lecithin/bile salt aggregates, as reported with other molecules [3]. In this work, systems with different proportions of sodium cholate (NaC), lecithin, and carboxymethyl cellulose were obtained. Zeta Potential (ZP) showed that systems with higher carboxymethyl cellulose content were more stable. Rheological properties show that systems with higher concentrations of bile salt and carboxymethyl cellulose were more structured and viscoelastic.

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Influence of sodium dodecyl sulfate in organically modified silicate xerogels for the adsorption of crystal violet dye

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Synthetic dyes, commonly used industrially, when discarded incorrectly in water, can damage aquatic life, such as fish and plants [1]. Crystal Violet (CV) is a dye used mainly in the textile industry. It can cause severe irritation if in contact with the human skin [1]. A promising method for removing such dyes from water is adsorption, where porous materials can encapsulate compounds in their pores. Very few studies exist in the literature with organically modified silicate xerogels and surfactants as adsorbents for dyes. In this work, the efficiency of two materials for the adsorption of CV was evaluated, one containing the surfactant sodium dodecyl sulfate (SDS) and another without SDS. The xerogels were prepared following the methodology described in [2] using basic catalysis. One of the materials was prepared without modification (SiO_2-NM), and in the second material, glycidyl propyl trimethoxysilane and SDS were added (SiO_2-G-SDS). Results have shown that in higher concentrations, SiO_2-G-SDS showed higher values of quantity of dye adsorbed per gram of adsorbent material (q_e). The values of q_e and concentration in equilibrium (C_e) for both xerogels are best adjusted to the non-linear Langmuir isotherm model. The values for the maximum quantity adsorbed (q_{max}) were 29,54 mg g^{-1} and 40,87 mg g^{-1} for SiO_2-NM and SiO_2-G-SDS, respectively. SiO_2-G-SDS has shown promising efficiency for the adsorption of CV due to the electrostatic interaction between the anionic SDS micelles and the cationic dye. Results have shown that these materials can help treat industrial wastewater.

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Mesoporous Nitrogen-Doped Holey Reduced Graphene Oxide: Preparation, Purification, and Application for Metal-Free Electrochemical Sensing of Dopamine

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Holey graphenic nanomaterials with porosity within the basal plane attract significant interest. It is observed that the perforation of graphene can enhance the specific surface area of the nanosheet, ensuring effective wetting and penetration of electrolytes to the electrode surface, facilitating rapid charge transfer, and boosting the electrocatalytic efficacy of the transducers. This study reports the first example of nitrogen-doped holey reduced graphene oxide with a mesoporous morphology of the graphene basal plane (N-MHG). It is shown that N-MHG can be synthesized through a one-step hydrothermal treatment of GO using NH3 and H2O2. A straightforward procedure for the purification of N-MHG has also been developed. AFM, TEM, and Raman analyses have revealed that N-MHG possesses a highly mesoporous network structure with a pore ranging from 10 to 50 nm. X-ray photoelectron spectroscopy data have indicated a partial reduction of the graphene oxide sheets during the etching process but also show a 3–5 times higher content of C=O and O–C=O fragments compared to rGO. This could account for the remarkable stability of the N-MHG aqueous suspension. The mesoporous morphology, strong functionalization of the particle edges, and the high degree of aromatization of the core indicate the high potential of N-MHG in membrane technology, including membranes for electrochemical sensors. N-MHG was used to construct an electrocatalytically active membrane on a glassy carbon electrode (GCE) for electroanalytical dopamine (DA) determination. DA is an important neurotransmitter that is essential in modulating brain function. N-MHG demonstrates better electrochemical characteristics than non-porous GO in DA determination. When immobilized on GCE, it not only enhances the current of the sensor but also reduces the overpotential of DA oxidation and reduction, shifting the peaks to lower voltages. This makes the DA redox process on GCE-Nf/N-MHG quasi-reversible.

Molecular interaction of heparin and proteins- A relationship with SARS-CoV-2

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Interactions between proteins and drugs can lead to the formation of stable complexes and have important implications for several processes related to human health. These interactions can affect, for example, the distribution, free concentration, biological activity and metabolism of drugs in the bloodstream. This work presents an investigation based on spectrophotometry (UV–Vis) on the interaction of albumin with heparin (HEP) in aqueous solution and in the form of films, under physiological conditions. Results from analytical models, molecular dynamics and calculations of binding constants indicate that increasing temperature leads to a decrease in the molecular interaction of HEP with albumin, with dynamic interaction, and secondary bonds. Morphological analyzes with fractality assessment corroborate the results. Simulation results suggest that the interaction of HEP with the SARS-CoV-2 spike protein should be stronger, with little variation over time. The weak interaction between HEP and albumin contributes to greater availability of the drug, which inhibits viral invasion in addition to disrupting microthrombi that prevent oxygenation in patients infected with SARS-CoV-2. The investigation of biological systems in solutions or in the form of films has allowed the analysis of complex formation using unconventional pharmacokinetic techniques.

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NANOSTRUCTURED FILMS FOR INVESTIGATION OF NON-CONVENTIONAL MATERIALS IN THE TREATMENT OF LEISHMANIASIS

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Cutaneous Leishmaniasis, CL, is a neglected disease that remains a relevant public health problem. Considering the low interest of the pharmaceutical market in the research and development of new drugs for neglected diseases, the lack of innovation and the scarce therapeutic alternatives for the treatment of CL, new strategies are needed to increase access to treatment and reduce the time taken to cure CL. The interaction between proteins and drugs has important implications for processes directly related to health, and can result in the formation of stable complexes that have important effects on distribution, free concentration and biological activity. One way to investigate the interaction mechanisms between these molecules is to seek to understand the physicochemical properties of these materials in the form of films. Therefore, in this work, the interaction of albumin protein with conventional drugs used in the treatment of leishmaniasis was investigated. The study is complemented by the estimation of the binding constant, in addition to the investigation of theoretical models in order to obtain results that contribute to a better understanding of the physical processes involved in the formation of layers by self-assembly. The use of theoretical models to describe the interaction processes and how this changes the properties of the interface, in addition to the quantitative analysis of microscopy results, contribute to the analysis of non-conventional healing surfaces for the treatment of leishmaniasis.

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Rheological properties of bile salt and nanocellulose hydrogels: kinetic study

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Bile salts, such as sodium deoxycholate (NaDC) and sodium taurodeoxycholate (NaTDC), are biosurfactants that, above their critical micellar concentration (cmc), form self-aggregates spontaneously. These self-aggregates can be modulated through intermolecular interactions established with other species, such as cellulose nanocrystals (CNCs) and nanofibrils (CNFs), resulting in systems with different rheological properties [1]. Those properties can change over time as aggregates evolve into different morphologies [2,3]. In this work, simple and binary samples of NaDC and NaTDC containing CNC and CNF were obtained. The viscoelasticity of the systems was evaluated over time, showing an evolution from more fluidic systems to stronger hydrogels at 1 week and at 16 weeks, respectively. This result indicated that a higher entanglement density between bile salts and nanocellulose particles was formed in a longer time [3]. The rheological properties of systems formed by NaTDC were more affected by time than NaDC systems, suggesting that the kinetic of formation of more entangled aggregates is slower for systems formed by NaTDC.

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Tungsten oxides for photocatalytic degradation of Rhodamine-B

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Abstract

Photocatalysis is a green technology whith can be used mainly in environmental remediation. We obtained tungsten oxides through the reaction of tungstic acid (TA) with hydrogen peroxide and ammonium hydroxide, in presence of ascorbic acid (AA). The photocatalysts degrade Rhodamine B (RhB) solution (values between 65.6% and 75.0%).

Keywords: tungsten oxide, ascorbic acid, rhodamine-B degradation

Introduction

Tungsten oxides have attracted much interest in recent years due to their excellent physicochemical properties. Its applications include photocatalysis, in addition to their good stability [1]. Among its main uses, we highlight photocatalysis for environmental applications. RhB can accumulate in the digestive system, causing diseases, in addition to being potentially carcinogenic [2]. Tungsten oxides were synthed and the photocatalytic performance on degradation of RhB investigated.

Methodology

Tungstic acid (4 mmol/L) were mixed with 100 ml of H2O2 and added to the structuring agent (0, 4, or 20 mmol of ascorbic acid, AA) in 100 ml of ammonium hydroxide. Systems were evaporated and calcined at 650 ºC. Similar systems were examined but underwent heat treatment via reflux after complete system solubilization.

Results

Raman spectra of all samples showed characteristic vibration bands of tungsten oxide and x-ray diffractograms have shown monoclinic phase. The band gaps of the samples decrease slightly with increasing AA proportion, independent of the chosen method. The main species are W(VI) and W(V). Conclusions AA is responsible for a decrease in band gap values. The amount of AA, as well as the processing, are responsible for materials with different photocatalytic performances.

Acknowledgments

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BS03-Advanced Materials and Surface Treatments for Biological, Dental, and Medical Applications

Hierarchical materials for biomedical application by additive manufacturing and liquid metal dealloying

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The close match between the elastic properties of an implant material and the bone is crucial to avoid the stress shielding effect. Therefore, low modulus biomaterials are desirable for biomedical implants that ensure rapid healing of hard tissue. In this work, novel hierarchical metal-polymer composites that "break" the common trend between strength and elastic modulus were synthesized by additive manufacturing and liquid metal dealloying. In the first step, the porous precursor TiCu-based scaffold was manufactured by laser powder bed fusion. Second, this additively manufactured precursor scaffold was subjected to liquid metal dealloying using liquid magnesium. Third, the magnesium was removed by chemical etching to obtain hierarhical porous titanium alloy. The large submillimeter porosity of this hierarchical porous alloy is induced by additive manufacturing, while its fine micrometer scale porosity is due to the processing by liquid metal dealoying. To obtain the hierarhical metal-polymer composite, the hierarhical porous titanium alloy was impregnated by a polymer. The mechanical characterization of the hierarhical metal-polymer composite reveals moderate strength and low elastic modulus in the range of that found for bone. The results suggest that these novel composite materials, which mimic the structure and mechanical behavior of bone, are potential candidates for biomedical applications.

HIERARCHICAL NANOSTRUCTURED BIO-INTERFACES TOWARDS ENHANCED CELL GUIDANCE

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In tissue engineering, biological, physical, and chemical inputs are combined to mimic cellular environments for different biomedical needs. The study of the tripeptide Arg-Gly-Asp (RGD), the binding site of different extracellular matrix proteins, has allowed the production of a wide range of cell adhesive surfaces. Although the surface density and spacing of the RGD peptide at the nanoscale have already shown a significant influence on cell adhesion, the impact of its hierarchical nanostructure is still rather unexplored. Accordingly, a versatile colloidal system named quatsomes, based on fluid nanovesicles formed by the self-assembling of cholesterol and surfactant molecules, has been devised as a novel template to achieve hierarchical nanostructures of the RGD peptide dramatically enhancing cell adhesion as a novel tissue engineering strategy.[3]
We will also present: i) The use of protein nanoparticles (pNPs) to provide simultaneously physical and biochemical stimuli to cells in 2D and 3D scaffolds; ii) A cell adhesion study with spatio temporal control using SAMs of an electroactive molecule as a dynamic interface to immobilize RGD upon the application of a low electric potential.[1,2]

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How cells surf the waves?

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Biological cells are strongly influenced by their environment which can be described in terms of chemical, topographical and mechanical properties. More specifically, the influence on cell fate of mechanical stimuli applied directly or by changing topography of their microenvironment has been extensively studied over the past three decades. The capacity of mechanical forces or of the cell-scale microenvironment to modulate cytoskeletal organization and cell contractility and to induce downstream signaling events is defined as mechanotransduction. The mechanotransduction mechanism justifies the existence of mechanosensors that will translate the mechanical input into a biochemical input inside the cells. The role of the cell nucleus as a mechanosensor has been only recently confirmed [1]. In this talk, I will illustrate the role of the nucleus in the response of cells to topography at their own scale. Our recent discovery of a new cellular migration ability which we term "Curvotaxis" will be detailed [2,3].

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Innovations in 3D Skin Models on a chip: Mechanical Stimulation and Melanoma Research

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This study presents advancements in 3D in vitro skin models on a chip, focusing on the effects of mechanical stimulation and their application in melanoma research. Using a state-of-the-art skin-on-a-chip platform, we explored how cyclic mechanical forces influence skin model differentiation and integrity. Our bioimaging and RNA sequencing results revealed increased expression of Keratin 10 and Keratin 14, as well as enhanced formation of desmosomes and tight junctions, indicating improved skin structure and mechanical strength. Gene expression analysis suggested significant cellular responses, potentially linked to the Hippo pathway. Concurrently, we characterized 3D skin models, including those with integrated melanoma, to assess their structural and genetic accuracy. These models closely mimicked human skin morphology and gene expression, with full-thickness models showing the highest resemblance. Incorporating melanoma cells preserved skin-like properties and gene expression profiles, confirming these models as robust platforms for cancer research. The models' responsiveness to vemurafenib treatment validated their use in drug testing and highlighted the importance of the microenvironment in cancer progression. These findings highlight the potential of advanced 3D skin models in biomaterials research, providing ethical and effective alternatives for studying skin biology and developing cancer therapies.

Nanostructures in life: bone is a nanomaterial

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In this lecture, the concept of bone as a nanomaterial will be introduced. Examples of biomimetic synthesis of biomaterials inspired by the composition and structure of the bone tissue will be also presented and related to the treatment of diseases.

Progress in the Design of New Low-Cost β Ti-Alloys for Bio-Implants

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There is an ever-increase in the world demand of more biocompatible metallic implants for long term implantation. A perfect bio-implant should show excellent chemical, mechanical and biological compatibility. In the commercial biomedical alloys, there are many concerns on its mechanical properties mismatching with human bone, corrosion resistance and ion release or toxicity after implantation. Many researches are being done to develop new alloys for long-life implantation with excellent biocompatibility (represented by low Young's modulus, high strength, high wear resistance, high fatigue strength, high specific strength, high corrosion resistance and high biological compatibility) through developing new Ti-alloys composed mainly of the high compatible alloying elements. Therefore, in the last two decades, many β Ti-Alloys were developed consisting of biocompatible elements such as Zr, Nb, Mo, and Ta and show excellent mechanical properties including low Young's modulus. However, a recent attention was directed towards the development of low cost β Ti-Alloys that have a minimum amount of the high melting point and high cost rare-elements such as Ta, Nb, Mo, and W. This comes with substituting these metals with the common low-cost and biocompatible metals such as Fe, Mn, Sn, and Si, while keeping excellent mechanical properties without deterioration. Therefore, the investigation of mechanical and biological biocompatibility of those low-cost alloys is highly recommended now to guide for a commercial alloys with excellent biocompatibility for long-term implantation. Among these low-cost alloys, Ti-5Fe-3Nb-3Zr alloy showed excellent biocompatibility confirmed by animal tests in addition to its high mechanical properties compared to the commercial Ti-6Al-4V ELI alloy. Also, the α+β Ti-2Mo-0.5Fe, Ti-3Mo-0.5Fe and near-β Ti-5.7Mo-5.4Fe alloys showed high corrosion resistance, high hardness and strength and high cytocompatibility.

Umbilical cord derivatives and bone regenerative medicine

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The perinatal tissues including human placenta and umbilical cord are housing numerous bioactive macromolecules, growth factors, with an array of high-quality mesenchymal stromal cells. These cells are utilized in both research and medical applications due to their sustainable sourcing (natural birth biowaste), high viability, low immunogenicity, multipotent lineage and immunomodulatory properties. Perinatal tissue-derived macromolecules present also an opportunity in the tissue engineering and regenerative medicine fields with minimal ethical constraints. The Wharton’s jelly, a part of the umbilical cord, is mainly composed by type I, III, V and XV collagens, hyaluronic acid and various growth factors and peptides that exert various beneficial biological effects, such as antibacterial activity, antifibrotic influence and immunomodulation. Mechanically, Wharton’s jelly is highly deformable (isotropic tissue) and withstands the progressive stretching of the growing embryo as well as protects it from external traumas. In view of such advantages, recently, hydrogels derived from Wharton’s jelly matrix are developed. These hydrogels are expected to support in situ cell attachment, proliferation and function while avoiding infection. However, due to the fast degradation and low elastic modulus in biological environment, the application of Wharton’s jelly derived materials (i.e. tissue and hydrogels) in bone regeneration is compromised. An overview of umbilical cord biomaterials and their application in bone regenerative medicine will be presented.

Advancements in dual-setting cements for medical applications: the synergy of magnesium potassium phosphate with natural hydrogels

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Bone tissue has inherent regenerative capabilities. However, the integration of biomaterials is sometimes critical to enhance the healing process. Bone cements are particularly noteworthy for their biofunctional properties. Among them, magnesium phosphate cement (MPC) is recognized for its rapid setting, high mechanical strength, and osteogenic benefits. Nonetheless, it faces issues such as brittleness and injection challenges. Therefore, this study focuses on developing biocomposite cements based on MPC and various natural hydrogels to address these limitations. The study involves fabricating cements by combining calcined MgO and KH2PO4, along with aqueous solutions of polymers: sodium alginate, gellan gum, and kappa-carrageenan, cross-linked ionically or physically with various parameters. The resulting biocomposites underwent comprehensive analysis, including physicochemical, mechanical, and biological assessments. Research reveals that the developed cements exhibit a diverse and complex microstructure, effectively incorporating k-struvite crystals within a hydrogel matrix. The materials demonstrate more controlled setting times due to the additional gelation reaction and reduced thermal emissions, alongside marked enhancements in paste consistency, injection capabilities, and reduced brittleness. Furthermore, the cement’s biocompatibility, as demonstrated through assays with human osteoblasts, underscores their potential for biomedical applications. In conclusion, the creation of these novel dual-setting biocomposite cements surpasses the common limitations of traditional bone cements, offering a notable alternative that may significantly enhance bone repair, particularly through their application in minimally invasive procedures.

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A novel strontium-flavonoid complex for bone regenerative medicine

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Among the issues studied in regenerative medicine are those related to bone defects. Although bone has the ability to self-regenerate, factors, such as age, fracture extent, and diseases, could hinder this ability. Currently, one of the ultimate choices for osteoporosis treatment is strontium ranelate (SrR). Despite its beneficial effect on bone homeostasis, there are several adverse effects related to its administration reported in the literature, which demands the development of more tolerable and bioactive Sr2+ carriers. Therefore, we used quercetin (Q), a natural flavonoid with antioxidant activity as a new ligand for Sr2+ by synthesizing a complex (SrQ). The complex was characterized by elemental analysis, thermogravimetry, UV-vis, infrared spectroscopies and nuclear magnetic resonance, and the results confirmed the complexation of Sr2+ among the 3-OH and 4CQO groups of quercetin, resulting with the following chemical formula [(C15H7O7)Sr2].6(H2O). The effect of SrQ complex on pre-osteoblast (MC3T3 Subclone 14; ATCC CRL-2594) differentiation was investigated. According to our results, no cytotoxicity was detected for treatment with 10 e 80 µM of SrQ at the end of 72 h exposure, although only quercetin showed high cytotoxicity at 80 µM. In addition, the treatment of pre-osteoblasts with the higher concentration of SrQ complex increased phosphatase alkaline activity by about 167% at the end of 7 d of exposure. Alizarin red-S staining revealed an increase of 204.9 ± 2.3 and 247.4 ± 1.9% in extracellular matrix mineralization for treatment of the cells with 10 and 80 µM of SrQ at the end of 14 d exposure. Taken together, our results showed the beneficial effect of the new synthetized SrQ complex on osteoblast differentiation and its potential as a biomaterial for bone regenerative medicine.

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Antibacterial Tannic acid-enzyme-based multilayer coatings

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Biofilm formation on synthetic materials presents formidable challenges due to its hygienic and functional problems, particularly in healthcare settings where it contributes to hospital-acquired infections. Methods to functionalize materials and design effective antibacterial coatings are the extreme importance to prevent biofilm formation. Among functionalization methods, layer-by-layer (LbL) stands out because it enables a multifaceted defense mechanism by combining antimicrobial agents and physical barriers to inhibit bacterial growth and can be performed under mild conditions which is favorable to preserve the activity of bioactive compounds [1]. A multitude of compounds can be assembled to design antibacterial multilayer coatings such as antibiotics, metal nanoparticles, and surfactants. However, the immobilization of these substances is limited due to antibiotic resistance, toxicity, and efficiency. Tannic acid (TA), a natural polyphenol, can be complexed with proteins and displays antioxidant and antibacterial properties. Antibacterial enzymes, effective in targeting components of the extracellular polymeric matrix, offer a strategy to disrupt biofilm without affecting planktonic growth or increasing bacterial resistance [2]. In this study, we propose a bio-inspired approach utilizing TA and antibacterial enzymes to develop antibacterial LbL coatings. The multilayer film was monitored by Quartz Crystal Microbalance, and the enzymatic activity of the films and TA release were investigated using a spectrofluorometer. Preliminary findings indicate reproducible films that release TA in physiological conditions and exhibit tunable enzymatic activity based on the number of deposited bilayers.

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Bactericidal activity of Cu-doped porous TiO2 coatings produced via MAO

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The Micro-Arc Oxidation (MAO) technique is a very versatile and uncomplicated alternative for the functionalization of titanium alloys [1]. It is widely known that titanium and its alloys are among the most used metallic biomaterials. This use is because they have excellent biocompatibility, corrosion, and wear resistance, and good mechanical properties [2]. However, these materials are bioinert, can cause infections, and do not have high osseointegration capacity, contributing to the increase in cases of implant failure [3]. The Ti-30Nb-5Mo alloy is a recently developed β alloy with a low elastic modulus and hardness and better wear resistance than Commercially Pure titanium (CP-Ti) [2]. Thus, this study aimed to functionalize the surface of this alloy via MAO to increase its biological activity, bringing the ability to better adhere to osteoblastic cells.

Furthermore, different concentrations of copper chloride were incorporated into the electrolyte solution to analyze the influence of different amounts of copper incorporated into TiO2 coatings on the bactericidal activity of the materials. The results showed that the presence of copper in the coatings effectively reduced the growth of Staphylococcus aureus, Enterococcus faecalis, Pseudomonas aeruginosa, and Candida albicans strains on the treated surfaces. The oxidation process induced the formation of a porous anodic coating, which created a rougher surface that enhanced its osseointegration. Furthermore, copper did not make the material cytotoxic in in-vitro tests and did not affect the differentiation of adipose tissue-derived mesenchymal stem cells (AMSCs).

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Biodegradable Mg-3Y Alloy Prepared by Selective Laser Melting and Spark Plasma Sintering

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This work explored possibilities of biodegradable magnesium alloy Mg-3Y preparation by two modern powder metallurgy techniques – spark plasma sintering (SPS) and selective laser melting (SLM). The powder material was consolidated by both methods utilising optimised parameters, which led to very low porosity (~0.3%) in the SLM material and unmeasurably low porosity in the SPS material. The main aim of the study was the thorough microstructure characterisation and interrelation between the microstructure and the functional properties, such as mechanical strength, deformability, and corrosion resistance. Both materials showed comparable strength of ~110 MPa in tension and compression and relatively good deformability of ~9% and ~21% for the SLM and SPS materials, respectively. The corrosion resistance of the SPS material in 0.1 M NaCl solution was superior to the SLM one and comparable to the conventional extruded material. The digital image correlation during loading and the cross-section analysis of the corrosion layers revealed that the residual porosity and large strained grains have the dominant negative effect on the functional properties of the SLM material. On the other hand, one of the primary outcomes of this study is that the SPS consolidation method is very effective in the preparation of the W3 biodegradable alloy, resulting in material with convenient mechanical and degradation properties that might find practical applications.

Chitosan-based antibacterial coating on PDMS surfaces for medical devices: Sustained Moxifloxacin released and superior coating adhesion over time

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Central venous catheters (CVCs) are widely used to administer chemotherapy, hemodialysis and other treatments. Often made of polydimethylsiloxane (PDMS), these devices pose an intrinsic risk of long-term infection due to potential biofilm formation, increasing the risk of complications. Drug-releasing polymer coatings are a well-known strategy for tackling these type of infections. However, controlling 1) the release of the antibacterial agent, and 2) the adhesion of the coating to the substrate over time remain major challenges. Consequently, this work aimed to design a chitosan-based coating engineered for maximum adhesion and stability to ensure sustained drug release and antibacterial properties for at least 14 days.

A coating composed of chitosan (CS) as drug carrier, caffeic acid (CA) and copper sulphate (Cu) as crosslinkers, and moxifloxacin (Mox) as an antibiotic, was deposited by casting process a PDMS surface functionalized with dopamine. PDMS surface modifications were assessed by X-ray photoelectron spectroscopy (XPS), and Fourier-transfer infrared (FTIR). Antibiotic release over time was assessed in pseudo-physiological conditions and quantified by fluorescence. Coating adhesion was evaluated over time using a specially designed pull-off test, before and after 14 days of ageing.

XPS and FTIR analyses demonstrated the successful modification of the PDMS surface. The CS-CA-Cu-Mox coating exhibited sustained moxifloxacin release for up to 49 days. In addition, the coatings displayed antibacterial activity for 21 days against E. coli, and for 14 days against S. aureus. Importantly, the coating remained stable and showed high adhesion even after ageing.

In conclusion, this study provides new insights into the adhesion behavior of chitosan-based coatings, with sustained drug release and antibacterial properties, on polymer medical devices, which is rarely reported in the literature.

Chitosan-based antibacterial films: Focus on relationship between crosslinkers and drug release kinetics

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Biofilm formation is one of the primary causes of biomaterial-associated infections (BAIs). Antibacterial coatings offer a promising solution to preserve the success of implanted biomaterials. Chitosan is a biocompatible biopolymer used to produce films for antibiotics controlled release. Despite several advantages, crosslinking is mandatory for tuning drug release, and rare are the studies that report how crosslinkers affect the drug release kinetics [1]. Therefore, the influence of two antibiotics (gentamicin or moxifloxacin) and two crosslinkers (tannic acid/iron or caffeic acid/sodium periodate) was evaluated on the release kinetics in chitosan-based films. The kinetics was assessed using HPLC/UV-Vis for moxifloxacin, and HPLC/MS for gentamicin, respectively. Additionally, antibacterial activity against S. aureus and E. coli was assessed through disk diffusion testing and indirect antibacterial activity over time. Results indicate that moxifloxacin showed prolonged release in the films with tannic acid when compared to caffeic acid. For films with gentamicin, the opposite effect was observed. Swelling and mass loss results were similar among the films, indicating that these parameters had no influence on release time. The differences in kinetics may be associated with the intermolecular interactions between the drug and the crosslinker. In conclusion, in order to produce coatings for short-term or long-term antibiotic release, it is necessary to consider the nature of the antibiotic interaction with the polymer matrix and the crosslinker. Therefore, these insights are useful to design coatings for medical devices with on demand release time.

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Development and characterization of a novel low-cost high-entropy alloy for potential application as bone fixation devices

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High entropy alloys (HEAs) are recognized for their emerging biomedical applications owing to their diverse crystalline structures, including HCP, BCC, or FCC. Coupled with a low elastic modulus and remarkable mechanical strength, HEAs offer a compelling combination of properties sought in biomedical implants [1]. Even though the current HEAs do not fully accommodate the complex biomechanical loads of the human body and lack optimal interaction with the biological host, they still hold potential for significant advancement in biomedical applications [2]. This study aimed to create a novel Bio-HEA based on non-toxic, low-cost, and non-refractory alloying elements, including Ti, Zr, Mn, Al, Nb, and Fe. The ingots were produced by argon arc melting and subjected to a homogenization heat treatment. The chemical composition was assessed using density, XRF, and EDS measurements. Structural and microstructural analyses were carried out using XRD, optical microscopy, and SEM. Finally, Vickers microhardness and elastic modulus measurements were taken to evaluate the selected mechanical properties. The samples demonstrated a complete mixture of all alloying elements in a solid solution, with an overall density of around 6.0 g·cm-3. The XRD profiles exhibited the formation of a dual-phase composition (BCC and HCP). Vickers microhardness measurements showed an average value above 450 HV, higher than some commercial metallic biomaterials. Besides that, the elastic modulus values remained close to 95 GPa. The results indicated that the obtained Bio-HEA grouped promising characteristics for potential use in biomedical applications, especially as implants and fixation devices.

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Development of Artificial Tendon using PCL fibers and Type I Collagen. An evaluation of 3T3-NIH Growth and Differentiation into Tenoblasts.

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There is significant interest in tendon tissue research due to thousands of people worldwide suffering from injuries or diseases[1]. Research in tissue engineering aims to improve conventional repair methods by offering parameters such as cells, structures, mediums and others[2]. Interesting scaffolds and three-dimensional structures can be obtained by the process of Rotary Jet Spinning by collecting fibrous material through various ways. Collagen type I is also proven to be a scaffold like material. This work aims to study cellular growth and differentiation within a type I collagen matrix and a fibrous Polycaprolactone (PCL) scaffold, forming a three-dimensional composite scaffold. PCL polymer fibers was prepared at suitable conditions and processed using a rotating jet spinning equipment, then, type I collagen was incorporated into this PCL scaffold to mimic the biochemical properties of natural tendon tissue. Morphology and surface structure of this final composite scaffold was analyzed by scanning electron microscopy (SEM) and optical microscopy. Subsequently, 3T3-NIH cells were added onto the final material to compose an artificial tendon.

Scanning Electron Microscopy (SEM) showed efficient fiber/matrix contact and Live and Dead staining after 7 days cellular culture showed that 3T3-NIH cells have successfully adhered within the composite. This study demonstrates the feasibility of the composite scaffold for tendon tissue engineering.

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Development of Bioactive Grafts via Tape Casting for Biomedical Applications

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Bioactive grafts have attracted significant attention in biomedical research, particularly in the field of bone tissue engineering, due to their potential in promoting bone regeneration [1]. This study investigates the development of bioactive grafts for biomedical applications, as an alternative potential for tissue engineering. The synthesis of these composite material involves the incorporation of bioactive glass particles into natural polymeric matrices such as collagen using tape casting technology. The bioactive glass stimulates bioactivity and tissue regeneration within the grafts, while the natural polymeric matrix provides a biocompatible and flexible structure for the cells [2]. The methodology comprises the selection of appropriate biomaterials for the graft development; the preparation of the slurry that will undergo tape casting processing; the production, drying, and crosslinking of the grafts. Characterization techniques, including scanning electron microscopy (SEM) and X-ray diffraction (XRD), are employed to evaluate the structural and morphological properties of bioactive grafts. These analyzes play a fundamental role in optimizing composition and processing parameters, ensuring desired properties including particle/matrix adhesion, morphology, and porosity, crucial requirements for effective grafts in tissue engineering applications. Overall, bioactive glass/natural polymer grafts represent promising biomaterials with immense potential for advancing biomedical technologies and improving patient outcomes.

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Elaboration of calcium phosphate composites beta tricalcium phosphate/copper-doped hydroxyapatite

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Calcium phosphate ceramics-based bone substitutes are constantly evolving. These materials of choice, known for their bioactive and osteoconductive properties (hydroxyapatite: HA, $Ca_{10}(PO_4)_6(OH)_2$) and even resorbable (beta tricalcium phosphate: βTCP, $Ca_3(PO_4)_2$), individually do not meet all the required criteria [1]. However, doping with ions of interest (Cu^+, Si^{4+}, etc.) can be used to modulate material degradation, adjust osteoinduction, and has been found beneficial for angiogenesis and osteogenesis. The purpose of this study is to combine copper-doped HA (CuHA) [2], with low solubility and promoting angiogenesis, with a resorbable βTCP matrix to adjust and control the dissolution rate of the produced biphasic compound while stimulating prolonged angiogenesis.

The undoped HA and βTCP were synthed by aqueous co-precipitation. βTCP-CuHA pellets were prepared by mixing CuO, HA and βTCP powders (at different powder ratios βTCP/CuO+HA), and sintering. The thermal behavior was studied by dilatometric and thermogravimetric analysis. X-ray diffraction (XRD) and temperature programmed XRD, scanning electron microscopy (SEM), and Archimedes' method were performed to characterize the composites microstructure and chemical composition.

The addition of CuO + HA powder up to 50 % in βTCP powder did not affect the densification of biphasic materials, however the grain growth was reduced. Dense pellets were produced after a thermal cycle at 1100°C during 1 hour. Structural analyses showed that copper ions could enter the bTCP lattice or the HA one depending of the sintering temperature, which can be of particular interest to adjust copper release and the biological behaviour of the composites. Dissolution experiments and cell culture are under progress.

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Engineered Protein to Control Biomolecular Phase Separation from Intrinsically Disordered Proteins

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Intrinsically disordered proteins (IDPs) have attracted a huge amount of interest in fundamental biology, as it has been discovered that they can drive the formation of membraneless organelles through a phase separation process within cells [1]. In this work, IDPs were mined [2] for consensus repeat sequences to develop a biomaterials platform capable of undergoing liquid-liquid phase separation (LLPS). First, amino acids were classified into four categories. Then, the protein sequences and subsequences were encoded into these classes to form a simplified protein sequence. The algorithm aligned the simplified sequence to various repeat unit cassette lengths and compared the repeats *via* a one-hot encoding strategy. Later, we translated the consensus repeat cassette length into possible sequences. Among the outputs of the algorithm, we found sequences and explored their phase separation in the presence of a panel of different biomolecules. The engineered proteins and their parent IDPs were ordered for expression in *E. coli.* Proteins were purified under denaturing conditions and lyophilized for coacervation tests. The ability of the proteins to form phase separation complexes was verified *via* turbidometry. Results showed that the engineered protein exhibited similar coacervation behavior to native protein. Therefore, by probing sequences of IDPs for areas of high repetition, we hypothe that new consensus repeat sequences can be prospectively mined and extracted to establish an engineered protein material platform around these systems.

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Enhanced synergistic therapy: Gold Nanorods/MCM-41 nanocarrier for chemotherapy and photohyperthermia

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The optical properties of gold nanoparticles are widely investigated with interest in their application in photohyperthermia cancer treatments [1]. Coating these nanoparticles with MCM-41 silica not only protects the gold nanoparticles but also has the potential for use as a nanocarrier, due to its textural properties [2]. This nanocarrier allows the incorporation of drugs, such as methotrexate (MTX), for use in chemotherapy [3]. Therefore, this work investigates the incorporation and release of MTX from the nanoplatform of gold nanorods coated with MCM-41, for application in chemotherapy together with photohyperthermia. The nanomaterial incorporated with MTX drug was developed with significant MTX incorporated into the material. The drug release assays demonstrated that the incorporated MTX was released in a controlled way and the profile of the MTX release curves indicate that the main drug release mechanism was by Fickian diffusion. Drug release results under laser radiation showed a greater increase in temperature and drug release, suggesting that these two therapies can be combined for more effective results. The nanomaterials do not present cytotoxicity to tumor and non-tumor cells, while the nanomaterials incorporated with MTX showed toxicity only to tumor cells, highlighting the relevance of nanoplatforms developed for therapeutic applications. Subcellular localization assays showed that nanomaterials were located within the cytoplasm and close to the nucleus, demonstrating that the delivery of the therapy, photohyperthermia and/or chemotherapy would be more efficient due to the proximity of the cell nucleus, causing greater damage to the tumor cells.

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Exploiting the MAO Oxide Growth in High-Entropy Alloys under Diverse Anodic Voltage Conditions

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This study evaluated the effect of alloying elements, applied voltage, and bioactive species (Ca, P, and Mg) enrichment in the micro-arc oxidation (MAO) treatment of novel high entropy alloys (HEAs) targeted for biomedical applications [1]. The non-equiatomic TiZrNbTaMo (TaMo), TiZrNbTaMn (TaMn), and TiZrNbFeMo (FeMo) samples were submitted to MAO treatment at distinct voltages (100, 200, and 300 V) [2], then their chemical, phase, and morphological aspects were evaluated by x-ray photoelectron spectroscopy (XPS), x-ray diffraction (XRD), and electron microscopy (SEM and TEM). Finally, the physicochemical behavior regarding contact angle measurements in distilled water at room temperature was evaluated. The results indicated that the alloying elements played a role in the phase composition, possessing distinct proportions of BCC and HCP phases. The MAO-treated surfaces depicted different mechanisms of anodic oxide growth and dielectric breakdown, forming the typical porous surface at distinct applied potentials. The bioactive species (Ca, P, and Mg) were gradually enriched in the oxide layer, composed of nano-crystalline and amorphous layers, typical of MAO-treated surfaces. As a result, the contact angle values of the MAO-treated samples were dependent on the applied voltage, indicating potential for use in the biomedical field, especially as temporary implants and bone fixation devices.

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Formulation with coffee pulp extract for wound healing

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Coffee pulp stands out as a significant by-product generated during coffee processing [1]. These by-products hold potential for application in the pharmaceutical and cosmetic industries [2]. The aim of this study was to develop a formulation utilizing coffee pulp extract to improve wound healing. To accomplish this coffee pulp extract was incorporated in a water-in-oil emulsion and available its cytotoxicity, antibacterial and, healing properties. It showed non-cytotoxicity and exhibited a minimum inhibitory concentration of 3 mg/mL against S. aureus. The formulation was stable with a white, creamy appearance, a slightly yellowish color in the presence of the extract, a pH close to 6, density of 0.96 g/mL, and viscosity of 51,333 ± 2,309 cP. Over 90 days, the formulation maintained stability. Additionally, a keratinocyte scratch assay indicated that the formulation promoted cell migration, leading to increased scratch retraction after 24 hours. In summary, the development of a formulation utilizing coffee pulp has shown promising results with antibacterial properties for potential use in wound healing products.

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Microstructure and defect structure evolution in magnesium alloys processed by severe plastic deformation

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Commercial Mg alloys MgAlZn and MgZnZr were processed by hot extrusion and equal channel angular pressing (ECAP) known as EX-ECAP. Microstructure and defect structure evolution with strain introduced to the material by severe plastic deformation were investigated by TEM, positron annihilation spectroscopy (PAS), and X-ray diffraction. Significant grain refinement and the bimodal structure was obtained for smaller number of passes. Further ECAP pressing resulted homogeneous gain distribution and the average grain of 500 nm. The dislocation density evolution with strain as determined by PAS followed the same scheme in both alloys. In the ex-extruded condition a very low density of dislocations of the order of 10^{14} m^{-2} was observed. Sharp increase of dislocation density by the factor of 2 occurred during the first two passes of ECAP, followed by saturation and even a decline manifesting the dynamic recovery at higher strains. After 8 ECAP passes the density of $1.1x10^{-14}$ m^{-2} was observed. XRD line-profile analysis confirmed the results of PAS with slightly higher values of dislocation densities in individual conditions, in average by the factor of 5. Detail analysis of contrast factors allows to determine the type of dislocations, in particular the fraction of screw dislocations in the extruded condition was 13, while in EACP deformed specimens, the fraction increased by a factor of 5 and corresponds to the evolution of the total density of dislocations with the highest value of 70% in the condition after 2 ECAP passes and slight decline to 47 and 42% after 4 and 8 passes respectively. The influence of microstructure on mechanical properties is rather complex and controlled by the dislocation density, texture and grain evolution with strain due to ECAP.

Osteoblast cell migration and abrogated cell contact guidance on radio-frequency plasma polymerized allylamine thin films

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The increase in instances of age-related diseases like osteoporosis drives a greater demand for bioactive orthopedic implants that have the ability to integrate into osteoporotic bones. One method of creating bioactive implants is coating materials with amino-rich polymers such as trimethoxysilylpropyl modified poly(ethyleneimine) and poly(allylamine) [1-2]. In this study, we prepared radio-frequency plasma polymerized allylamine (rf-PPAAm) thin films on titanium substrates with varying amine content, and we investigated the osteoblast cell migration and the abrogated cell contact guidance behavior on the surfaces of these materials. The thin films were prepared by plasma polymerization of allylamine on 1 x 1 cm titanium-coated flat and micro-grooved silicon wafer substrates using a custom-built radio frequency plasma with a vertical configuration [2-3]. The plasma polymerization of allylamine was performed at a controlled pressure of 0.2-0.4 mbar with power ranging from 20 W to 60 W, polymerization time of 10 mins, and duty cycle varying from 2% to 100%. The thin films were then characterized by water contact angle measurements, Zeta potential measurement, profilometry, and X-ray photoelectron spectroscopy. Cell spreading, cell migration, and cellular contact guidance abrogation assay using MG-63 osteoblastic-like cells were investigated using LSM780 and LSM800 confocal microscopes. Results show varying osteoblast cell behaviors, depending on the quantity and quality of amine groups on the surfaces of the thin films.

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Osteocompatible tannic acid cross-linked wharton jelly hydrogel: new guide for bone regeneration

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New multifunctional hydrogels with antioxidant and antibacterial properties are today needed to meet the modern challenges in tissue regeneration. One popular approach to generate these hydrogels is to use decellularized tissues. The as- hydrogels have weak mechanically properties, are unstable against reactive oxygen species and challenging to handle. By taking advantage of the polyphenol chemistry[1], we herein aimed to design a new family of Wharton Jelly (WJ) derived hydrogel, using a dual cross-linking strategy. WJ-derived macromolecules were extracted from decellularized WJ according to Freytes method[2,3]. The self-standing hydrogel was obtained in physiological conditions (pH7, 37°C). A dual WJ-hydrogel network using tannic acid (TA) infusion was applied to improve the hydrogel features. To circumvent the cytotoxicity of TA an oxidation with periodate was performed. The TA oxidation was limited to the edge of the hydrogel, suggesting the formation of a TA "reservoir" within the hydrogels. Compared to WJ hydrogel, the covalently cross-linked TA-WJ hydrogel showed an increase in the gel fraction, elastic modulus along with an increase in the resistance to the collagenase degradation. The TA was released from the "reservoir", exerting therefore its biological effects. Indeed, in comparison with WJ hydrogel, the crosslinked TA-WJ hydrogels showed a limited bacteria proliferation; scavenging of the excessive intracellular accumulation of ROS; osteosarcoma cell apoptosis; and osteogenic properties with an increase in parietal bone volume and hardness after 12 weeks of implantation in rat calvaria critical defects. Taken together, these results showed the osteo-biocompatibility and the great potential of TA-WJ-based hydrogel for bone regeneration.

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pH-Responsive Microparticles Derived from Novel PDPA-Containing Copolymers: Synthesis, Characterization, and Potential Applications

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This study investigates the properties and potential applications of novel random copolymers, namely poly(2-(diisopropylamino)ethyl methacrylate))-rand-polymethylmethacrylate (PDPA-rand-PMMA) and poly(2-(diisopropylamino)ethyl methacrylate))-rand-butyl methacrylate (PDPA-rand-PBMA). Synthed via reversible addition-fragmentation chain transfer (RAFT), these copolymers were utilized to fabricate highly monodisperse pH responsive microparticles using the microfluidics droplet generation technique. Microparticles exhibits pH-responsiveness due to the presence there of the PDPA block with the pKa ~6.8. When the pH is lower than the pKa of PDPA, the amine groups become protonated making the PDPA block soluble in an acidic environment that leads to the alternation in chain properties of microparticles and to the release of potentially encapsulated cargo molecules. Furthermore, this phenomenon leads to the positively charged surface of microparticles that may be used for the attachment of negatively charged bacteria which can be applied for the decontamination of aquatic environments or as biofilm management. To demonstrate changes in charge on the microparticles caused by the protonation of amino groups on the PDPA block, we examined the interaction between microparticles and negatively charged latex resin beads using confocal microscopy imaging. Importantly, when the pH exceeds the pKa of PDPA, no significant interaction between the beads and microparticles is observed.This comprehensive approach provides valuable insights into the pH responsiveness of PDPA-containing copolymers and their behavior in biological environments, offering promising avenues ranging from targeted drug delivery to bacteria entrapment.

Prolonged antibacterial activity of chitosan-based coatings on PDMS and polyethylene for medical device applications

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Biomaterial-associated infections (BAIs) are a global concern. To prevent such infections, antibacterial coatings for medical devices can be a promising solution. These coatings can be produced using biocompatible natural polymers, such as chitosan, which have shown prolonged antibacterial activity in previous works [1,2]. In this study, two different formulations were used to produce coatings on polydimethylsiloxane (PDMS) and polyethylene (PE), materials commonly used in medical devices. To ensure coating adherence, flat specimens of 1.5x1.5x0.2 cm3 underwent pre-treatments. PDMS was treated with NaOH 2.5 M for 20 min in ultrasonic bath, while PE was treated with piranha solution for 6h. Next, the samples were soaked in polydopamine (DOPA) 2 mg/mL at pH: 8.5 overnight, dried and cleaned. Finally, samples were drop-coated with mixtures of 1% chitosan, 5% moxifloxacin, 20% tannic acid and 5% iron (TA-Fe) or 1% chitosan, 5% moxifloxacin, 5% caffeic acid and 5% sodium periodate (CA-PS) and dried at 40ºC. The coatings were analyzed for moxifloxacin release kinetics in phosphate buffer saline by HPLC/UV-Vis, during 6 months. The results showed that coatings containing TA-Fe sustained the antibiotic release for over 4 months, while coatings containing CA-PS sustained it for two weeks. Antibacterial activity was confirmed against E. coli and S. aureus. Both coatings remained attached to the substrate during the release study. In conclusion, antibacterial coatings suitable for long-term and short-term applications were obtained, providing valuable insights for modifying medical surfaces aiming prevention of BAIs.

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Silicone breast implants and the biological risks associated to their degradation or rupture

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Silicone breast implants for cosmetic or reconstructive purposes are among the most widely used medical devices. It is now accepted that they can cause a wide range of chronic inflammatory diseases or cancer. Breast implants trigger a foreign body reaction which leads to the formation of a fibrotic tissue called capsule that isolates the implant from the rest of the body. The capsule, and the immune cells that patrol it, then become the first recipients of silicone substances released from the implant, including silicone oils leached from the gel through the shell and eroded shell debris. We have previously published a transcriptomic analysis of explanted capsules showing that the expression of certain inflammatory genes was significantly higher in fibrous capsules formed around macrotextured implants (1). Our current focus is to analyze changes in tissue organization and transcriptomic signatures in human periprosthetic tissues exposed to silicone. We combined histological analysis (43 patients) and gene expression profiling (RNA sequencing, 21 patients) of samples from patients with silicone breast implants and performed systematic cross-comparisons. In this pilot study, we considered implant integrity (intact vs ruptured), surface texture (macro- vs micro-texture) and implant filling (serum vs silicone). Overall, this work shows that silicone exposure induces immune responses, including pathology-related markers. Furthermore, it shows that the immune system is able to discriminate between different sources of silicone and that serum-filled and gel-filled microtextured implants are the least immunogenic implants. In conclusion, this study provides the first biological evidence of an association between silicone implants and autoimmune markers, highlighting the need for further research and stricter implant safety regulations.

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Structural characterization of novel multicomponent Ti-based alloys for use as hard tissue replacements

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Metallic biomaterials play a crucial role in medicine, especially as replacements of hard tissues and bones for orthopedy and dentistry. In this scenario, evaluating their physical properties is imperative for a proper lifespan adjustment of the material after implantation [1]. With the coming of novel multicomponent Ti-based alloys, with the chemical composition set up by theoretical design methods, like the molecular orbital theory and entropy concept, the comprehension of the phase stability and chemical composition relationship is essential to promote a complete understanding of their mechanical properties [2]. In this study, the phase stability and crystalline structure of some novel multicomponent Ti-based alloys (Ti-Al-V, Ti-Al-Fe, and Ti-Al-Fe-Cr) were evaluated by in situ X-ray diffraction (XRD) measurements and correlated with the microstructural and mechanical aspects. The results indicated that Bragg's peaks of the Ti's phases (α and β) moved toward low angles, resulting in an augment of the lattice parameters with the temperature. From the lattice parameters vs. temperature plot, it was possible to note that the thermal expansion coefficient was anisotropic on the hexagonal close-packed structure and depended on the solid solution's chemical and phase composition. These results were then correlated with the changes in the atomic bonding provided by each alloying element, and their impacts on the manufacture of biomedical implants were evaluated. Acknowledgments: FAPESP (grants #2023/15812-2, #2021/13921-3, and #2024/03148-3) and CAPES PrInt (grant #88887.898681/2023-00). References: [1] Pinto, B. O. et al., Scientific Reports, v. 13, p. 4349 (2023).
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Surface Characterization of Ti-Nb-Zr Ternary Alloy Coatings Sputter Deposited on Si (100) Substrate

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Ti, Nb, and Zr are non-toxic and non-allergenic biocompatible metals, and their ternary alloys with body-centered cubic structure (β phase) present lower elastic moduli, shape memory effect, and superelastic characteristics that are desirable for biomedical applications [1]. Nevertheless, bulk β-Ti-Nb-Zr alloys are much more costly than stainless steel and Co-Cr alloys commonly used as implants. An interesting approach to dealing with this limitation would be to coat an implant with a β-Ti-Nb-Zr thin film with adequate composition to enhance the material biocompatibility [2]. However, the ideal amounts of the constituent elements in the Ti-Nb-Zr ternary system are undetermined. Combinatorial strategies allow for the simultaneous production and characterization of many alloys, and magnetron sputtering is suitable for producing ternary alloy coatings with various compositions. In this work, Ti, Nb, and Zr targets were positioned in a triangular configuration below a Si(100) wafer substrate, and a composition gradient was formed over the substrate area by magnetron co-sputtering. Five samples were cut from different patches of the coated wafer with the following compositions (at.%): $Ti_{67}Nb_{21}Zr_{12}$, $Ti_{49}Nb_{13}Zr_{38}$, $Ti_{43}Nb_{42}Zr_{15}$, $Ti_{36}Nb_{59}Zr_{5,}$ and $Ti_{22}Nb_{58}Zr_{20}$. The physicochemical characteristics of the Ti-Nb-Zr coatings were characterized by SEM-EDS, XRD, AFM, and XPS. Mainly the β phase was detected and the coating surfaces were oxidized, providing better corrosion protection, and benefitting biomedical applications.

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Surface Evaluation of 361L Stainless Steel for Orthopedic Implants

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In the Brazilian Unified Health System (SUS), stainless steel is widely used in orthopedic applications for its mechanical strength, corrosion resistance, and cost-effectiveness. However, it has drawbacks such as high density and susceptibility to bacterial biofilm formation post-surgery. This study aims to enhance 316L stainless steel surfaces to prevent surgical site infections, a common issue in orthopedic trauma surgeries. Electrochemical methods like anodization were used to modify the surface, improving osseointegration and reducing infection risks. Mechanical polishing was done to remove surface irregularities before anodization with galvanostatic control in an acidic solution. Surface characteristics were evaluated using optical microscopy, and roughness was measured via mechanical roughimetry. Five current parameters were tested, showing a correlation between applied current and surface roughness. SEM-EDX was used to identify metallic components of the alloys. A nonlinear relationship between current and voltage was observed during electrochemical polishing. Optical microscopy at 100x and 200x magnifications revealed changes in surface texture, such as pitting at different currents. Roughness measurements with an SJ-210 roughness meter showed a decrease in roughness with lower currents. The results indicate that electrochemical polishing significantly reduces surface roughness, potentially lowering infection risks and enhancing implant performance in SUS orthopedic applications.

Synthesis and evaluation of the hemolytic potential of cassava gum hydrogel incorporated with thymol

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Low-cost, highly biocompatible biomaterials drive research linking biotechnology to regenerative medicine. Cassava derivative-based hydrogels, noted for their exceptional absorbency, facilitate effective integration of bioactive compounds like thymol. Thus, the aim was to analyze the cytotoxicity of cassava gum hydrogel with thymol (HGMT) through the hemolysis assay to evaluate its hemolytic potential. The hydrogel was prepared as described by Lima[1] followed by adding necessary components and thymol. Initially, a leachate of the lyophilized material was produced at four concentrations [2]. A hemolysis test was conducted according to a previously described protocol[3]. Erythrocytes were diluted and incubated with leachate, results were assessed by measuring absorbance at 405 nm. Statistical analysis was performed by ANOVA followed by Dunnett's test (*$p<0.05$).The hydrogel at the lowest concentration exhibited the lowest percentage (6%) of hemolysis, while the leachate from the hydrogel at its maximum concentration showed the highest hemolytic potential of the material (18%). Although this difference did not reach statistical significance. The results suggest that, regardless of variations in diluted hydrogel concentration, HGMT extracts did not show significant differences in their ability to induce hemolysis under the evaluated experimental conditions. Consequently, the analyzed biomaterial exhibits no apparent residual hemolytic activity, being considered potentially innocuous for medical applications.

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Acid-actived vermiculites as adsorbents for ranitidine

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The presence of drugs in water has become an ecological problem and the focus of many different studies, due to the low biodegradability and high toxicity of these organic contaminants [1]. Ranitidine (N-[2-[[[-5-[(dimethylamino)methyl)]-2-furanyl] methyl] thio] ethyl] -N'-methyl-2-nitro-1,1-ethenediamine hydrochloride) is a drug used in the treatment of gastrointestinal diseases and generates harmful subproducts when photodegraded, making it highly toxic to living beings [2]. Among water treatments, adsorption is an alternative, and natural adsorbents, including clay minerals, have been evaluated in recent years [3]. In this work, vermiculite (V_0) was activated with 2.0 and 3.0 mol L^{-1} HNO_3 resulting in Va2 and Va3, respectively. The activated solids were applied in ranitidine removal and parameters such as pH, adsorbent dosage, contact time, and initial drug concentration, were evaluated. The solids were characterized by X-ray diffractometry, chemical analysis, infrared spectroscopy, thermogravimetry, textural analysis, and scanning electron microscopy. The XRD results showed a reduction in the intensity of the reflection of plane (002), indicating loss of crystallinity as the acid concentration increased. The infrared spectra presented changes in the 1082-673 cm^{-1} region, related to structural modification after the acid activation. The Va2 and Va3 exhibited the better performance at pH 10, 100 mg of adsorbent at 60 min, resulting in removals of 84.1 and 85.1%, respectively. The drug removal by V_0 was 20.5% using 125 mg of adsorbent.

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Alternative Chemical Route in Low-Pressure Plasmas for Disinfection of Medical-Doctor Devices Fabric

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Aprons and surgical drapes, gloves, and masks are devices used in medical-hospital procedures that are discarded after use. Despite presenting conditions for reuse, disposal is necessary because there is no validated sterilization method for these devices. In addition to adding costs to medical-hospital procedures, disposal has environmental impact. In this work, new chemical sterilization routes for fabrics in low-pressure plasma are proposed. Polypropylene fabric, from commercial N95 respirators, were exposed to plasmas excited from mixtures of 50% of citric acid alcoholic solution (C6H8O7), 25% of nitrogen, and 25% of oxygen. The base, gas, and working pressures were respectively adjusted to 2X10-2 Torr, 5X10-2 Torr, and 7X10-2 Torr. The plasma was established by applying radiofrequency signal (13.56 MHz) to the lower electrode, grounding the upper one. The fabric samples were attached to both electrodes, and the treatment time was 10 minutes. The effect of plasma excitation power, ranging from 100 to 300 W, as well as the of the treatment electrical configuration (driven or grounded electrode), on the morphology, elemental composition, chemical structure, wettability, and sterilization efficiency of the fabric contaminated with Saccharomyces cerevisiae fungi was investigated. Results reveal that the polypropylene fibers remained intact, regardless of the electrical treatment configuration and the excitation power. Compositional, structural, and morphological changes were observed only on the surface of the fibers. The material's water receptivity was altered only for the treatment conducted at 300 W, on the driven electrode. The highest sterilization efficiency was provided by 100 W plasmas, which also resulted in the least alteration of the fiber structures. These results will be correlated with the plasma composition under each excitation condition for full interpretation.

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Analysis of Biocompatibility of Innovative Titanium Alloys: Modulation of Signaling Pathways and Epigenetic Regulation

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The trajectory of biomaterials is marked by continuous evolution, from the early metallic implants used in orthopedics to the more advanced and personalized materials developed today. Titanium and its alloys play a crucial role in orthopedic and dental implants due to their outstanding biocompatibility, corrosion resistance, and excellent strength-to-density ratio compared to other biomedical alloys. Among the titanium alloys used globally for orthopedic implants, the most commonly used is the Ti-6Al-4V alloy [1]. However, concerns have recently arisen regarding releasing aluminum and vanadium from corrosion or wear processes in such alloys, prompting increased scrutiny of their widespread use [2]. Recent research has shown that these elements may pose long-term health risks, with vanadium associated with cytotoxic effects in tissues and aluminum linked to neurological disorders, including Alzheimer's disease [3]. Surface modifications, such as micro-arc oxidation (MAO), are widely recognized in the biomedical field for their benefits. These modifications achieve greater control over protein absorption, increase corrosion and wear resistance, and enhance cellular adhesion. The research focused on analyzing the biocompatibility of Ti6Al4V alloys with specific surface modifications, namely Ti6Al4V with calcium and phosphorus addition and Ti6Al4V with calcium, phosphorus, and oxides addition. To this end, in vitro cytotoxicity assessments were conducted to investigate the viability of these new materials for biomedical applications, with their ability not to interfere with cellular growth processes being the primary criterion. The results showed no cytotoxic effects in all studied samples. In addition to preliminary cytotoxicity tests, a more in-depth analysis of the effects on cellular and molecular responses was made to elucidate how the new alloys influence gene expression and epigenetic patterns in bone cells. Financial support: FAPESP - Proc. 2021/12073-9.

Antimicrobial cellulose nanofibers/ silver niobate aerogels for tissue engineering

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Human tissues, like skin, bone and cartilage are often damage by mechanical trauma, chronic diseases and tumors [1]. To improve patients' life quality different materials have been developed to regenerate human tissues, however, there is a lack of multifunctional materials with capacity of not only regenerate the injured tissue, but also act as an antibiotic agent. Aerogels are porous ultralight solid materials with very low density and high specific surface area [2]. These are essential properties for tissue regeneration, since it allows cell growth and nutrients and oxygen transport. In this work, we developed a composite aerogel based on cellulose nanofibers and silver niobate. Cellulose can provide high flexibility and strength to the scaffolds, while silver niobate has potential to act as antimicrobial and regenerative agent. The composite aerogels were obtained by freeze drying and four compositions were evaluated (10, 30 and 50% w/w). The materials were characterized by FTIR and SEM analysis. In addition, the materials were evaluated about the antimicrobial properties against *E. coli* and *S. aureus*. The FTIR analysis suggests that cellulose and silver niobate can form compatible mixture. All the composite aerogels possess porous 3D structure, with open and interconnected porous. The presence of silver niobate particles is noticed. Regarding the antimicrobial properties, the samples with 30% and 50% (w/w) of silver niobate were effective on inhibit bacteria growth. Therefore, the developed composite aerogels are multifunctional scaffolds and have potential to be applied for tissue regeneration.

Acknowledgments:
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Assessing the Efficacy of Silver Nanoparticle-Infused Plant-Based Nanocellulose Membranes in Treating Burn Wounds in Rabbits

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This study investigates the effectiveness of nanocellulose membranes embedded with silver nanoparticles for treating burn wounds in rabbits. Silver nanoparticles were synthed using the Tollens reagent method and impregnated onto cellulose films. Results demonstrated efficient silver release in moist environments, vital for antibacterial action. Characterization confirmed uniform distribution of silver nanoparticles without compromising structural integrity. Anesthesia and burn induction proceeded smoothly, with effective postoperative pain management. Histological examination and statistical analysis affirmed successful wound regeneration with silver nanoparticle-containing membranes. By day three, wounds appeared clean with mild drying and contraction of wound edges. By day seven, initial crust formation was observed, followed by increased formation and dark areas resembling necrosis by day fourteen. Silver-impregnated membranes exhibited reduced dark coloration and a drier appearance. Further research with a 28-day treatment period is warranted for comprehensive analysis. Consideration of pore presence and treatment duration remains pivotal for optimal outcomes [1].

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Assessment of antibacterial potential of calcium phosphate-AgNPs biomaterials designed for bone applications

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The development of biomaterials for bone applications has explored combining different constituents to produce biomedical devices with optimized properties to meet the quality and functionality requirements for bone substitutes. In particular, the literature reports the use of calcium phosphate derivates in association with additives (ions, polymers, and nanomaterials) for the production of scaffolds. In this context, calcium polyphosphate (CPP) emerges as an alternative to develop bone biomaterials because it has biocompatibility, low toxicity, osteoconductive, osteoinductive, and osteogenic potential, as well as controlled porosity. However, the use of bone grafts can lead to the emergence of infections due to bacterial invasion and proliferation at the site of application. To mitigate this issue, scaffolds have been associated with antimicrobial agents, such as antibiotics and silver nanoparticles (AgNPs). Therefore, this work pretended to develop CPP-based materials for bone applications, incorporating alginate and AgNPs. The biomaterials based on CPP, alginate, and AgNPs were characterized by FTIR and SEM, confirming the formation of the composites. Besides, X-ray diffractograms revealed that composites have crystalline phases of hydroxyapatite, dicalcium phosphate, and tricalcium phosphate. Moreover, preliminary results showed that the composites exhibited antibacterial potential against S. epidermidis and S. aureus. Thus, our results showed that these composites have the potential to be used as antibacterial biomaterials for bone applications.

Bacterial cellulose (BC) and konjac glucomannan (KGM) films for potential biomedical applications

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Chronic wounds represent a significant challenge in medical practice, demanding innovative approaches for effective healing. Bacterial cellulose (BC), naturally produced by bacteria (e.g., K. xylinus), is highlighted for its purity and versatility, because of its three-dimensional nanofiber structure [1]. Konjac glucomannan (KGM), obtained from Amorphophallus konjac, possesses gel-forming and swelling properties due to hydroxyl groups in its structure. This study aimed to develop a film composed of BC and KGM for wound dressings. Initially, hydrogels of BC and deacetylated KGM were prepared in a 1:3 ratio (BC:KGM), followed by casting to produce the films. The BC:KGM resulted in thin films resistant to handling, also BC added opacity to the material, contrasting with the inherent transparency of pure KGM films. Scanning electron microscopy (SEM) analysis revealed a rough surface on the BC:KGM films, with BC nanofibers covered by a compact layer of KGM, highlighting fiber networks in some regions. Evaluation of the film's surface topography by atomic force microscopy (AFM) resulted an average roughness (Ra) of 204.4 nm, a value higher than that found in the literature [3]. This value may be related to the interaction between BC and KGM, due to the biomaterials' characteristics and packaging during the casting process. These findings indicate promising applications for KGM and BC films for wound dressing applications. KGM offers a compact structure as an external barrier, while BC fibers enhance roughness, enabling greater tissue interaction and aiding dressing adhesion and fixation.

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Biocompatibility Analyses of New Titanium-Based Alloys for Biomedical Applications

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The evolution of biomaterials is characterized by continuous progress, from the first metallic implants used in orthopedics to the most advanced and personalized materials developed today. The most commonly used alloys in Brazil and worldwide for orthopedic applications are Ti6Al4V due to their corrosion resistance and excellent mechanical strength-to-density ratio [1]. However, it is known that this alloy incorporates elements considered cytotoxic, such as vanadium, which is associated with adverse tissue effects, and aluminum, which is linked to neurological problems, including Alzheimer's disease [2]. It is important to note that the selection of biomaterials was previously based predominantly on their mechanical durability; however, nowadays, the crucial importance of the interaction between the material and cells is recognized. Considering this critical perspective, an essential innovation emerges: developing new titanium alloys free of these elements, specially designed for implantable medical devices [3]. Thus, the present work aimed to conduct preliminary biocompatibility analyses of the new titanium alloys developed at the Laboratory of Anelasticity and Biomaterials, aiming for safer and more effective biomedical applications in the future. From a biological standpoint, biocompatibility demands low or no toxicity levels. This characteristic is crucial, as systemic toxicity can potentially impair the complete functionality of biological systems. The results showed that none of the sets of Ti alloys presented cytotoxic effects. (Financial support: CNPq, grant #314.810/2021-8 and FAPESP, grant #2021/12073-9)

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Biological and Mechanical Evaluation of a GelMA-PCL Scaffold for Bone Tissue Engineering

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Biomimetic scaffolds, fabricated through 3D bioprinting techniques, offer a promising avenue for accelerating bone regeneration, mirroring the characteristics of native tissue conducive to cellular growth within living organisms. Gelatin Methacryloyl (GelMA) is a polymer known for presenting biocompatibility and biodegradability; when integrated into bioprinting alongside polycaprolactone, it has the potential to enhance the structural stability and mechanical strength, requirements for bone tissue function. GelMA undergoes crosslinking upon exposure to UV irradiation facilitated by an appropriate photoinitiator, such as lithium phenyl-2,4,6-trimethylbenzoylphosphinate (LAP), which plays a crucial role in regulating the degree of crosslinking within these scaffolds. Such modulation contributes to enhancing both the modulus of elasticity and the structural stability of the implants. The present study systematically investigated the effects of LAP concentrations (0.075% and 0.1%) and photoactivation timeframe (30, 60, and 90 seconds) in rheological capabilities, bioink printability, and degradability. Biological assessments, including cellular viability, cytocompatibility, and mineralized matrix deposition, were conducted to explore the effectiveness of these scaffolds. Our findings reveal that, during 3D bioprinting, cell viability typically decreases with increasing photoinitiator concentration and printing time when utilizing LAP. However, the concentration of 0.1% LAP exhibited greater shape fidelity and stability, whereas 0.075% LAP demonstrated increased cellular response at 60-second interval ($p < 0.01$). This result underscores the critical balance between scaffold integrity and cellular viability, highlighting the significance of optimizing photoinitiator parameters for enhanced tissue engineering outcomes. Overall, the biofabrication technique proposed herein may be translated to the pre-clinic repair of bone defects aiming at future medical application.

Bioplastic based on silk fibroin, bacterial cellulose, curcumin and silver nanoparticles as an alternative for food packaging

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Conventional petroleum-derived plastics are difficult to degrade in the environment [1]. Some of this waste comes from food industries which, in addition to plastic waste, generate food waste due to the lack of better packaging technologies for their products [2]. One solution is the use of bioplastics made from biodegradable materials, silk fibroin (SF) and bacterial cellulose (BC) [1,3]. The use of curcumin (Cur) can assist in UV/Visible and antimicrobial protection and silver nanoparticles (AgNPs) can further enhance antimicrobial properties, ensuring an extension of the food's shelf life [2]. Infrared spectroscopy of the SF/BC bioplastic showed that the chemical properties of each material were maintained. By inserting Cur into the SF/BC, SF/BC/Cur bioplastic film, it was possible to verify the stability of Cur in acidic (yellow color) and basic (red color) media. This property can be exploited as a freshness indicator packaging. Furthermore, Cur can provide UV-Visible and antimicrobial protection. AgNPs were obtained with maximum absorption at 398 nm characteristic of nanospheres, average of 10 nm and zeta potential of -36.8 mV, indicating good stability. The next step will be to insert the AgNPs into the SF/BC/Cur bioplastic, verifying whether the halochromic and antimicrobial properties are maintained and whether there is a synergism of these properties when inserted into the bioplastic.

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Caffeine controlled release device associated with ADHD treatment

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Attention Deficit Disorder (ADHD) is a neurobiological disorder characterized by symptoms of lack of attention, concentration and restlessness. Caffeine is responsible for blocking the neurotransmitter adenosine, responsible for the feeling of relaxation [1] and also stimulates the normalization of dopamine levels, so it provides satisfactory results to avoid the unwanted symptoms of the disorder. Usual administration of caffeine is done orally, however, intraperitoneal administration presented satisfying results in animal models, showing there is a high potential for the substance to treat ADHD by promoting neuromodulation [2].

Therefore, this work aims to study the effects of caffeine and develop an implantable device for the controlled release of caffeine for the treatment of ADHD. Devices will be manufactured through a combination of extrusion and additive manufacturing by fused filament fabrication (FFF), using TPU and EVA polymers which are medical grade and FDA approved, as well as a 10% concentration of anhydrous caffeine in their composition. Safety and effectiveness of devices will be verified through drug release assays, cytotoxicity and mechanical testing. Drug tolerance and the reduction of adverse effects can be improved with drug releasing devices, with a reduction of side-effects and the need of oral administration.

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Cellulose-Derived Polymers/Curcumin for Tissue Engineering and Drug Delivery: Synthesis and Physical-Chemical Characterization And Biological Assay

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The most commonly used cellulose-derived esters for biomedical applications are cellulose triacetate (CTA) and cellulose phthalate acetate (CAP). Some of their applications are related to tissue engineering, controlled drug release, antimicrobial matrices, thermosensitive gels, and pH-responsive fibers. Thus, this study aims to obtain cellulose triacetate and cellulose phthalate acetate from purified cellulose from corn husk to be used as scaffolds for tissue engineering and drug delivery systems (DDS). The goals also include the characterization of the synthed polymers, preparation of cellulose triacetate and cellulose phthalate acetate with curcumin in the form of films scaffolds for conducting embryotoxicity tests in Zebrafish (Danio rerio). The CAP and CTA were structural characterized by FT-IR spectroscopy. The CAP and CTA spectra showed its characteristic bands, which suggests that polymers were successfully synthed. The thermogravimetric analysis showed that CAP degradation occurs in several stages, in interval of 180 oC to 380 oC. Alread CTA present the onset decomposition temperature at 145 oC. A significant amount of residue was observed following the decomposition of all prepared polymers, which can be attributable to the materials preparation processes. The UV-Vis spectra showed that CTA and CAP no present absorption visible region, but the Curcumin/CTA and Curcumin/CAP present the large band in visible region, this band is attributed that curcumin molecule. Embryotoxicity assays using zebrafish show that the materials prepared in this study are not cytotoxic and teratogenic for embryos. This is of fundamental importance for the use of these materials as scaffolds for tissue engineering.

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Characterization of biocompatible fibers for cardiac tissue regeneration

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Cardiovascular diseases are the leading cause of death worldwide, affecting thousands of people every year. Several techniques such as transplants and implants have been improved and allow to save lives, but the limitation of genetic compatibility between patient and donor, the dependence on medications for the rest of life and the high chances of reoperation are limiting factors of these procedures. For these reasons, tissue engineering has emerged as a promising alternative for replacing organs and tissues by growing cells on supports called scaffolds. It is of the utmost importance that these supports are biocompatible, biodegradable and allow good cell adhesion to avoid immune responses. These characteristics can be found in some polymeric materials, which are increasingly proving to be suitable options for manufacturing scaffolds [1]. The aim of this work was to characterize poly(lactic acid)/polyethylene glycol/polyaniline (PLA/PEG/PANI) fiber scaffolds. The fibers were obtained by electrospinning mechanism and Fourier transform spectroscopy (FTIR), scanning electron microscopy (SEM) and contact angle measurements were used to characterize the chemical composition, morphology and surface properties. The SEM results showed that fibers with nanometer-scale diameters were obtained with non-uniform distribution and many showed granule formation. The contact angle test indicated the formation of hydrophilic fibers, but the wettability of the samples was influenced by the entrapment of air in the structure of the blankets and by the possible effect of the hydrophilicity of the aluminum substrate. The FTIR results confirmed the structure of the PLA, PANI and PEG used.

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Characterization of high entropy oxide-like coatings on the biomedical Ti-6Al-4V alloyproduced by PEO treatment

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Metallic biomaterials are crucial in medicine,but can cause damage due to the release of toxic ions Advanced techniques like plasma electrolytic oxidation (PEO) create enriched coatings with bioactive elements. [1]. In this study, we explored a new approach to modify the surface of the Ti-6Al-4V alloy with PEO. We aimed to obtain a coating composed of multiple oxides (Fe, Mo, Mn, Ti, and Al) and bioactive elements (Ca, P), which were added in powder form to the electrolyte. This strategy isexpected to result in a unique biological response at the cellular level, providing more excellent to wear and corrosion and contributing to advances in biomaterials and their biomedical applications. Surface modification was performed under two conditions, varying the total concentration of metal oxides added to the electrolyte solution (1 g/l and 3 g/l). After treatment, the samples were characterized using various techniques such as scanning electronmicroscopy (SEM), X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS). The SEM images showed a porous morphology characteristic of the PEO treatment in both conditions. The diffractograms showed an amorphous region (20-35°) with anatase and rutile peaks, but no metal oxide peaks were observed. XPS analysis indicated higher concentrations of $TiO2$, Ca and P, with lower concentrations of metal oxides and no Mn spectrum detected. The results were satisfactory, suggesting improvements for the alloy studied. This research has significant implications for the development of efficient medical biomaterials.

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Development and characterization of the Zr-25Ta-25Ti-Ag alloy for biomedicalapplications.

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Titanium alloys are gaining visibility in a lot of studies due to their high biocompatibility. The transition to alloys that blend α and β crystalline structures extends beyond the scope of pure titanium, representing a leap forward in biomaterials science. Central to this advancement is the exploration of β-type alloys, integrated with elements like molybdenum, zirconium, tantalum, and niobium, designed to enhance biocompatibility and reduce Young's modulus, thus addressing the challenge of "stress shielding" [1]. This phenomenon occurs when an implant's high elastic modulus results in the implant, rather than the bone, absorbing mechanical loads, potentially leading to decreased bone density. Crucially, the inclusion of silver is spotlighted for its contribution to the alloys' structural, antimicrobial, mechanical, and biocompatible properties, showcasing its multifaceted benefits [2]. Following this strategic integration of elements, the Zr-25Ta-25Ti-xAg (x = 0, 1 or 3 wt.%) alloy experienced rigorous characterization to confirm their suitability for biomedical use. This analysis involved evaluating structural and microstructural aspects using advanced techniques such as X-ray diffraction and scanning electron microscopy. Mechanical properties were assessed through tests like XRD and elastic modulus measurements, which showed expected values, since the XRD measurement showed that most of the alloys crystalline structures are β-type and the Young's modulus measured for the samples containing Ag were in the range of 57 GPa being lower than the marketed Ti-6Al-4V alloy.

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Development and Characterization of the Zr-25Ta-25Ti-Cu Alloy for Biomedical Applications.

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Due to their high biocompatibility, Titanium alloys have attracted significant interest in developing biomaterials. Initially, Ti alloys were α-type crystalline structures with a molecular structure similar to commercial pure titanium. Over time, α+β-type alloys gained attention for their wide range of properties, with Ti-6Al-4V becoming one of the most utilized alloys. However, aluminum and vanadium ions were detected in patients' bloodstream, leading to cytotoxic effects and a predisposition to neurological problems, including Alzheimer's disease. Consequently, a new class of Ti alloys, primarily with a β-type crystalline structure, was developed, aiming at a lower Young's modulus, adding Mo, Zr, Ta, and Nb to enhance its biocompatibility. Previous studies extensively examined the Ti-25Zr-Ta system, with Ti-25Ta-50Zr showing the best mechanical and biocompatible properties, promising for orthopedic and dental applications. This work aimed to prepare and characterize novel Zr-25Ta-25Ti-Cu alloys for the understanding of the effects of copper on its structural, antimicrobial, mechanical, and biocompatible properties through techniques such as X-ray diffraction, elastic modulus through impulse excitation, scanning electronic microscopy, Vickers' microhardness, and biocompatibility tests. The results indicated favorable properties for the use of biomedical implants.

Acknowledgements:

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DEVELOPMENT AND CHARACTERIZATION OF Ti-20Ta-Nb ALLOYS SYSTEM AIMING BIOMEDICAL APPLICATIONS

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In recent decades, the search for biomaterials that can meet project requirements in order to improve implant performance has become a topic of great importance. Recent studies have shown the growth of the use of implants in patients of all ages. A class of Ti system alloys has attracted the attention of researchers due to its properties such as low density/mechanical strength ratio, low elastic modulus value, good resistance to corrosion in body fluids, and good biocompatibility. Brazil has the largest reserves of Ta and Nb, especially in the Amazonas state, and with the increase in demand for these minerals, it is necessary to develop technology to add value to the reserves and seek regional technological development. Hence, the objective of this work was to produce four Ti-based alloys with the following compositions: Ti-20Ta, Ti-20Ta-10Nb, Ti-20Ta-20Nb, and Ti-20Ta-30Nb. After melting, the alloys were characterized using the XRF, EDS, density measurements, X-ray diffraction, optical microscopy, scanning electron microscopy, and Vickers microhardness. The theoretical and experimental results of densities were very close and it was observed that with an increase in the percentage of niobium increased the density of the samples. X-ray diffraction measurements showed the presence of α, α′, α″ and β phases. With the increase of the percentage of niobium, the presence of the β phase also increased, demonstrating the effect of the beta-stabilizer of the niobium. Regarding hardness values, the compositions Ti-20Ta-10Nb and Ti-20Ta-20Nb presented close hardness values, and the alloy containing 30 wt% of Nb showed a lower hardness value. No cytotoxic effects were observed in all produced alloys. (Financial support: CNPq and FAPESP, grant #2021/12073-9).

Development and Characterization of Ti-25Ta-xNb Alloys for Orthopedic Applications

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Titanium and its alloys are widely employed in biomaterials due to their biocompatibility, good corrosion resistance, low modulus of elasticity, and attractive relationship between tensile strength and density [1]. Tantalum and niobium metals enhance these properties, as they are beta-stabilizing elements that reduce the titanium beta-transus temperature [2]. This study aims to develop alloys of the Ti-25Ta-xNb system (x=10, 20, 30, and 40% in weight) with a modulus of elasticity closer to cortical bone and high osseointegration capacity. After cleaning the elements, the metals were melted in an electric arc furnace under a controlled argon atmosphere using a water-cooled copper crucible. Homogenization heat treatment was performed after melting, and solubilization heat treatment was conducted after hot-rolling. The alloys underwent structural, microstructural, mechanical, and biological analyses. Chemical mapping indicated that the samples exhibit good homogeneity. The semi-quantitative chemical analysis obtained through EDS measurements confirmed that the alloys have adequate stoichiometry. According to X-ray diffraction patterns and scanning electron micrographs, adding niobium resulted in stabilizing the body-centered cubic structure (β phase). The Ti-25Ta-xNb system demonstrated promising modulus of elasticity values, lower than currently marketed alloys such as Ti-cp and Ti-6Al-4V, indicating the beta-stabilizing nature of tantalum and niobium elements, with the Ti-25Ta-20Nb alloy showing the lowest modulus of elasticity (66 GPa). Biological tests indicated that none of the alloys in the system caused toxicity to the organism, leading to cell death. (Financial support: Capes, CNPq and FAPESP).

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Development of a dengue aptasensor using thin films

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The development of fast, selective, and low-cost diagnostic devices, such as biosensors, is a major concern for researchers due to the emergence of diseases [1] . This work aims to demonstrate the development of a thin-film platform for detecting diseases, including Dengue. To achieve this, FTO substrates and gold thin films were deposited via Sputter with varying deposition times (2, 3, 4, and 5 minutes). Various techniques were employed to characterize the surface of the thin film, including X-ray diffraction, UV-Vis spectrophotometry, and electrochemical impedance spectroscopy (EIS). Subsequently, the platform was functionalized by co-immobilizing aptamers (apt) and 6-mercapto-1-hexanol (MCH) in varying proportions. The biosensor was characterized using EIS techniques. The results indicate that deposition times shorter than 2 or 3 minutes did not provide complete coverage of the FTO substrate. Longer deposition times, specifically 4 and 5 minutes, resulted in satisfactory coatings [2]. Surface functionalization was performed using FTO/Au deposited for 4 minutes. To optimize the FTO/Au films, various ratios of aptamers and MCH were tested, with a ratio of 1:25 (Apt: total thiol) ultimately selected. The biosensor was optimized to achieve a sensitivity of 40.2 ± 3.7% per decade and a low detection limit of 12.46 pg/mL, enabling dengue detection in the clinical range for first and second infections [3].
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Development of an electrochemical biosensor based on carbon fiber-coupled antibodies as a strategy for diagnosing hypogonadism.

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Diseases related to testosterone deficiency, particularly hypogonadism, pose significant challenges, especially among older male adults. Symptoms such as depression, decreased libido and bone density, and erectile dysfunction highlight the importance of early detection [1]. This research focuses on the development of electrochemical biosensors using flexible carbon nanofibers [2] to quickly detect testosterone deficiency. The biosensor utilizes the immunoassay technique, where an antibody is adsorbed on the fiber surface [3]. The first step involved in this study ensured the efficiency of the voltammetry and impedance signals by cleaning the carbon fiber with a (K4MnO2) + (H2SO4 [1 mol/L]) solution. The results demonstrate that the sensitivity of the biosensor depends on the quality of the carbon fibers and the electrolytic solution of a redox par (K4Fe(CN)6 • 3 H2O + K3Fe(CN)6 • 3 H2O + KCl) used in the potentiostat. This redox solution exhibits fully reversible behavior, as observed through voltammetry tests conducted between -0.2 to 0.8 V at scan rates of 0.1 and 0.01 V/s. This behavior was also observed in impedance tests with frequencies ranging from 0.01 to 100 kHz. These tests allowed us to characterize the effect of the fiber in this solution through its redox peaks.

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Development of Cutaneous Biocurative by Decellularization of Nile Tilapia Skin: A Promising Approach

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The preserved skin of Nile Tilapia (Oreochromis niloticus) has been used as a dressing for cutaneous wounds in various species. However, the presence of proteins in the cell membrane can lead to severe inflammatory processes and rejection in the recipient individual [1]. The aim of this study was to develop a biocurative for cutaneous use through the decellularization of tilapia skin. Adult tilapia skins were dissected to remove subcutaneous tissues and washed in a physiological solution. Subsequently, 5x3cm fragments, extracted from three regions of the skin (dorsal, median, and ventral), were subjected to different times (12, 16, 24, and 72 hours) of alkaline treatment in NaOH solution. After treatment, they were submerged in sodium hypochlorite for disinfection, washed in distilled water, dried on paper towels, frozen in liquid nitrogen, and lyophilized for 20 hours. Samples from the control group were washed in distilled water, frozen, and lyophilized without being treated in an alkaline solution. Permanent histological slides of the samples were prepared, stained with hematoxylin-eosin and Gomori trichrome, and evaluated under optical microscopy. Effective decellularization of the dermis was observed at all treatment times, which showed either no fibroblasts or a significant reduction in their quantity. Additionally, it was noted that alkaline treatment removed the amorphous part of the extracellular matrix, further contributing to improved biocompatibility. However, the increase in treatment time was directly proportional to the disorganization and fragmentation of collagen fibers. It was concluded that a 12-hour treatment is sufficient for effective decellularization and removal of the antigenic part of the extracellular matrix with good preservation of collagen fiber structure.

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Development of halloysite nanoclay composites based on *Scaptotrigona postica* propolis extracts for antimicrobial applications.

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The emergence of a wide variety of resistant microorganisms to antibiotics has prompted a massive study to develop alternative mechanisms capable of inhibiting bacterial growth [1]. Photodynamic inactivation [2], for example, is an auspicious alternative that, associated with a propolis-based composite with nanoclay, as our project aims, instead of a conventional photosensitizer, can successfully combat microbial resistance in a sustainable manner. In this work, we produced a series of nanocomposites, based on *Scaptotrigona postica* propolis extracts and halloysite nanoclay (HNT) for antimicrobial application. Using a methodology developed by our group [3], three propolis extracts were prepared (using ethanol, chloroform, and toluene as solvents) and they were successfully mixed with pre-treated HNT (basic, neutral and acid treatments). Both extracts and nanocomposites were characterized by absorption spectroscopy, photoluminescence (PL) and photoluminescence excitation (PLE) and were tested against *Staphylococcus aureus* and *Escherichia coli* bacteria strains to evaluate the pro-oxidant effectiveness of the substance. The photophysical characterization showed the presence of several flavonols. For experiments against *E. coli*, all composites reduced the bacterial growth, being the chloroform extract-based composites more effective. In the case of *S. aureus* bacterial strain, all composites showed similar activity. The more effective composites will be tested against resistant bacterial strains.

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Development of Ti-10Al-2(Cr, Fe) (%) alloys for use in ankle-foot joint prostheses

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Considering titanium is one of the most used materials in the world, essentially in the biomedical area, it will be the basis for seeking improvements and increasing the useful life of alloys by adding chromium and iron elements, applied in the metallurgical industry as economic drivers, improving hardness properties, tenacity, malleability, wear, elastic modulus, and biocompatibility [1]. Therefore, this project aims to study the chemical, physical, structural, microstructural, mechanical, electrochemical, biological, and tribological properties of alloys based on Ti-Al-Fe-Cr combined with different thermal treatments and proportions of the alloy elements aiming to use as prosthetics of the ankle-foot joint [2]. An initial check of the mechanical properties was verified by Vickers microhardness measurements, microstructural properties by optical microscopy, and structural properties by XRD. The results indicated that the Ti-10Al alloy predominates the α phase in the form of lamellas. The other alloys in the study have characteristics of the α +β phase, with precipitation of martensite structure with the addition of β elements. It was also possible to analyze the increase in microhardness by adding the chemical element chromium to prepare alloys through electric arc melting.

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Effect of cold plasma on Ti surfaces decorated witch silver nanoparticles

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Biocompatible materials for prostheses are extremely necessary and sought after in the medical field. From this perspective, titanium has become widely used, but prostheses made from this metal are not without the risk of infection [1]. An alternative to this would be to implement silver nanoparticles, with proven efficacy in eliminating bacteria, on its surface [1]. To promote adhesion of nanoparticles, surface modification using cold plasma treatment is an option. This has been used industrially to effectively alter the surface properties of various materials [2].

Therefore, the main objective of this work is to modify the surface of titanium with silver nanoparticles to give it antibacterial properties. Plasma treatment took place before and after the application of the nanoparticles, making it possible to compare the results by checking which treatment promotes better adhesion of the nanoparticles to the metal surface.

The AgNPs, synthed by the chemical reduction method without stabilizing agents, were characterized by UV-VIS spectroscopy before application, in order to prove their existence and estimate their . The modified titanium surfaces were analyzed by optical microscopy, atomic force microscopy (AFM) and scanning electron microscopy with energy dispersive spectroscopy (SEM/EDS) before and after the treatment in order to evaluate the morphology and topography of the surfaces obtained. The shape and the height of the nanoparticles on the titanium surface was shown to be strongly influenced by the energy inferred during the cold plasma treatment.

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Effect of heat treatment on the growth of bioactive oxide films obtained by plasma electrolytic oxidation on the Ti-6Al-4V alloy

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Technological innovation promoted essential advances in developing metallic alloys and surface engineering techniques. Among the materials applied as biomaterials, titanium alloys have been extensively studied. The attractive properties of titanium have promoted the creation of several alloys, such as α- (commercially pure Ti), α+β- (Ti–6Al–4V), and β-type (Ti-13Nb-13Zr), through the design of the chemical composition of the alloy with stabilizing α and β elements. The α+β type alloys have two phases at room temperature and can be considered the most common and versatile form of titanium alloys. The proportion, , and distribution of the phases can be changed through heat treatments under specific parameters, which can promote changes in the properties of the alloy. On the other hand, an essential aspect of titanium alloys is the possibility of modifying their surface. Bioactive coatings containing calcium phosphate (Ca-P) are similar to biomimetic materials used for bone tissue. In this aspect, surface treatments of Ti alloys, such as plasma-assisted electrolytic oxidation (or PEO), stand out due to their ability to promote surface characteristics that meet the human body's requirements. The PEO technique has the potential to produce layers that increase the resistance to corrosion and wear, bioactivity, and biocompatibility, among other factors. Based on this context, in the present study, heat-treated Ti-6Al-4V alloy was subjected to PEO treatment for the growth of bioactive oxide films. The structural, microstructural, mechanical, electrochemical, chemical, and physical results indicated evidence that the bulk's phase composition influenced the surface characteristics of the sample, being useful for biomedical applications.

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Effect of heat treatment on the optical and structural properties of natural andalusite

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Andalusite is an aluminosilicate mineral with an orthorhombic structure and Pnnm space group and constitutes one of the Al2SiO5 polymorphs with kyanite and sillimanite [1]. Andalusite forms under low pressure and low to high-temperature conditions and has an orthorhombic structure with a Pnnm space group[1]. Their ideal composition is 62.92 wt% alumina and 37.08 wt% silica [1]. Under natural conditions, these minerals present significant impurities in their structure, which are responsible for the different colors. In this work, reddish-green andalusite samples from Minas Gerais were ground using an agate mortar and pestle. The samples were sieved to obtain two different particle groups, one lower than 75 µm and the other 75 µm – 180 µm. The 75 µm – 180 µm powders were submitted to heating treatment in an air atmosphere furnace for 1 hour at 700 ºC and 800 ºC. The microstructural and optical characterizations were performed using X-ray diffraction (XRD), Raman, Fourier transformed infrared (FTIR), and ultraviolet–visible (UV-vis) spectroscopy. From DRX analysis, the orthorhombic structure was identified in the sample studied. The optical absorption profile indicates a broad absorption band centered around 490 nm, which decreased for the sample submitted to 800 ºC heat treatment. The registered Raman and FTIR spectra show agreement with the data published in the literature for andalusite. The effect of the heating treatment on the Raman was estimated by comparing the intensity and full width at half maximum values with the as-received sample, and the observed results indicate modifications in the spectra registered for the sample heated at 800 ºC, with broadening of some bands and decreased intensity. Grant Fapesp #2021-13132-9, #2023/12201-2, CNPq; #23038.000776/201754, #420798/2023-4, NIPE-Unifesp; and CEMUD-ICAQF/UNIFESP. [1]. Zhai, K., et al. Raman spectra of sillimanite, andalusite, and kyanite at various temperatures. Phys Chem Minerals 47, 23 (2020).

Effect of NaOH etching and oxygen plasma post-treatments on surface characteristics and their potential to activate micro-arc oxidized TiO2 coatings.

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Activation post-treatments such as NaOH etching or O2 plasma exposure can play an essential role in surface conjugation of titanium with organic molecules and biomolecules, in order to achieve a better interaction at the bone and implant interface. However, their application on complex titanium dioxide (TiO2) surfaces is still not explored. In this contribution, bioactive and porous TiO2 coatings produced by micro-arc oxidation (MAO) were post-treated with NaOH etching or O2 plasma, and then placed in contact with reactive isocyanate organic compounds to evaluate the potential of molecule conjugation. Results suggested that O2 plasma treatment has only changed the surface chemistry of the coating through carbon contaminants removal, plasma-driven oxidation and generation of functional OH species, including reactive carboxyl groups. This surface chemical modification by plasma has made the surface superhydrophilic. After NaOH etching, the coating became rougher and also superhydrophilic, containing titanate structures on its surface and also inside the inner pores. These newly structures presented sodium and calcium (and no content of phosphorus), which may indicate the formation of sodium and calcium titanates. Upon reaction with isocyanate molecules, the oxygen-containing functional groups derived from plasma exposure seem to provide a more stable and reliable interface to the covalent grafting compared to the aggressive NaOH etching, introducing characteristic conjugation bonds and also making the activated MAO coating more hydrophobic due to the surface-terminated methyl chains from isocyanate (Financial support: FAPESP grant # 2020/10125-9).

Effect of phase composition of Ti-6Al-4V alloy on oxide growth obtained by micro-arc oxidation.

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Titanium is an allotropic metal extensively employed as biomaterials for diverse applications in Medicine. Its unique combination of properties, including biocompatibility, corrosion resistance, lightweight, and high mechanical strength, makes it a valuable material for use in a variety of medical devices and implants [1]. The understanding the physical and chemical properties of titanium, as well as its interaction with the human body, plays a fundamental role in the research and development of the current biomaterials. Thus, research involving titanium alloys has been contributing to significant advances in the health and quality of life of patients [2]. Given that, the Ti-6Al-4V alloy represents the most widely used form of titanium worldwide, with a market share ranging from 50% to 70% in aerospace, engineering, and biomedical industries. The improvement of the properties of this alloy is attributed to the ability of aluminum (Al) to function as an α-stabilizer and vanadium (V) to play the role in the β phase stabilization [1,2]. This research aims to investigate the effect of distinct α and β proportion in the surface aspects of the Ti-6Al-4V alloy submitted to micro-arc oxidation treatment. The results indicated that the heat treatments performed at 600, 800, and 1000°C promoted a significative change in the quantity, distribution, and morphology of α and β phases in the sample which resulted in variations in the pore and shape of the porous oxide layer on the surface. The quantity of chemical species incorporated into the coating (Ca, P, and Mg) and the surface phase composition (anatase and rutile) exhibited dependence with the α and β phase proportion. The findings show that the controlling of the bulk's phase composition of the Ti-6Al-4V alloy can be useful for the manufacture of bioactive surfaces by MAO treatment.

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Elaboration of electrochemical sensor based on cobalt metal-organic framework for detection of dopamine from biological samples

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Dopamine (DA) is an important neurotransmitter that acts on essential functions of the human brain. Assessment of DA levels in human biological fluids is critical for identifying neurological disorders related to stress, substance abuse, and neurochemical imbalances [1]. In this context, this study aims to develop a new electrochemical sensor based on a modified electrode using metal-organic framework of cobalt, [Co(BDC)]n. The sensor was successfully synthed by the solvothermal method using 1,4-benzenodicarboxilic acid (BDC) as ligand and Co salt as metal source. [Co(BDC)]n was characterized by FT-IR, XRD, SEM-EDS and TGA analyses. For AD detection, some parameters were optimized, (i) the percentage of the modifier; (ii) pH; and (iii) tension for electrode modification. As a result, the ideal conditions for AD detection were achieved using pH 6.0 solution, 25% (w/w) modification of [Co(BDC)]n, potential increment of 5 mV, frequency of 75 Hz and amplitude of 100 mV. The sensor was tested on two synthetic biological samples (urine and saliva). In synthetic urine samples, the LOD and LOQ were 1.7 µmol L-1 and 5.7 µmol L-1, respectively, while in synthetic saliva samples they were 0.5 µmol L-1 and 1.7 µmol L -1. The sensor showed good linearity (R2 > 0.9922) and recovery rates between 84.9% and 97.1%, with RSD < 8.0% (n=3). These results suggest the potential of the [Co(BDC)]n based electrochemical sensor for clinical applications in the diagnosis of neurological diseases related to AD.

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Electrochemical detection of ciprofloxacin in urine and egg samples using [Cu(BDC)]n coordination compound

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Ciprofloxacin (CIP) is a widely used antibiotic, mainly in the production of foods of animal origin. The detection of in biological and food samples is essential due to its potential for the development of antibiotic resistance, resulting in a serious public health problem. [1]. This study describes the development of an electrochemical sensor for detecting CIP, focusing on synthetic samples of urine and eggs, using an electrode modified with Metal-Organic Frameworks (MOFs) based on copper, specifically [Cu(BDC)]n. The MOF was successfully synthed via the solvothermal method, employing 1,4-benzenedicarboxylic acid as the organic ligand and copper salt as the metal source. Characterization of [Cu(BDC)]n was conducted using FT-IR, XRD, SEM-EDS, and TGA analysis. The electrode modification was optimized using the parameters the (i) percentage of the modifier; (ii) pH; and (iii) tension. Optimization of sensor parameters in DPV, including a pH 6.0 solution, 20% (m/m) [Cu(BDC)]n, was conducted. The calculated number of electrons was 1.92 (α = 0.06), suggesting that the electrochemical oxidation of CIP involves two electrons. The increase in scan rate (ν) induced a linear augmentation in peak currents: $Ipa = 0.3656\nu + 0.7237$. The slope value of 0.37 suggests that electron transfer at the electrode surface follows a diffusion-controlled behavior. The sensor exhibited considerably good linearity (R2 = 0.992) for recoveries ranging from 70 to 111%. In synthetic urine samples, the LOD and LOQ were 0.5 µmol L-1 and 1.7 µmol L-1, respectively, while in eggs they were 3.0 µmol L-1 and 10.1 µmol L-1. By offering enhanced sensitivity and accuracy, this sensor holds promise for monitoring CIP residues in food products, thereby contributing to food safety and public health.

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Encapsulation of synergies of essential oils in polymeric matrix for therapeutic applications

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Essential oils, extracted from plants, have various therapeutic properties and have been used in therapeutic, cosmetic, and wellness practices for centuries. Aromatherapy, which utilizes these aromas to promote physical and emotional balance, has been gaining increasing popularity. The potential of essential oils to alleviate conditions such as stress, anxiety, insomnia, and muscular pain is recognized [1]. Lavender is known for its calming properties, while peppermint oil is stimulating and analgesic [2]. In this study, the encapsulation of synergies of these oils in a polymer matrix of alginate and chitosan was proposed [3]. A Central Composite Design was adopted, varying the concentrations of chitosan, alginate, and calcium chloride to optimize the process. The results indicated efficacy in the protection and stabilization of the oils, with encapsulation efficiency above 68% and controlled release of the compounds.

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Evaluation of Genotoxicity and Cytotoxicity: Biosilica and Spongin in Bone Tissue Repair

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Bone fractures have become a significant public health concern in recent years, necessitating effective treatments for non-consolidated fractures [1]. Surgical procedures employing metallic devices and biomaterials, both natural and synthetic, are commonly utilized for bone fixation [2]. In this regard, Biosilica (BS) and marine spongin (SPG) extracted from marine sponges emerge as promising biomaterials for bone healing. This study posits that BS/SPG scaffolds can enhance material biological performance. Accordingly, the study aimed to assess and compare the morphological properties, cytotoxicity, genotoxicity, and mineralization potential of BS and BS/SPG scaffolds. Scanning electron microscopy (SEM) was employed for sample characterization. Furthermore, the impact of BS and BS/SPG scaffolds on cell viability, genotoxicity, and biomineralization in L929, MC3T3-E1, and CHOK-1 cell lineages was evaluated through MTT assay, comet assay, micronucleus assay, and alizarin red staining, respectively. Results revealed needle-shaped BS and fibrillar aspects of SPG granules in morphological characterization. Moreover, BS and BS/SPG scaffolds exhibited approximately 70% cytotoxicity for L929 lineage at 1 and 3 days. No genotoxicity was observed in CHOK-1 cell lineage after 24 hours for all extract concentrations. Additionally, BS demonstrated intense alizarin red staining after 7 days, while BS/SPG showed light staining after 14 days, indicating in vitro biomineralization potential. In conclusion, BS and BS/SPG scaffolds demonstrated in vitro biocompatibility, absence of genotoxicity, and in vitro biomineralization potential, suggesting their promising utility in bone regeneration applications.

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Evaluation of hybrid chitosan-gelatin-ZnSrTCP hydrogel and PCL scaffolds for bone regeneration

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This study investigated the effects of β-TCP doped with Zn and Sr when associated with a chitosan hydrogel/gelatin hybrid scaffold for bone tissue engineering. Considering the benefits already shown of using ZnSr doped β-TCP combined with silk fibroin for osteochondral regeneration[1,2], this work sought to understand the impact of ZnSr-TCP associated with chitosan/ gelatin hydrogel on a 3D PCL structure for bone regeneration. Physicochemical characterization was performed. The porosity of the scaffolds was approximately 18%. The proposed scaffolds exhibited significant swelling within the first 15 minutes, maintaining stability for up to 180 minutes. The *in vitro* degradation showed a progressive increase over a period of 90 days. *In vitro* tests using Saos-2 cultured on the scaffolds were conducted at different time points (1, 3, 7, and 14 days) to evaluate cell proliferation, DNA quantification, and ALP production. The quantitative results indicated increased cell proliferation compared to the control group. These findings suggest that the ZnSr-doped β-TCP combined with chitosan/gelatin/PCL can be valuable in tissue engineering applications, promoting the proliferation of bone cells and having a versatile application for different materials. By corroborating previous studies and providing yet another successful use for this material, this study contributes to a solid basis for future investigations into the therapeutic use of this material in tissue regeneration.

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Evaluation of the healing process in oncological wounds treated with fibrin natural polymer using the BATES-JENSEN Wound Assessment Tool

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Chronic wounds are characterized by a persistent inflammatory phase, prolonged infection, and failure of defense cells to respond to environmental stimuli. These injuries do not heal and represent a challenge for health professionals since the conventional dressings show refractoriness, causing the wounds to remain open for months or even years [1]. Wound assessment is pivotal in oncological care, particularly in monitoring the healing process and optimizing treatment strategies. The BATES-JENSEN Wound Assessment Tool (BJWAT) is widely used to evaluate wound healing in various contexts [2]. However, its direct applicability in the context of oncological wounds in Brazil remains largely unexplored. This article proposes using BJWAT as an index for evaluating the oncological wound healing of two participants treated with the natural polymer fibrin membrane. Both had been treated with conventional dressings for one year (Case 1) and two years (Case 2) with no sign of healing. The wounds were treated weekly with an autologous dressing formed by fibrin membranes, isolated from blood, and irrigated with membrane exudate until healing. The BJWAT parameters were evaluated to compute the score between 1 (tissue health) and 60 (wound degeneration). Complete healing of the two wounds occurred within six weeks. In case 1, a male, 65 years old, with a wound of 66 cm2, the BJWAT score went from 35, closer to wound degeneration, to 12, reaching complete regeneration. In case 2, a female, 58 years old, with breast carcinoma, the BJWAT score went from 33, also closer to wound degeneration, to 13, also with complete regeneration. No adverse effects or hypertrophic scars were reported, showing that the fibrin membrane dressing is effective in healing chronic oncological wounds.

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Exploring Wettability on Ti-6Al-4V Alloy Surfaces: Strategies for reducing bacterial adhesion

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Titanium and its alloys are the most commonly used and suitable materials for biomedical applications such as implants. The Ti-6Al-4V ELI (Extra Low Interstitials Alloy) alloy is the most requested for this purpose due to its excellent mechanical performance and notable biocompatibility. Surface treatments such as electropolishing must be added to minimize bacterial adhesion after implantation. The aim of this study was to evaluate the wettability and surface energy after electropolishing of the Ti-6Al-4V ELI alloy. Samples were sectioned and subjected to electropolishing at potentials ranging from 13 to 18 V with times of 5, 10, and 15 minutes, using a solution of $HClO_4$, CH_3COOH, and $C_3H_8O_3$. After electropolishing, the samples were characterized by SEM (Scanning Electron Microscopy), contact angle measurements, and surface energy. The surface morphology after the electropolishing process was evidenced by SEM. The best results were obtained with the sample electropolished at 18 V for 15 minutes, with a contact angle measurement of 107.25° and surface energy of -21.59 mNm. These data confirm that electropolishing contributes to the achievement of hydrophobic surfaces and that the relationship between contact angle and surface energy determines bacterial adhesion.

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First insights of the Ti-15Nb alloy reinforced with TiC particles and TiB whiskers to combine low elastic modulus with high wear resistance for biomedical applications

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Ti-Nb alloys, such as the Ti-15Nb alloy, emerge as promising candidates for orthopedic prostheses, because they can achieve elastic modulus values closest to that of bone, which is crucial to prevent bone embrittlement [1]. However, joint prostheses, like hip and knee replacements, also involve tribological requirements, because cyclic sliding movements usually occur between their components. This condition limits the success of metallic materials, which generally have low wear resistance. To attend these requirements, a strategy may involve the addition of hard particles as the reinforcement of Ti-Nb alloys, yielding Ti-based Matrix Composites (TMCs). Indeed, the critical factor for achieving the desired properties lies in the strong bond between the reinforcement and the matrix, which can be achieved when chemical reactions occur during the TMC production, known as in-situ conditions [2,3]. In this way, the present work aimed to produce new in-situ TMCs with the Ti-15Nb alloy and the addition of different amounts of B4C powder during melting. The preliminary characterization performed after melting evidenced the absence B4C, while TiC particles and TiB whiskers were detected as the reinforcements, proving the in-situ condition. The reduced B4C addition decreased the reinforcements' contents, lowering the elastic modulus values. Therefore, this study introduces promising alternatives for wear-resistant load-bearing implant applications.

Acknowledgments

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Fracture strength and toughness of Biosilicate glass-ceramic

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Bioactive materials, designed to interact with and promote healing in natural tissues, face a critical challenge: achieving both desirable mechanical properties and biocompatibility. BiosilicateTM glass-ceramic aims to address this challenge by offering a unique combination of these two crucial features.

Understanding the relationship between a material's microstructure and its mechanical behavior is essential for designing bioactive glass-ceramics with tailored properties. This project focuses on systematically characterizing the mechanical properties of BiosilicateTM by independently controlling the crystal and volume fraction within the material [1].

We will investigate the mechanical response of BiosilicateTM glass with a composition of 1.5Na2O.1.5CaO.3SiO2 + 4P2O5 (wt%) by varying the crystallized volume fraction from 0% (glassy) to 100% (fully crystalline). Additionally, we will explore the effect of crystal (5, 15, and 45 µm) on mechanical behavior. By measuring fracture strength and toughness, this project aims to elucidate the key toughening mechanisms operative within BiosilicateTM, paving the way for its optimized design and application [2].

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Gadolinium-doped hydroxyapatite-based theranostic nanoparticles for targeted delivery of curcumin

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Nanotechnology in medicine offers promising opportunities to improve cancer diagnosis and treatment. Specifically, the creation of theranostic nanostructures drives advances toward personalized medicine. Hydroxyapatite (HAp) nanoparticles have multiple applications in diverse fields, including modern oncology, where they are employed in diagnostic imaging, drug delivery, and controlled release, as well as in bone regeneration [1]. Gadolinium ions (Gd^{3+}) are common as contrast agents in nuclear magnetic resonance imaging (MRI), but their release into the bloodstream can be highly toxic. Prolonged exposure to these contrast agents can lead to health problems due to the accumulation of Gd^{3+} in tissues and organs. In this sense, due to the high stability of the HAp structure, the production of HAp nanoparticles doped with Gd^{3+} can be an alternative to toxicity problems. Doping HAp with rare earth elements such as Gd allows diagnostic imaging, while functionalization with folic acid allows selective tumor targeting. Furthermore, nanoparticles can serve as a vehicle for natural substances such as curcumin, known for its anti-cancer properties [2]. This study explored the synthesis of HAp-Gd nanoparticles using microwaves, followed by functionalization with folic acid and incorporation of curcumin. The synthed nanostructures were characterized by XRD, nano-FRX, TEM, FTIR, TGA, CHN, and VSM techniques. The results indicated the obtaining of HAp-Gd nanoparticles with paramagnetic properties with the potential to be used not only as a contrast agent in MRI but also in the targeted delivery of curcumin for cancer therapy.

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HAp powder and HAp precursors as filler changing the PVDF phase formation of the polymeric fibers.

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PVDF is a thermoplastic polymer with wide application in several areas due to its special properties [1]. Among the properties that stand out most for this polymer is polymorphism. PVDF has five distinct phases that can be obtained during and after processing. The most easily obtained phase is the α phase, however, when talking about applications in the biomedical area, the β phase is the most recommended due to its greater biocompatibility and piezoelectricity [1], [2]. With this application in mind, it is necessary to be aware of the influence of processing and materials incorporated into the polymer matrix on the formation of PVDF phases. Thinking about the final application and the effect of fillers on this product, PVDF fibers made by electroblowing were carried out to check the effects of the presence of hydroxyapatite (HAp) in powder and HAp precursors on the formation of the β phase. The PVDF fiber samples obtained using the electroblowing technique were analysed by XRD, SEM, EDS and FTIR to observe how the fillers interfere in the presence of the α and β phase. In the end, the addition of 5% HAp powder and 5% HAp precursors proved to be an approach with great effects on the morphology of the fibers obtained, increasing their diameter and also influencing the conversion from the phase α to the phase β [3]. Furthermore, it was observed that the fibers were easier to handle due to the lower electrostatic interactions between the fibers with HAp powder and HAp precursors. Another change observed was the formation of a calcium phosphate structures that joins the fibers and makes it possible to obtain a final product in the form of a blanket.

Heterogeneous nucleation of protein crystals using graphene oxide

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X-ray diffraction crystallography is recognized as the primary means to elucidate the three-dimensional structure of macromolecules. However, obtaining high-quality protein crystals poses a challenge due to the empirical process of crystallization, which relies on trial and error, and high costs [1]. Heterogeneous nucleation using nanomaterials has emerged as an alternative to enhance this process. Among nanomaterials, graphene oxide (GO) stands out due to their diversity in surface topographies, porosities, and length scales [2]. In this study, the influence of GO and its chemical derivatives on lysozyme crystallization, a model enzyme, was investigated. GO was synthed following the modified Hümmer's method and subsequently functionalized with polyethylene glycol (PEGGO) and reduced (rGO) with ascorbic acid. The three variants were applied to lysozyme solutions using the hanging drop vapor diffusion technique. The study also evaluated the impact of nanomaterials on the protein's crystal structure using synchrotron X-ray diffraction. The results revealed the presence of nanomaterials stimulated the crystallization process, with approximately 75% of wells showing crystals, in contrast with the control group, which showed no crystallization. Furthermore, it was found that nanomaterials did not affect the crystal diffraction quality, suggesting promising potential for future applications. These findings open opportunities to explore GO and its chemical derivatives for crystallization of other proteins of interest, particularly those considered challenging to crystallize using conventional crystallization methods.

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How Langmuir Trough technique could be useful for osteogenesis study?

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In order to increase the efficiency and bioactivity of bone implants, we generally search for functionalized surfaces that optimizes the implant-bone interface. In this sense, coating the surface of these materials with monolayers that stimulate osteogenesis is a possible strategy. This study focuses on the investigation of lipid monolayers produced in a Langmuir Trough containing two proteins of interest, Alkaline Phosphatase and Vitronectin (TNAP and VN, respectively), which are related to the formation of bone hydroxyapatite (HAp). The aim is to determine which protein-protein and lipid-protein interactions are associated with an increase in the enzymatic activity of TNAP in the presence of VN (as indicated by experiments with Langmuir-Blodgett films), which would be crucial to elucidate osteogenic propagation from Extracellular Vesicles (EVs) and understanding the relationship between the amount of vitronectin found in these vesicles and bone diseases [1]. The results show that while monolayers containing only TNAP are expanded due to the insertion of the enzyme, the presence of VN with TNAP is responsible for keeping the monolayer with minimal expansion, behaving similarly to monolayers built in the absence of both proteins. This reveals that VN is not only able to increase the enzymatic activity of TNAP, but it is also associated to the stabilization of the monolayer, reinforcing the hypothesis that this protein would be an important component of EVs lipid bilayer. With all these data, a new aspect of osteogenic propagation will be clarified, as well as enabling the development of a new technique aimed at functionalizing the surface of bone implants, seeking greater efficiency and bioactivity, what have been the target of our research group.

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How laser surface treatment of a beta Ti alloy affects fatigue

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Surface modification of titanium alloys is a necessary factor for the success of the osseointegration process. Newly developed beta alloys require surface modification just like the traditional alpha+beta Ti-6Al-4V alloy. This is the case with the commercial beta Ti-15Mo alloy, which was subjected to laser modification in this study. Laser modification promotes substantial changes to the surface, which can act as major stress concentrators from a mechanical point of view. This fact was observed in the work, which resulted in an intense reduction in the material's fatigue performance. The results show that the application of lasers to a beta type titanium alloy, despite the excellent biological response reported in the literature, requires an in-depth feasibility analysis.

IMPACT RESISTANCE, MORPHOLOGICAL AND MELT FLOW BEHAVIOR OF PLA/CELLULOSE NANOFIBRILS COMPOSITES

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Cellulose has been identified as a promising material in several applications such as packaging, textile, and paper sectors, and it is used as a raw to obtain nanostructures. Cellulose nanofibrils (CNF) are nanostructured materials that have been investigated and reported in the literature. The visibility given to CNFs is explained by their high impact resistance, good thermal stability and additionally by the reason to are isolated from renewable [1]. Poly (lactic acid), PLA, is a biodegradable polymer that originated from renewable sources and presents high rigidity and good processability [2]. Those outstanding characteristics explain the reason PLA is receiving a lot of attention in the scientific community regarding the development of new products. However, in some applications, PLA presents insufficient impact resistance that may limit its use. In this sense, the addition of CNF may improve these shortcomings, and additionally improve the melt flow index (MFI) of the molten polymer, which is dependent on the dispersion and adhesion of CNF in the polymer matrix. Therefore, this study aimed to evaluate the impact performance of PLA composites prepared by extrusion and 3D printing reinforced with two CNF concentrations. Based on the results, it was observed a good acting of the nanofibril in the impact resistance of the composites when compared to pure PLA. Based on the impact resistance results, it was observed that the formulations with the lowest and highest nanocellulose content presented similar values, which were equal to 6.58 and 6.08 KJ/m2. Good adhesion among the PLA and nanofibrils was also observed by Scanning Electron Microscopy. It was possible to verify that CNF affected the MFI of the PLA.

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INFLUENCE OF INTERSTITIAL OXYGEN ON THE STRUCTURE, MICROSTRUCTURE, MECHANICAL PROPERTIES AND BIOCOMPATIBILITY OF Ti-25Ta ALLOY, AIMING AT BIOMEDICAL APPLICATIONS

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The present study addresses the influence of interstitial oxygen on the mechanical properties and biocompatibility of Ti-25Ta alloy for biomedical device applications, particularly in orthopedic implants. The alloy production involved varying oxygen concentrations through arc melting and thermomechanical treatments, such as hot-rolling and annealing [1]. Different characterization techniques were employed to analyze the alloy properties, including density measurements, optical and electron microscopy, X-ray diffraction, hardness and elastic modulus measurements, and biological analyses. The main objective was to develop a biomaterial with optimized mechanical properties and enhanced biological compatibility. The results indicate that the alloy exhibits the orthorhombic crystalline phase (α'') in all samples [2]. Oxygen doping proved effective in adjusting the mechanical properties of the alloy, contributing to improved compatibility with human bone tissue [3]. Biological assays demonstrate that the material is non-toxic and suitable for use as a biomaterial. Studies on gas analysis present in the alloy are being conducted for a more conclusive understanding of the methods used in the study, aiming to provide a broader perspective on the use of Ti-25Ta alloy as a biomaterial (Financial support: Capes, CNPq and FAPESP). <div>References:
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Influence of Mineral Oil in 3D Printing of CMC-Laponite Emulsified Gels

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Advancements in 3D hydrogel printing are revolutionizing tissue and organ fabrication [1]. This research delves into the printability and biocompatibility of CMC and Laponite hydrogels, enhanced with mineral oil, to increase porosity and cell viability.

In this work, we assessed the hydrogels' structural integrity and compatibility with cellular processes by employing dental pulp Mesenchymal stem cells (DMSCs) and a 3D Bio X bioprinter. The optimized hydrogels demonstrated post-printing shape retention and supported high DMSC viability and proliferation. Adding mineral oil significantly improved porosity, facilitating cell growth and 3D interactions. The viability results indicate the hydrogel's potential in tissue regeneration and drug delivery. This study confirms the viability of using mineral oil-enriched CMC-Laponite hydrogels for 3D printing, suggesting a potential for patient-specific constructs in regenerative therapies and a range of clinical applications.

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Influence of the growth pressure on the structural, optical, and photoelectrical properties of magnetron sputtered ZnO thin films for gas sensing

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Nanostructured oxide materials are currently used as biosensors in technological applications. These materials are of great interest due to their potential for use in medical diagnostics, as they enable rapid, non-invasive, and low-cost evaluations. In this work, zinc oxide (ZnO) films were produced by the sputtering deposition method, varying the work pressure [1], [2], in order to obtain materials with specific features which can be used as gas sensors. X-ray diffraction analysis revealed the formation of ZnO's wurtzite phase with preferential orientation along the [001], [002], and [101] directions. It was determined that the film thickness decreases as the work pressure is increased. XRD data analysis also indicates that the mean crystallite and lattices constants decreases as the work pressure is increased. Good crystallinity was obtained after subjecting the films to thermal annealing in air and vacuum. UV-Vis spectroscopy results revealed that the band gap energy of the films does not show a clear tendency with the work pressure. With the same response time, photocurrent measurements for the films showed a good sensitivity to UV light [3]. Tests with a methane gas showed that the films can also be used as a gas sensor material.

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Innovative composite for orthopedic applications: synthesis and characterization of a multifunctional system composed by hydroxyapatite, boron nitride nanostructures, collagen, and tannic acid.

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The increase in life expectancy has raised worries about declining functional capacity, especially in bone health, where reduced resistance and higher fracture susceptibility present significant orthopedic challenges. Synthetic materials have emerged as promising alternatives for bone repair. This study focuses on developing an innovative composite consisting of hydroxyapatite (HA), boron nitride nanostructures (BNNs), collagen, and tannic acid (TA). This combination harnesses the mineral properties of HA(1) and collagen, the superior mechanical characteristics of BNNs(2), and the biological benefits of TA(3). The composites underwent thorough characterization utilizing several techniques including XRD, FTIR, TGA and SEM, confirming the presence of all components. Mechanical assessments demonstrated increase in Vickers hardness when BNNs and TA were added (118% and 139%, respectively). Also, an expressive enhancement of 1236% in the fracture resistance was noted when adding the reinforcement phase and TA. Drug release studies revealed the composite's capability to deliver ciprofloxacin, providing a multifunctional character to the nanocomposite, expanding its applicability. The nanocomposite presented a satisfactory release, reaching equilibrium after 96 hours of testing with 75% of the drug diffusing to the medium. Biological evaluations demonstrated the composite's biocompatibility with non-tumor cells and its toxicity towards osteosarcoma cells, evidencing a decrease in tumor cells viability at 50, 100, and 200µg/ml-1 concentrations with adding TA, highlighting its anti-tumor properties. These findings collectively suggest that the synthed composite holds promise as a biomaterial for orthopedic applications. Acknowledgments: FAPEMIG, CNPq an FINEP. (1)Klacic, T. et al. Coll. Surf. A: Physicochem. Eng. Aspects, 648, 2022.(2)Antillon, M. et al. Adv. Eng. Mater., 1800122, 2018.(3)Kaczmarek B. Materials. V.13,p.1-13,2020.

In Silico Investigation of Cell-Penetrating Peptide Properties and Their Potential as Transport Vectors Across the Blood-Brain Barrier

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The Blood-Brain Barrier (BBB) hinders the entry of therapeutic molecules into the central nervous system . The precise control of membrane permeability, which regulates the passage of molecules through passive diffusion or active transport, can be an obstacle to the delivery of some therapeutic compounds [1]. Cell-penetrating peptides (CPPs) emerge as structures designed to overcome lipid barriers, based on a series of distinct mechanisms, such as amino acid structure and hydrophobicity, often being cationic [2].

However, the pharmacological parameters defining penetration efficiency and the use of peptides as vectors for transporting these CPPs are unknown. In this study, we calculated the efficiency of peptides based on the parameter of lipid membrane permeability, as well as their potential as transport vectors. We performed molecular dynamics simulations in a bilayer area of 5 × 5 nm^2 , located in the middle of a 7.5 nm-high box, to calculate the free energy surface. Through the Replica Exchange Umbrella Sampling (REUS) methodology, we identified transition probabilities between different conformational states of the compounds and measured the permeability of the biomolecules used.

It is known that the transport of medium and large molecules across the BBB is complex and poorly understood. Pharmacological parameters are not always consistent with patterns observed in vitro and in vivo. Given this gap, molecular dynamics simulations can aid in understanding this mechanism and broaden our perspectives for the controlled transport of drugs.

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In situ production of a high entropy alloy reinforced with B4C for potential use as a biomaterial

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High entropy alloys (HEAs), composed of five or more elements, have been recently developed. These materials have been recognized for their high ductility, mechanical strength, and corrosion resistance, sparking interest in their use in the biomedical field. The development of new high entropy alloys has flourished, as currently developed HEAs do not exhibit suitable mechanical, electrochemical, and biological properties for biomaterials [1]. Metal matrix composites (MMCs), particularly with ceramic B4C material reinforcement, have emerged as high-performance materials for applications in aerospace and automotive industries, ensuring more excellent mechanical and corrosion resistance in aluminum, magnesium, and titanium alloys [2]. The objective of this study was to pioneer the development of a new high entropy alloy matrix, incorporating non-toxic and non-allergenic alloying elements, TiNbZrTaMo, non-equiatomic, with in-situ B4C reinforcement using electric arc melting. Chemical, structural, and microstructural details were investigated through x-ray diffraction, optical microscopy, scanning electron microscopy, density, and microhardness tests. The XRD and SEM results showed the presence of TiC and TiB precipitates, in the aspect of whiskers and particles, in the microstructure composed by grains of BCC-type phase and laths of HCP-type phase. Furthermore, the experimental density value was distinct from the theoretical one, evidencing the presence of in situ reactions between titanium atoms with B4C. Besides this, the precipitates did not compromise the plastic behavior of the material, having similar level of Vickers micro-hardness. The main findings shed light on the processability of novel composites based on high entropy alloys, which can open new horizons for biomedical materials.

Investigation by Electrochemical Impedance Spectroscopy of the Stability of Chitosan and Graphene Oxide Films

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The characterization of chitosan (CS) and graphene oxide (GO) coatings is already the focus of different studies aiming to obtain advanced materials. This combination exhibits regenerative capacity due to the re-pairing of chemical bonds, potentially returning to the pre-damage configuration and maintaining conductivity, which is crucial for the development of surfaces with good adhesion and cell proliferation [1]. Therefore, the aim of this article is to analyze the degradation kinetics of Ti6Al4V sample surfaces and investigate the protective performance of chitosan and graphene oxide coatings through the study and optimization of parameters in the electrochemical impedance spectroscopy (EIS) technique and self healing. Accordingly, this procedure was carried out using an alternating current impedance bridge with a 20 mV perturbation ranging from 10^4 Hz to 0,01 Hz in a 3,5% NaCl solution [2]. Additionally, confocal microscopic monitoring at 100x magnification and topographic study of the metal surface were conducted. A variation in polarization resistance values was observed between the samples before and after mechanical damage, indicating the corrosive process of the uncoated samples and the protective stability of chitosan and graphene oxide films.

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Investigation of the Influence Training on the Thermomechanical Behavior of Pseudoelastic NiTi Thin Plates using Digital Image Correlation and Thermography

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Shape Memory Alloys (SMAs) are renowned for their thermo-mechanical coupling associated with phase transformation processes. With unique attributes in stress-strain-temperature behavior, SMAs find diverse engineering applications, including actuators, smart structures, and mechanical vibration dampers. SMAs typically exhibit two main phases, austenite and martensite, showcasing macroscopic behaviors linked to phase transformation induced by mechanical or temperature loadings: pseudoelasticity, prevalent at high temperatures with austenite as the stable phase under stress-free conditions; and the shape memory effect, manifesting at low temperatures with martensite as the stable phase under stress-free conditions. Digital Image Correlation (DIC) emerges as an adequate technique in SMA studies, enabling the analysis of strain fields. By tracking displacement and strain fields during thermomechanical loading, DIC offers insights into material response to external load. In addition to DIC, thermography serves as an useful tool in the study of SMAs, allowing for the visualization of temperature distribution and thermal gradients during phase transformation processes. The integration of thermography provides complementary information to DIC, enhancing the understanding of the thermomechanical behavior of SMAs. This study presents an investigation into the influence of heat treatment and training on the thermomechanical behavior of pseudoelastic NiTi thin plates. Tensile tests, coupled with Differential Scanning Calorimetry (DSC), DIC, and thermography, were conducted to comprehensively assess the material's response. The integration of experimental techniques sheds light on the complex interplay between heat treatment, training, and thermomechanical properties, contributing to the understanding of SMA-based systems in engineering applications.

In vitro Foreign Body Reaction (FBR) model to evaluate the influence of silicone breast implants on protein conformation and immune cells

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Silicone breast implants for cosmetic or reconstructive purposes are among the most used medical devices. Despite an ongoing debate on implant biocompatibility, it is now widely accepted that silicone implants may cause a broad spectrum of chronic inflammatory diseases [1-2]. Breast implants trigger a cascade of stereotype immune events so called Foreign Body Reaction (FBR). This process starts with plasma protein (such as fibrinogen) deposition onto to the implant surface, which in turn triggers immune cell activation (especially macrophage) and results in the formation of a fibrotic tissue surrounding the implant (capsule), isolating it from the rest of body. Capsule then becomes the first recipient of silicone substances released by the implant, that could influence protein conformation and affect the proper mechanisms underlying the FBR. In this study, we proposed a simplified *in vitro* FBR model to evaluate the influence of silicone exposure on protein conformation and immune cells behavior. First, gel permeation chromatography and mass spectrometry were used to identify silicone species permeating from breast implant gel. Second, fibrinogen conformation after silicone exposure was analyzed by Fourier-transform infrared spectroscopy (FTIR). Third, the pro-healing (M1) or pro-inflammatory (M2) state of macrophages after silicone exposure was characterized using M1/M2 molecular markers by qPCR. Results showed that fibrinogen and macrophage behavior are affected depending on the physical characteristics and coatings of silicone films.

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Isolation and characterization of type II collagen isolated from pig ears

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Collagen (COLL) is the main component of the connective tissues of all multicellular organisms. Type II COLL is the main constituent of cartilage. Its primary structure is constituted by the aminoacids glycine, proline and lysine, arranged in a helicoidal structure. Due to its structural importance, various biomaterials have been prepared based on COLL, either in its pure form or mixed with other bioactive compounds. In the present study, type II COLL was isolated from pig ears and used to prepare biopolymeric membranes by casting. The methodology involved digestion in an acidic medium, centrifugation, dialysis and washing [1]. The characterization of the samples revealed the presence of two bands at 190 and 250 nm in the circular dichroism, supporting the anisotropic helical organization of the COLL fibrils. SDS-PAGE results showed 3 main bands with molecular weights close to 192.5 kDa; 156.6 kDa; 114.9 kDa. The COLL solution was placed in a Teflon mold, left in ammonium carbonate and dried in an oven to prepare membranes. Mechanical tests were carried out to determine the tensile strength, elongation and Young's modulus of the samples. Finally, scanning electron microscopy was used to observe the alignment of collagen fibrils in the membranes. The images revealed a cholesteric organization, similar to that found in the bone tissue. This study validated the methodology for isolation of type II collagen and its use for the preparation of biopolymeric membranes.

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Laser Synthesized Nanoparticles-Polycaprolactone heterogeneous membranes for Guided Bone Regeneration

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Regulation of biological activities such as angiogenesis or osteogenesis is critical for tissue engineering. Drugs induce cell differentiation, but high doses cause side effects and costs[1]. Exploring drugs with new pathways, with low hormone concentration for synergetic effects is an alternative. This work investigates antimicrobial and osteogenic properties of nanoparticles (NPs) produced by pulsed laser ablation in liquid. We studied silver NPs (AgNPs), nickel oxide NPs (NiONPs), and carbon monoxide-rich gold NPs (COR-NPs) obtained by pulsed laser-driven CO2 reduction reaction [2]. AgNPs and NiONPs were effective against Staphylococcus aureus, while COR-NPs induced cellular differentiation in adipose-derived stem cells (ADSC), as confirmed by alkaline phosphatase activity, osteocalcin staining, and calcium deposition assays. The polycaprolactone-metal nanoparticle blend, verified by scanning electron microscopy, showed no cytotoxicity in (ADSC), suggesting potential for future in vivo Guided Bone Regeneration applications [3].

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Live imaging of cell migration on self-assembled monolayers with well-controlled ratios of methyl- and amino-terminal groups

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Response of cells on the surface of materials used for implants can be understood by examining the physico-chemical properties of these surfaces and by carrying out dynamic biological studies. This knowledge may help us to creat novel bioactive materials that addresses the increasing cases of bone deficiencies due to pathologies such as osteoporosis in developed countries (1-2). In this study, we observed the spreading and migration of MG-63 osteoblastic-like cells on self-assembled monolayers with well-controlled ratios of amine and methyl contents on the surface. The surfaces were prepared by fabricating self-assembled monolayers (SAMs) with different and methyl densities on 1 x 1 cm silicon wafer substrates using a protocol that involves silanization using bromine-terminated silane, SN2 substitution of bromine to azide, and reduction of azide to amine (3). The resulting surfaces were characterized by water contact angle measurements and X-ray photoelectron spectroscopy. Live cell imaging experiments on the SAMs were performed by staining MG-63 cells with 1/2000 SPY620-DNA and 1/2000 SPY555-FastAct™ and then inoculated on the surface and were observed up to 16.5 hours using a LSM800 upright confocal microscope. The physico-chemical characterizations confirmed the presence of self-assembled monolayers on the silicon substrates with well-defined ratios of methyl- and amine-terminal groups. The cell spreading behavior and their slower migration on SAMs with higher amine groups are confirmed by the live cell imaging experiment. These results confirm the important role of amine groups on cell responsiveness on implant surfaces.

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Development of kaolinite nanoclay composites based on Brazilian stingless bees propolis for antimicrobial applications.

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Microbial resistance causes millions of deaths and, in recent years, has become an important area of research. Therefore, research involving new routes capable of dealing with multidrug-resistant bacteria is essential [1]. This study presents a system for photodynamic inactivation, using composites based on nanoclays and propolis as a more sustainable alternative to traditional photosensitizers. The nanocomposites were produced from extracts of the propolis Scaptotrigona postica (Mandaçaia, Mdg) and kaolinite (Kaolinite, KAO) - with pre-treatment at different pHs (Acid, Basic and Neutral) - for antimicrobial applications. Three extracts were used, produced from Ethanol, Chloroform and Toluene, following the protocol established by the group [2]. These were successfully mixed with the different Kaolin. The extracts and their respective nanocomposites were characterized using absorption spectroscopy, photoluminescence (PL) and photoluminescence excitation (PLE). They were also tested against Gram-negative (E. coli) and Gram-positive (S. aureus) bacteria to evaluate the pro-oxidant activity of the system. The Mdg ethanol and chloroform extracts and its composites showed a reduction of one log in the bacterial growth (E. coli) and two logs for (S. aureus).

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Experimental-analytical study of stainless steels for orthopedic implants under controlled deformation conditions

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High-N austenitic stainless steels have been used in orthopedic implants due to their mechanical properties and biocompatibility, proving to be economically viable options. However, they face challenges related to metallurgical production and processing. Physical simulation of thermomechanical processing allows estimating the dependence of parameters on the mechanical-microstructural responses of the alloy under conditions similar to industrial ones, as well as understanding metallurgical phenomena of work hardening (HW), dynamic recovery (DRV), and dynamic recrystallization (DRX) and their relation to the stacking fault energy (γ_{SFE}). In the present study, continuous isothermal hot torsion tests were conducted to simulate the thermomechanical processing of ASTM F-1586 steels, obtaining curves at different temperatures (900 ºC – 1200 ºC), deformation rates (0.01, 0.5, 1, and 10 s^{-1}), and a constant strain of $\varepsilon=5$. To determine the onset of DRX, the Poliak and Jonas method was used, which takes into account the work hardening rate (θ) relative to stress (σ), adjusted to a 3rd order polynomial equation, whose inflection point represents the critical stress for the onset of DRX. The results obtained indicate that $\sigma_{sat} = 1.05\sigma_p$, $\sigma_c = 0.96\sigma_p$, and $\sigma ss = 0.90\sigma_p$. Furthermore, the critical stress (σ_c) is reached at high deformations. This suggests a predominance of softening due to DRV. Microstructural aspects by optical and scanning electron microscopy confirm the presence of elongated strain-hardened grains in the first part of the curve, resulting from the HW-DRV synergy. After the peak, it is noted that DRX is slow and only completes at large deformations, as a result of the moderate value of stacking fault energy $\gamma SFE = 68$ mJ/m². Regarding the processing route, it is observed that for higher deformation rates, there is a delay in the onset of DRX, due to the time required for nucleation of new grains, while at higher temperatures, DRX is favored.

Luminescent nanosystems based on hydroxyapatite co-doping with Gd^{3+} and Eu^{3+}

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Nanomaterials have been widely studied for early diagnosis of tumors. Among these materials, hydroxyapatite (HA) has shown promise due to its bioactivity and chemical similarity with the inorganic phase of bone, in addition to having a structure that makes it possible to make substitutions, making the material obtain new properties [1]. Doping with rare earth elements is favored because they are similar to the atomic radius of calcium (Ca^{2+}). Among these elements, Europium (Eu^{3+}), due to its luminescence, can be used as dopants, forming an interesting system for imaging diagnosis. However, according to the literature [2], excess dopant can cause cytotoxicity. For an increase in the luminescence signal to occur, it is possible to perform co-doping so that Gadolinium acts as a sensitizing ion, based on energy transfer and the electron transfer process between rare earth elements. The objective of this work is to synthe a co-doped hydroxyapatite with different percentages of Europium and Gadolinium through hydrothermal treatment so that the properties for imaging diagnosis can be evaluated. The samples were characterized by XRD, SEM, FTIR, XRF, VSM, Zeta potential and photoluminescence. The results evidenced luminescent and magnetic properties of the materials and showed characteristics suitable for application in imaging diagnosis.

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Mesoporous Silica Materials Loaded with Tannic Acid as a promising potential in Biomedical Application

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The use of nanostructured carriers modified with specific molecules has presented notable advances in cancer cell therapy, improving the capacity for selective action in specific areas of the organism [1]. The properties of mesoporous silica, such as MCM-41, qualify it as an excellent option for carrying therapeutic agents due to its extensive surface area, well-defined pore diameter, and known biocompatibility [2]. In addition, tannic acid is a herbal medicine with great potential for bioapplication, due to its pharmacological properties, including bactericidal, antioxidant, anti-inflammatory, and anticancer activities, with this last property being the focus of this project. The aim of this work was to synthe, characterize, and functionalize MCM-41 nanoparticles with APTES. Tannic acid was incorporated into this final material for subsequent biological evaluation. The samples were characterized with FTIR, TGA, CHN, nitrogen adsorption, SAXS, SEM, zeta potential and release assays. The results revealed that the nanomaterials were successfully synthed and an efficiency in the incorporation and release of tannic acid from the functionalized MCM-41 was observed, suggesting a potential nanocarrier of herbal medicines for therapeutic purposes in biomedical applications.

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Mesoporous silica nanoparticles loaded with gold nanoparticles and gadolinium as a potential theranostic system

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Mesoporous silica nanoparticles (MSNs), such as MCM-41, are frequently employed in drug delivery systems due to their extensive surface area, well-defined pore diameter, and known biocompatibility [1]. Gadolinium is a popular contrast agent used in Magnetic Resonance Imaging (MRI) that improves the signal intensity of the tissue of interest and can potentially serve as a radioisotope (^{159}Gd) [2]. Similarly, gold nanoparticles have shown promise as a radioisotope (^{198}Au) for biomedical applications, such as cancer therapy [3]. To create a theranostic system, a silica matrix was complexed with gold nanoparticles and gadolinium. Multiple techniques were used to characterize the nanocomposites synthed in this study, including FTIR, UV-Vis, TGA, Nitrogen Adsorption, SEM, DLS, XRF, X-ray Absorption Near Edge Structure (XANES), Electron Paramagnetic Resonance (EPR), Vibrating Sample Magnetometry (VSM), and Inductively Coupled Plasma-Optical Emission Spectrometry (ICP-OES). The results showed that the nanocomposites were successfully synthed and gold nanoparticles and gadolinium were incorporated into the MCM-41 matrix, indicating that the system has potential applications in cancer treatment and diagnosis.

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Microencapsulation of ionic liquid and claymineral compounds for application as chromium adsorbent in aqueous solution

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Water contaminated by potentially toxic elements has serious impacts on the ecosystem. Currently, chromium compounds are recognized as one of the most harmful pollutants to human health. This study focused on the development of alginate beads, incorporating clayminerals and ionic liquids, aiming for a promising application in water decontamination through the adsorption of chromium. The adsorbents were prepared with a base of sodium alginate (2%) and sodium cloisite (2%), supplemented with zwitterionic ionic liquid (ZIL) (1%) or pure ZIL (1%). Therefore, the production of beads through microencapsulation, involving active materials with a thin polymeric layer as support, is interesting for the formation of porous microparticles. The spheres were subjected to characterization by scanning electron microscopy (SEM) and Fourier transform infrared spectroscopy (FTIR). Preliminary adsorption tests were conducted in batch evaluation the influence of most important factors. The quantification of metal in solution was analyzed by Atomic Absorption Spectrometry (AAS). The characterizations confirmed the presence of pores in the samples and the incorporation of ionic liquid and sodium cloisite in the spheres produced. Adsorption tests demonstrated that this material has potential for application in chromium removal, reaching an adsorption percentage above 90%. Kinetic tests indicated that the speed mechanism of the adsorption process is chemical in nature. Therefore, this study makes it possible to prepare adsorbents with good viability for application in environmental remediation.

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Multi-drug Intrauterine Device associated with the treatment of HPV and cervical cancer

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Cervical cancer is a disease that affects 80% of women in Latin America, with some cases arising from persistent Human Papillomavirus (HPV) infection [1]. The most common treatment for cancer is chemotherapy or radiotherapy, causing undesirable effects. As an alternative for cancer treatment and HPV prevention, this work aimed to develop intrauterine devices that allow the release of a local amount of medication into the body. Copper is a material with antibacterial and antiviral properties, making it promising for cinergetc healthcare treatments together with other specific drugs. The devices were manufactured using the fused filament manufacturing (FFF) 3D printing technique using EVA with concentrations of 10 wt. % of each drug, namely copper sulfate, silver sulfadiazine and Fluorouracil. Multi-drug IUDs were subsequently manufactured, with 8 wt.% copper sulfate and silver sulfadiazine and 8 wt.% copper sulfate and Fluorouracil. To characterize the devices and filaments, DSC, DMA, FTIR, SEM tests and in vitro tests were carried out in order to verify the performance of the manufactured devices, analyzing the drug release profile to evaluate the viability for applications. EVA with 12% vinyl acetate performs well in the 3D printing process, with greater agility in the process and good filling of the manufactured devices. Finally, the feasibility of using these materials in the additive manufacturing process with potential for incorporation of medicines and controlled release capacity during certain periods is highlighted.

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NATURAL RUBBER-BASED FIBROUS BIOCOMPOSITE REINFORCED WITH BIOACTIVE GLASS-CERAMIC PARTICLES FOR BIOMEDICAL APPLICATIONS

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In this study, a new fibrous mat biocomposites formed with natural rubber (NR) and containing 45S5-K (BL0) or biosilicate (BioS) particles was developed using solution blow spinning technique. In order to assess fiber formation and BG dispersion in fibrous specimens, SEM morphological analyses were conducted. It was observed that average fiber diameter (dm) increased with the incorporation of BG in NR fibers, i.e., for pure NR, the dm value was 74.47 ± 24.54 µm, while for NR/BioS and NR/BL0 the values were 78.96 ± 30.54 µm and 84.75 ± 25.69 µm, respectively. The TG/DTG tests indicate that NR/BioS and NR/BL0 fibrous biocomposites display similar thermal profiles to neat NR, whose main events occur between 290°C and 450°C, indicative of structural degradation of NR chains. According to the mechanical tensile test, adding BioS or BL0 to the NR-based biocomposite enhanced the tensile strength at break and elastic modulus, as compared to neat NR. As a result of dynamic mechanical analysis (DMA), the stored modulus and loss factor of the fibrous specimens of NR/BioS (70/30) and NR/BL0 (70/30) displayed higher values than those of the NR fibrous sample, since the specimens became more rigid as BG quantity was increased. The indirect cytotoxicity tests showed that NR, NR/BL0, and NR/BioS fibrous biocomposite promoted MSC attachment, i.e., greater than 70% viability. In addition to improving tensile properties and biological properties of NR-based fibrous biocomposite, BioS and BL0 particles have been shown to have potential applications in biomedicine.

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Novel functional bone cement based on magnesium phosphate and poly(vinyl alcohol) hydrogel dedicated for minimally invasive surgical applications

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In the biomedical field, self-hardening cements play a crucial role in the reconstruction, implant fixation, and stabilization of complex fractures. Magnesium phosphate cement (MPC) is particularly valued for its rapid setting time, high mechanical strength, and excellent biodegradability. However, its clinical application is hindered by its brittleness and poor injectability. To address these limitations, this study aims to develop a novel cement by incorporating poly(vinyl alcohol) (PVA) hydrogel into the MPC matrix. This biocomposite is formulated by combining MgO with KH2PO4 (at a 4:1 Mg/P molar ratio) within a PVA (at a 2.5:1 g/mL P/L ratio), crosslinked with sodium borate. The evaluation includes assessments of setting time and temperature, microstructure, phases and chemical composition, compressive strength, injectability potential, biodegradability, and cytocompatibility with human osteoblasts. The MPC+PVA cement exhibits outstanding characteristics, including a lower setting temperature, increased compressive strength with potentially reduced brittleness, and enhanced functional properties such as paste cohesion and injectability. The gelation reaction did not adversely affect the hydration process, and a significant proportion of k-struvite was observed in the material. Additionally, the cement demonstrates excellent cytocompatibility and an appropriate biodegradation rate. In conclusion, the dual-setting MPC+PVA cement was successfully developed. This cement overcomes the common limitations of traditional bone cements, making it a promising candidate for widespread clinical application, and its enhanced properties potentially lead to better patient outcomes and more efficient repair processes.

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Optimizing prosthesis Dental Zirconia Manufacturing through Ultra-Fast Sintering

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Ultra-Fast High-Temperature Sintering (UHS) has emerged as a promising technique for rapidly consolidating ceramics, offering unprecedented processing speeds and energy efficiency. The UHS process provides significant advantages, such as reduced processing time, improved energy efficiency, and the potential for finer microstructure control. Therefore, it is a sintering process that enables extremely high heating rates through direct contact of samples with electrically heated thin carbon strips. This study explores the application of UHS for the sintering zirconia with 4 mol% $Y2O3$, a unique combination of mechanical, thermal, and biological properties suitable for different applications, including dental materials. However, conventional sintering processes for zirconia often require long processing times and energy consumption. Through a parametric study, this research investigates the behavior of zirconia under UHS conditions and proposes a setup (protocol) to mitigate heat loss and improve process efficiency. The sintering protocol involved applying 30 A for 30 seconds, 35 A for 30 seconds, 40 A for 30 seconds, 45 A for 30 seconds, 48 A for 7 minutes. Subsequently, a slow cooling protocol was performed at 45 A for 2 minutes, 35 A for 2 minutes, and 30 A for 2 minutes. Static strength and microstructure were investigated through static biaxial flexural strength tests, scanning electron microscopy and Archimedes density measurements. The highest static strength recorded was 588.76 MPa, and the sintering protocol demonstrated the ability to produce samples with up to 98% density in just 16 minutes. The results obtained thus far suggest that the UHS technique can significantly accelerate zirconia processing.

Optimizing Slurry Formulations for Tissue Engineering Using Design of Experiments

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This study investigates the application of a design of mixture experiments to optimize the formulation of slurries used in bioactive grafts manufactured by tape casting. The primary objective is to improve the tape casting process quality by determining the ideal composition of the additives. The methodology employed involved the use of experimental design and statistical analysis to identify the optimal mixture of additives. The results revealed that the statistical mixture design approach provided a significant enhancement in the properties of the bioactive grafts. The findings of this study have significant implications for the biomaterials development and bone tissue engineering. The use of statistical mixture design approaches in the development of optimized additive formulations has the potential to accelerate the development of new and improved bioglass-based materials for bone regeneration and tissue engineering applications.

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PCL nanofibers containing tetracycline-curcumin synergistic association applied to biocompatible wound dressings

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PCL nanofibers containing tetracycline-curcumin synergistic association applied to biocompatible wound dressings

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The WHO manual on prevention and management of wound infections advise for the importance of properly treatment of wounds.[1] The association of synergic combination of antibiotics with natural compounds is a beneficial strategy to wound healing.[2] In this study, a biocompatible nanofibrous wound dressing based on PLC nanofibers and a synergistic combination of tetracycline (TC) and curcumin (CC), was successfully developed. Specifically, the system was fabricated using the solution blow spinning technique, and the results showed large self-standing bandages, able to protect the wound against microorganisms from the environment. A sustained co-release profile for both components was verified, reaching a maximum release of 60% of CC content and 68% of TC content at 72 hours. Importantly, the extracts released from the wound dressings showed no cytotoxicity for human dermal fibroblasts, with cell viabilities above 95%. Ultimately, in vivo tests conducted on induced wounds in mice skin, associated to photodynamic therapy (PDT) technique, also demonstrated that the fibrous mats promoted effective healing, without causing any inflammation.

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Photocatalytic performance of Ag-TiO2 films under visible light

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Water pollution caused by the disposal of organic substances such as dyes, pesticides and antibiotics seriously affects the quality of water resources and, consequently, human health. Advanced oxidative processes present themselves as an effective alternative for removing these contaminants from water. In this work, the photocatalysis performance of Ag-TiO2 films under visible light in the removal of methyl orange dye was studied. The films were obtained from a solution containing titanium isopropoxide (IV) and ethyl alcohol in a ratio of 1:10 (v:v). The solution was kept under constant stirring at 70 °C for 60 min. Subsequently, the sol was deposited on borosilicate glass using an airbrush. The films were heat treated for 30 minutes at 500 ºC in a muffle furnace and then immersed for 30 minutes in an aqueous solution of 0.1 mol.L-1 of AgNO3, followed by rinsing in deionized water and drying. After that, these films were subjected to UVC radiation for periods of 60, 90, 120 and 150 minutes to allow the reduction of Ag+ to Ag0. X-ray diffraction and scanning electron microscopy techniques were used to characterize the films. In the photocatalysis tests, it was observed that the longer the irradiation time of the catalyst in UVC light, the better its photocatalytic performance, quantified by spectrophotometry, considering the discoloration of the methyl orange dye (5 mg.L-1). The best performance was attributed to the film subjected to 120 minutes of exposure to UVC light, reaching 80% of degradation after 300 minutes of exposure to visible light.

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Photogem-nanoclay composites to improve antimicrobial activity.

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Among the many research groups dedicated to drug delivery systems, a good portion challenge themselves to face the bacterial drug resistence problem. Moreover, in 2018, WHO declared the antimicrobial resistance as ‘(...) one of the top 10 global public health threats facing humanity’, along with a similar problem in cancer treatment: the chemotherapeutic drug resistant cells [1]. Photoinactivation systems and photodynamic therapy (PDT) are regarded as some of the main upcoming methods to overcome these issues, however, at the current stage, the prospection of more robust and efficient molecules that can act as photosensitizers (PS) are still needed. In this work, the PS derived from porphyrin, photogem (PG), was submitted to a set of physiochemical variations (pH 2, 7 and 10, and concentrations of 2.5, 6, 12, 16, 22, 25, 35 and 50 µg/mL) to promote new aggregation states with the aim of improving its antimicrobial activity. The aggregated states of PG were characterized by photoluminescence and photoluminescence excitation spectroscopies, showing different conformations at basic and at acidic pH, but not changing significantly with the increase in concentration. These samples were used to build composites with halloysite and kaolinite nanoclays, of which the acidic showed a more efficient formation. The antimicrobial activity of the composites were then tested against E. coli and S. aureus. The results and effect of the composites will be discussed in light of the photophysical behavior of PG and the near field effect.

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Preparation of hydrogels containing type II collagen and carrageenans and their potencial use for cartilage regeneration.

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Collagen is a potential candidate for the preparation of biomimetic materials able to stimulate bone mineralization and cartilage regeneration. The human cartilage has a low ability of regeneration due to its avascularity. Therefore tissue engineering aims at obtaining biomimetic materials with controlled biodegradability rates and able to improve specific local cell stimulation on site of defects. Chondroitin sulfate (CS) is one of the main glycosaminoglycan (GAG) component of cartilage and it can connect or retains growth factors [1]. Carrageenan has chemical and structural characteristics similar to CS, so it is a candidate as a substitute of this GAG. Furthermore, carrageenan has better rheological properties compared to CS and can be obtained from renewable sources. This study aimed at comparing mechanical properties or chondrocytes culture of type II collagen containing either kappa-carrageenan (K-carr) and CS. Type II collagen was isolated from pig's ear [2] at a concentration of 1.7 mg/mL. After concentration by tangential flow filtration, a solution containing 5.1 mg/mL of type II collagen was used to prepare the scaffolds. The tertiary helical structure of the collagen triple-helix was confirmed by circular dichroism spectrum. The molecular weight of collagen was obtained by SDS-page electrophoresis and it was found bands associated to the 3 α_1 polypeptide chains (192.5, 156.6 and 114.9 kDa). The scaffolds were prepared and characterized by FTIR and SEM. Bands associated to the chemical structure of collagen, K-carr and CS at 1540, 1225 and 1640 cm^{-1} were detected by FTIR. The modification of size and distribution of collagen fibrils caused by the addition of K-carr and CS was observed by SEM images, which indicates the potential of K-carr associated with collagen for cartilage regeneration.

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Preparation of type II collagen hydrogels with curcumin and curcumin A and effects on osteoblast mineralization

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Curcumin (1,7-bis(4-hydroxy-3-methoxy-phenyl)-hepta-1,6-dien-3,5-dione) is a yellowish hydrophobic phenolic compound present in the rhizomes of Curcuma longa that has anti-inflammatory properties. The literature indicates limitations of the use of curcumin as a bioactive molecule due its high hydrophobic character that led to low bioavailability and toxicity in high concentrations. In the present study, type II collagen hydrogels were prepared with curcumin and curcumin A, a monocetonic modified curcumin synthed by aldol condensation under acidic conditions between acetone and vanillin, which formed three-dimensional structures in the form of scaffolds. The effect of the scaffolds containing curcumin on the mineralization of osteoblastic cells was tested in vitro. Cell mineralization experiments, performed for periods of 7, 14 and 21 days, evaluated alkaline phosphatase activity and alizarin red staining were carried out in the presence of type II collagen scaffolds without addition of curcuminoids (control), type II collagen +curcumin scaffolds and type II collagen+curcumin A scaffolds, using a concentration of curcumin of 20 µg/mL. When free in the culture medium, curcumin nor curcumin A presented positive effects on osteoblasts mineralizations. However, when added to scaffolds containing type II collagen, curcumin A + type II collagen scaffolds induced higher alkaline phosphatase activity values compared to the control.The quantification data of mineralized nodules, demonstrate that there is no statistical difference over the days comparing the curcumin and curcumin A scaffolds with the control. The set of data highlights the importance of administration of curcumin on cells using a biomaterial as a carrier to guarantee assess to the cells.

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Production and characterization of PEO-treated AISI 1020 low-carbon steel enriched with Ta2O5 for use as a biomedical material

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Fe-based materials have extensive applications in the building and automobile industries due to their excellent mechanical properties and low cost. However, their biomedical usage is restricted by the corrosion propensity when in contact with body fluids. This study used PEO treatment in a TaOH-rich electrolyte to coat AISI 1020 low-carbon steel and to enhance its anti-corrosion and wear properties, targeting its employment as a medical device. The effect of potential, time, duty cycle, frequency, and Ta(OH)5 concentration on the chemical and phase composition, topography, wettability, and roughness of the obtained coatings were addressed. The results indicated that the Fe-based oxide coatings had a rough and super-hydrophilic surface. The phase composition of the coatings was formed mainly of Ta2O5, hematite (Fe2O3), and a minor amount of rust (Fe(OH)2), with the chemical analyses also indicating the presence of some absorbed molecules. Once the best PEO parameters were established (200 V, 5 min, 60%, 1000 Hz, and 40 g/L Ta(OH)5), the previous mechanical, corrosion, and wear tests evidenced the positive effect of the chemical species deposited in the surface when compared to the substrate. The corrosion resistance of the PEO-treated samples was better than that of the substrate against saline solution (0.9% NaCl) due to the Fe2O3 growth decorated with Ta particles, especially in the sample treated at 200 V. In this way, PEO treatment applied on AISI 1020 low-carbon steel in a TaOH-rich electrolyte can be an adequate alternative to produce low-cost materials for medical devices, especially as a potential substitute for stainless steel in surgical instruments. The results state that the Ta-enriched Fe-based oxide coatings could significantly improve the applicability of low-carbon steel SAE 1020 as a low-cost biomaterial, particularly for medical devices. (Financial support: CNPq and FAPESP)

Production of Zein-CMC-PEO by Electrospinning for application in controlled release of piperine

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The electrospinning technique can produce fibers or nanofibers, having characteristics such as lightweight, mechanical flexibility, chemical specificity, and high biocompatibility [1, 2]. Piperine is a potential bioactive compound found in black pepper (Piper nigrum), with many biological properties [3]. This work investigated the formation of zein, carboxymethylcellulose (CMC), and poly(ethylene oxide) (PEO) by electrospinning technique for application in piperine control release. Zein-CMC-PEO dispersion was prepared by mixing zein 9,5% (w/v), CMC 0,5% (m/v), and PEO600 kDa 5% (w/v) in a hydroalcoholic solution (water/ethanol 3:7 (v/v)) and kept under stirring at 200 rpm for 1h. The sample was pumped at a 5.0 mL h-1 flow rate through a stainless-steel needle acting as a spinneret upper electrode to which a 12 kV voltage was applied to obtain the fiber, which was collected in aluminum placed 10 cm from the needle. Scanning Electron Microscopy (SEM) revealed the formation of nanofibers with thickness ranging between 800 to 2000 nm. Piperine was extracted from black pepper using the soxhlet method. FTIR spectrum showed piperine formation with the bands: at υ1580 cm-1(C=C vibration of the aromatic chain), υ 2937 and 2850 cm-1 (aliphatic C–H), υ3000 cm-1 (aromatic C–H), υ 1630 cm-1 (C=O) and 1H NMR (δ/ppm, D 1,6Hz), δ 6,97 ppm (d, J = 1,6 Hz), e δ 7,38 ppm (dd, J = 14,6; 10,1 Hz). More experiments are in progress, such as Zeta Potential, DSC, and TGA.

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Release of metronidazole benzoate and/or metronidazole-incorporated frommicrofibers formed by zein/HPMC-AS/CNF for potential treatment ofperiodontitis.

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Periodontitis is a disease that results in damage to the supporting tissues of the teeth and the formation of periodontal pockets, caused by detachment of the epithelium and deterioration of the bones [1]. The drugs metronidazole (MDZ) and metronidazole benzoate (BMDZ) are microbial agents that can be used in the treatment of this infectious disease [2]. Several drug release platforms can be used to treat periodontal diseases, including fibers produced by electrospinning [3]. In this sense, fibers composed of 39.8% (w/w) zein, 59.7% (w/w) hydroxypropyl methylcellulose acetate succinate, 0.5% (w/w) poly(ethylene oxide) (PEO), and 1% (w/w) cellulose nanofibrils were evaluated as a platform for the release of 40% (w/w) MDZ and/or BMDZ. The fibers formed had a semi-crystalline character and lower temperature of drug crystallization, indicating a good interaction between the drugs and the biopolymers. The release tests showed that the presence of CNF contributed to prolonging the release of the drugs and the fibers containing both drugs have a better profile release for treating the disease for a longer period.

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Silky fibroin/alginate/carboxymethylcellulose hydrogel loaded with red propolis for wound healing

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A hydrogel-based wound dressing is important to promote post-injury functional skin integrity [1]. This study focuses on evaluating of physicochemical properties and antimicrobial activity of Alginate/Fibroin/Carboxymethyl cellulose (ALG/FB or ALG/FB/CMC) hydrogel under different conditions of Ca^{2+} crosslinker/glycerol plasticizer agents and red propolis extract. ALG/FB and ALG/FB/CMC-based films have been prepared by solvent casting process. It was obtained a homogeneous and flexible self-demoulding film. Mass proportions between silk fibroin and sodium alginate were 1:3 in order to provide a hydrogel formation [2]. The results of ATR-FTIR spectroscopy have showed a good compatibility among the protein/polysaccharide chains of the biopolymers. The swelling efficiency was observed from 200 to 977%, exhibiting an excellent ability to absorb wound exudate fast and completely. Likewise, the hydrolytic degradation has resulted in 30 to 74 wt% mass loss. It also observed a successfully red propolis-incorporated delivery system. After 30 days, the percentage of red propolis released was noted a significantly lower release between 30-45% for all samples, indicating a tailored controlled release rate. Furthermore, the red propolis loaded films have also showed antimicrobial activity against Staphylococcus aureus, Staphylococcus epidermidis and Pseudomonas aeruginosa. Therefore, this work has demonstrated the antibacterial activity of the films, taking into consideration its application on important adjuncts to treat contaminated or chronic wounds. Likewise, it is important to conclude the adding value products from beekeeping sector by potential use for drug delivery devices.

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Structural, magnetic and luminescent properties of kyanite samples

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Kyanite is the compound formed under the highest pressure among its polymorphs [1], with its main composition assigned to the Al2O3 and SiO2 structural units, and the remainder is generally dominated by impurities [2]. In this work, blue and green kyanite samples from Minas Gerais - Brazil, were pulverized to obtain particles in the range from 75 μm to 180 μm. The samples were subjected to heat treatment at 700, 800, 900 and 1100 °C. The effect of heating treatment was evaluated using Raman spectroscopy, optical absorption (OA), Infrared absorption spectroscopy (FTIR), X-ray diffraction (XRD), X-ray fluorescence spectrometry (XRF), Thermogravimetry (TGA), Thermoluminescence (TL) and Optically stimulated luminescence (OSL). The XRD evidenced the triclinic crystalline structure of the samples. Based on the Raman spectroscopy results, it was possible to identify the vibrational groups corresponding to the oxides SiO2, Al2O3 and Fe2O3. Energy dispersive spectroscopy data indicate the predominance of silicon, oxygen, and aluminum in the composition of the samples. XRF indicated the presence of impurities in the structure of the materials, such as Fe, V, Ti, Cr and Mn, with higher Fe concentrations in the green kyanite sample. The OA of green kyanite samples shows absorption bands attributed to substitutions of the Al3+ for Fe3+ and Cr3+ ions and indicates Ti4+-Fe2+ charge transfer. The magnetization data shows a pure paramagnetization only for the green kyanite treated at 1100 ºC. TGA results under nitrogen and synthetic air conditions evidenced the behavior of the sample's mass change in the temperature range from RT until 1100 ºC. TL and OSL results were used to evaluate the defect's depth and the potential application of the kyanite as a radiation sensor.Acknowledgments: this work was supported by FAPESP (#2023/12201-2 and #2021/13132-9) and CNPq. References: [1] A. E. Maftei et al., Minerals 10, 988 (2020). [2] A. Tarantola et al., Minerals 9, 252 (2019).

Study of Ceramic Suspensions for Porous Ceramic Production in order to Technological Purposes

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In recent years, the inclusion of porosity in ceramic materials has motivated the development of several technologies, such as ceramics for implants, aircraft components, filters, and others [1]. In this context, a series of methods have been used to create porous solids and the obtaining of ceramic suspensions through colloidal processing based on gelcasting has been a great alternative [2]. In this work, ceramic suspensions of the alumina were obtained by foam gelcasting using ovalbumin as consolidator and foaming agent. Viscosity and zeta potential measurements were made to ensure the best stability and homogeneity condition for the suspension. Also, the microstructure, morphology and pore distribution were investigated by SEM. The results of this study showed that the technique developed is efficient in obtaining porous ceramics with a solid content greater than 65 (wt%) using an organic content of around 6 (wt%), generating an interconnected microstructure of pores, which can be successfully applied to bioinert implants, filters, in addition to increase the reliability of ceramic materials for purposes such as these.

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Study of Laser-Induced Ablation of Polymethyl methacrylate (PMMA) for Ophthalmic Applications

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With the advancement of femtosecond laser technology, a new array of laser-based technologies for increasingly precise surgeries has emerged. Presently, there is a concerted effort to deepen our understanding to refine these technologies for safer, more precise treatments, and to develop more compact equipment. To better comprehend how laser-induced ablation parameters affect the human cornea, it is imperative to conduct ablation characterization across various attributes. To achieve this, Polymethyl methacrylate (PMMA) is utilized as a material that replicates the human cornea. By profiling the surgical process of current technologies and characterizing laser ablation with new parameters, the study aims to develop more sophisticated laser ablation techniques for ophthalmic surgeries that are replicable in subsequent studies involving the human cornea.

Study of the surface modification of commercial Ti laminates using cold plasma and silver nanoparticles

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In the medical field, there is a critical need to develop durable and infection-resistant prosthetic materials. Cold plasma surface modification of titanium followed by application of silver nanoparticles is a promising approach to prevent bacterial growth [1]. Titanium is inert and resistant to corrosive body fluids, while silver nanoparticles exhibit strong antimicrobial properties [2]. This work focuses on developing methods to modify the surface of titanium. The methods combine plasma techniques, heat treatments and the controlled introduction of superficial defects followed by the insertion of silver nanoparticles. Sample groups were divided based on the presence or absence of surface defects. After surface treatments and the application of silver nanoparticles synthed by chemical reduction method optical microscopy, scanning electron microscopy with energy dispersive spectroscopy (SEM/EDS), atomic force microscopy (AFM), evaluation of contact angle and surface energy (WCA) and attenuated reflectance infrared spectroscopy (FTIR- ATR) were applied to evaluate the samples surfaces. Additionally, UV-VIS-NIR spectroscopy was performed to confirm the synthesis of the nanoparticles and estimate their range. The nanoparticles stabilized on the surface even without the use of stabilizing agents during the synthesis process. The activation energy of the plasma is important in the adhesion process of the nanoparticles, which prefer defective regions. In addition, surface swabbing tests were conducted using a dry cloth and 70% alcohol to simulate a sterilization process on a modified surface.

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STUDY OF THE TL DOSIMETRIC PROPERTIES OF LITHIUM SILICATE PHOSPHOR FOR GAMMA DOSIMETRY

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Radiation quantification or dosimetry can be performed in several ways, generally based on the physical effects caused by radiation on a given material. One way of detecting radiation is by using thermoluminescent materials. These materials are capable of emitting light when heated provided they are previously exposed to ionizing radiation.

Silicates are an attractive class of materials among inorganic phosphors, due to a wide range of applications and certain properties, such as chemical stability, transparency to visible light, and physicochemical stability at high temperatures. A very important characteristic of silicates is the sensitivity to ionizing radiation for a certain energy range. Silicates with a cation in their crystal structure, such as pure and doped lithium silicate synthed by different methods, exhibit certain properties like luminescence in the visible region, physicochemical stability at high temperatures and radiation stability. In the present work, we have synthed lithium silicate (LSO) by solid-state reaction sintering method and studied the dosimetric properties in terms of its thermoluminescence (TL) response such as: linear response to γ-exposure, fading, sensitivity, minimum detection dose, repeatability, and its TL emission characteristics. The dosimetric properties of LSO in the form of pellets were studied by TL under the effect of different doses of γ-irradiation. The phosphor exhibited a TL emission curve with four TL peaks with a light emission band centered at 385 nm. The TL dose-dependent γ-radiation dose response of the TL peak at 182 °C was linear in the low-dose region, from the order of mGy to 50 Gy. In addition, the phosphor exhibits lower fading and good reproducibility.

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Superficial modification of CP 2 Titanium and Ti6Al4V ELI alloy for coating through biomimetic method

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Titanium (Ti) and the Ti6Al4V ELI alloy are essential metallic materials employed in implant applications. Surface modification of these materials is necessary to enhance their integration with host tissue. This research utilized a biomimetic process to coat the surface of commercially pure Grade 2 Titanium (Ti CP 2) substrates and Ti6Al4V ELI alloy. Initially, the materials underwent surface modification through techniques involving double acid etching and basic etching, resulting in increased roughness to facilitate better adhesion of the subsequent coating to be deposited. Afterward, the substrates were activated via thermal treatment and immersion in sodium silicate. These activated materials were then incubated in an SBF (Simulated Body Fluid) solution, mimicking the composition, pH, and temperature of human blood plasma. The roughness level post-chemical treatments and the resulting coating were analyzed using various characterization techniques, including Scanning Electron Microscopy (SEM/FEG), Energy Dispersive Spectroscopy (EDS), Optical Microscopy (OM), X-ray Diffraction (XRD), and Optical Profilometry. The Ti CP 2 and Ti6Al4V ELI substrates that underwent acid etching, followed by surface activation through thermal treatment and immersion in sodium silicate, and were subsequently incubated in SBF for 21 days exhibited superior efficiency in terms of the coating.

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Surface characterization of high entropy alloys MAO treated in Cu-rich electrolyte for potential use as biomaterials.

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High entropy alloys (HEAs), composed of five or more elements, have been developed in recent years, and have been attracting the attention for biomedical use, due to the promising solid solution hardening, superior mechanical strength, ductility, corrosion resistance and wear resistance when compared to conventionally used materials [1]. However, the current developed HEAs lack of proper mechanical, electrochemical, and biological properties for the usage as biomaterials at long-term. In addition, as their surface is bioinert, the HEAs do not present adequate bioactive or antimicrobial effect when in contact with the biological host [2]. Thus, surface modification methods, including micro-arco oxidation (MAO), have been used for the surface functionalization of metallic biomaterials, resulting in fast osseointegration, bone tissue recovery, and prevention of bacterial infection on the implant surface [3]. In this scenery, this study aims to develop a new Bio-HEA composed of non-toxic, low cost and melting point elements, such as Ti, Zr, Mn, Al, and Nb, for potential biomedical applications as bone fixation devices (pins, plates, and screws) with a surface functionalized by MAO in a Cu-rich electrolyte. The MAO-treated samples showed mostly amorphous TiO2 oxide decorated with calcium, phosphorus and magnesium, and traces of copper. The MAO treatment made the surface rougher and changed the contact angle and surface energy. The main findings of the study shows that the MAO treatment is a useful tool to coat HEAs with a porous Cu-rich and bioactive oxide layer which could be interesting for the next generation of metallic biomaterials.

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Surface modification of poly(lactic acid)/strontium-substituted hydroxyapatite scaffolds by polydopamine coating for bone tissue engineering

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Bone tissue engineering presents a promising solution for autogenous replacement. Bone fractures can be effectively treated through the utilization of supportive structures for tissue growth (scaffolds) [1]. Strontium-substituted hydroxyapatite (HASr) is a notable ceramic material, enhancing the properties of poly(lactic acid) (PLA) scaffolds [2]. Polydopamine (PDA) exhibits potential in functionalizing biomaterials as it has functional groups, such as catechol, amine, and imine, that allow it to establish connections between materials and cells [3]. This study proposes the application of PDA coating on PLA/HASr scaffolds to enhance their hydrophilicity and functional groups. Filaments of PLA and PLA/HASr were manufactured using a two-screw extruder. Fused Filament Fabrication 3D printer was used to produce scaffolds with trabecular biomimetic geometry [1]. The scaffolds were immersed in 3 mg/mL dopamine in Tris HCl buffer pH 8.5 solution for 24 h. Wettability analysis demonstrates that PLA/HASr/PDA resulted in improved material hydrophilicity (31.2±5.8°) compared to neat PLA (88.3±0.4°), PLA/PDA (40.6±1.6°) and PLA/HASr (64.8±0.1°). SEM images illustrate the presence of PDA microparticles on the surface of PLA/HASr/PDA scaffolds, suggesting enhanced surface area. FTIR analysis confirms the presence of catechol and amino groups on scaffolds coated with PDA. These scaffolds exhibit several characteristics for bone tissue engineering applications, such as the presence of signaling ions, improved adhesion properties, and biocompatibility.

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Surface modification of Ti6Al4V alloys with bioactive PMMA-silica coatings

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The development of multifunctional materials is the key to improving the properties of new generation of implantable medical devices based on titanium and its alloys. Incorporating bioactive agents into coatings is among the strategies for modifying surface properties to customize biological responses after implantation [1]. Thus, in this study, poly (methyl methacrylate) (PMMA)-silica coatings were modified with hydroxyapatite (HA), β-tricalcium phosphate (β-TCP), and cerium oxide (CeO_2) nanoparticles with bioactive and bactericidal properties, respectively. CeO_2 was synthed using a hydroxide-mediated precipitation method. PMMA-silica hybrids modified with HA, β-TCP, and CeO_2 were obtained by covalently coupling the polymeric phase of methyl methacrylate (MMA) and 3-methacryloxypropyl trimethoxysilane (MPTS) with the silica nanophase, synthed by sol-gel reactions of tetraethylorthosilicate (TEOS). The 17 µm-thick coatings deposited on Ti6Al4V are homogeneous and show a strong adhesion (>12 MPa) to the substrate. X-ray diffraction (XRD) and atomic force microscopy (AFM) showed that the CeO_2 particles have a cerianite structure and s in the range of 40−100 nm. The effect of HA, β-TCP, and CeO_2 on the structural properties was evaluated by infrared spectroscopy, X-ray diffraction, thermal analysis, atomic force microscopy, and contact angle measurements. The corrosion efficiency was studied by electrochemical impedance spectroscopy in a simulated body fluid (SBF) solution. The modified coatings showed an impedance modulus of up to 74 GΩ cm^2, which remains four decades higher than the uncoated Ti6A4V alloy after 300 days of exposure to SBF. The formation of apatite on the surface of the coatings was evaluated by scanning electron microscopy after 21 days of exposure to the SBF solution.

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Sustainable Calcium Nanoparticles based on Agroindustry Waste for Potential Odontologic Applications

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Development of sustainable proposals in various areas has been crucial nowadays. Climate changes and all environmental advances have caused many worries in society. Thus, this research evaluated a sustainable synthesis of calcium nanoparticles (CaO NPs), using an agroindustry waste from eggshells to promote dentistry tissue regeneration with antimicrobial activity. Then, eggshells were loaded to heat treatment with two different temperatures (700 ºC and 900 ºC) for three times (7, 15 and 24 hours). These CaO NPs were characterized using spectroscopies (UV Vis, FTIR, XRD) and morphological (ZP, SEM). Additionally, antimicrobial activity against Escherichia coli (ATCC 1597) and Candida albicans (ATCC 90029), cell viability, protein adsorption and alkaline phosphatase activity were evaluated. The results showed that CaO NPs were produced in both temperatures, but in the case of slow temperature Ca(OH)2 was still presented. Moreover, morphological analysis showed charges close to zero, indicating high agglomeration of nanoparticles proved by SEM images. CaO NPs average diameter were in the range of 52.27 and 104.23 nm, with band gap found by TAUC relation at 2.82.to 5.77 eV. The cell viability was great for biological proposals, mainly in the sample performed at high temperature (over 90%). Furthermore, the antimicrobial activity showed incredible results against both microbials, similar to protein adsorption and phosphatase activity. Thus, this research demonstrated a sustainable way to reusability for waste from agroindustry for improvement the economical final material for potential dentistry applications.

Synthesis and characterization of carrageenan nanoparticles containing flavonoid-Sr2+ complex for bone regeneration

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Bone regeneration is a global concern due to trauma, aging, and chronic diseases that could affect tissue integrity and function. Therefore, studies have been conducted on natural compounds as candidates for bone regeneration. In a previous study, our group demonstrated the osteogenic potential of a flavonoid-Sr^{2+} complex [1]. In the present study, we synthesized and characterized nanoparticles (NPs) composed by K-carrageenan (Kcarr) containing a complex of quercetin (a flavonoid with antioxidant activity) and Sr^{2+} (SrQ), as a potential biomaterial for bone regeneration. The NPs were prepared by mixing an aqueous solution of Kcarr with an ethanolic solution of SrQ at 65°C and then cooled to room temperature. The NPs were characterized by size, zeta potential and UV-vis spectroscopy. The DLS analysis showed an average size of 27.6 nm for bare NPs and 407.0 nm for NPs loaded with SrQ, suggesting the incorporation of SrQ into the NPs. Additionally, DLS analysis revealed zeta potential values of -16.4 mV for bare NPs and -28.2 mV for SrQ NPs, indicating that the NPs containing SrQ have greater physicochemical stability in suspension. Moreover, the incubation of the NPs at 37°C for different time intervals resulted in increase of size, related to changes in Kcarr conformation. Additionally, UV-Vis spectra indicated increased concentration of SrQ present in solution after incubation of the NPs at 37°C. These results provide fundamental insights into the properties of NPs containing SrQ, making them potential candidates for bone regeneration approaches.

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Synthesis and characterization of nanocomposites based on mesoporous silica incorporated with cobalt, magnesium and zinc for bioapplications

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Nanomaterials emerge as promising due to their properties for controlled drug release and targeting to specific regions of the body. MCM-41 stands out for the stability of the mesoporous matrix, extensive surface area, well-defined pores and functionalization capacity [1]. The incorporation of metals such as cobalt, magnesium and zinc in mesoporous matrices has the potential for tissue regeneration, anti-cancer properties and influence on diabetes [2]. This study aims to explore the properties of MCM-41 incorporated with metals to develop therapies to cancer, diabetes complications and promote tissue regeneration, contributing to significant advances in medicine and the quality of life of patients [3]. The techniques used to characterize the nanocomposites were infrared spectroscopy (FTIR), thermogravimetric analysis (TGA), X-ray Fluorescence (XRF), X-ray diffraction (XRD), scanning electron microscopy (SEM), small angle scattering (SAXS), nitrogen adsorption, zeta potential and optical emission spectroscopy (ICP-OES) for stability assey. The results revealed that the nanocomposites were successfully synthed and metals were incorporated into the matrix withal the hydrodynamic particle of around 200-300 nm allows it to take advantage of the EPR effect, demonstrating its biomedical potential.

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SYNTHESIS AND THERMOLUMINESCENCE PROPERTIES OF CALCIUM SILICATE PHOSPHOR

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Calcium silicate phosphor (CSO) pure and doped with different impurities have been investigated by several authors due to their interesting thermoluminescence properties and their potential application in radiation dosimetry. Despite these studies, no systematic studies have been performed to identify defect centers involved during TL emission.

In this work, calcium silicate (CSO) phosphor was synthed using the sol-gel technique. The crystal structure analysis was carried out by the X-ray diffraction (XRD) technique at room temperature. The CSO sample presented the pseudo-wollastonite phase of calcium silicate phosphor. The TL glow curves of CSO irradiated with a gamma source show a very intense peak at 190 °C and two peaks of lower intensity at 120 °C and 280 °C. The TL intensity was observed to increase with gamma dose, and its kinetic parameters have been determined by Tm-Tstop and deconvolution methods. Both peaks centered at 190 and 280 °C correspond to deep traps with good thermal stability. Electron paramagnetic resonance (EPR) properties study has been carried out to identify the defective centers responsible for the TL emission. The EPR results show a first center (g values of 2.014, 2.011, and 2.0080) assigned to an O- ion; the second center (g values of 2.015, 2.013, and 2.010) is also attributed to an O^- ion and is associated with the TL peak at 280 °C; and the last center (g value of 2.0011) is due to the F^+ center (singly ionized oxygen vacancy), and this center correlates to the TL peak at 280 °C.

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The effect of adding nanocellulose in the preparation of pectin/zein/HPMC-AS/PEO fibers for controlled release of hydroxychloroquine

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The search for new drug release methods has attracted the attention of several researchers. Electrospinning is one of those techniques that can be used to prepare platforms for drug delivery. This technique consists of applying a potential difference to form nano and microfibers [1]. Biopolymers, such as zein and pectin, have been widely used in the production of electrospun fibers because they are biodegradable, biocompatible, and abundant. [2]. Hydroxychloroquine is a derivative of chloroquine, widely used to treat malaria and autoimmune diseases, such as lupus erythematosus and rheumatoid arthritis. Recent studies point to its role as an adjuvant in the treatment of cancer cells, by inhibiting cellular autophagy [3]. The present work involves obtaining fibers through electrospinning composed of 1% (w/w) pectin, 5% (w/w) zein, 7.5% (w/w) hydroxypropyl methylcellulose acetate succinate (HPMC-AS) and 4% (w/w) poly(ethylene oxide) (PEO), for controlled release of hydroxychloroquine (HCQ) with and without the addition of 1% (w/w) of cellulose nanocrystals (CNC) or cellulose nanofibrils (CNF). Images obtained through SEM showed that the addition of HCQ does not drastically influence the fiber diameter values, the addition of CNC showed a greater formation of clusters indicating low solvent evaporation. The controlled release tests were carried out in phosphate buffer (pH 6.8) and it was observed that the addition of nanocellulose promotes a slower release of HCQ, especially in the CNC system.

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The Effect of Electropolishing on the Surface Roughness of Ti-6Al-4V Surfaces for Implants: an Analysis by Optical Profilometry

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Titanium and its alloys are the most commonly used and suitable materials for biomedical applications, such as implants. The Ti-6Al-4V ELI (Extra Low Interstitials Alloy) alloy is particularly sought after for its excellent mechanical performance and notable biocompatibility. In order to optimize the metal surface to improve osseointegration after implantation, electropolishing was adopted as the baseline treatment capable of controlling the surface roughness to be subsequently modified. The samples were sectioned and subjected to electropolishing at potentials ranging from 13 to 18 V with times of 5, 10, and 15 minutes, using a solution of $HClO_4$, CH_3COOH, and $C_3H_8O_3$. After electropolishing, the samples were characterized by SEM (Scanning Electron Microscopy), which revealed the entire electropolishing process, followed by analysis using optical profilometry, which demonstrated significant differences in roughness profiles depending on the applied potential. Electropolishing contributed to the control of surface roughness of the Ti-6Al-4V ELI alloy, thus favoring enhanced osseointegration in implants.

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The use of co-electrospinning to produce PVA/CMC-PCL/Ibu nanostructured hybrid mats for wound healing

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Electrospinning is an established technique capable of producing nanofibrous mats with high surface area and high porosity, which make them excellent candidates for wound dressing. Co-electrospinning is characterized by spinning two solutions simultaneously, forming hybrid mats with combined properties. Carboxymethyl cellulose (CMC) is a low-cost and effective polymer in wound healing treatment. However, it is a non-spinnable material and thus, should be blended with another hydrophilic polymer, such as polyvinyl alcohol (PVA), to be processed by electrospinning. Ibuprofen (ibu) is an analgesic and anti-inflammatory drug. Polycaprolactone (PCL) is a polyester widely applied to obtain nanofibers, which can be used to encapsulate Ibu. In this work, PVA/CMC - PCL/Ibu hybrid mats were produced aiming to obtain a novel wound dressing, that combines high exudate absorption capacity and drug delivery system. PVA: CMC 4 :1 (m/m) was blended in 3%(m/m) Pluronic aqueous solution. Ibu was solubilized in dimethylformamide (DMF) (10% m/m) and added to a 10%(m/v) PCL solution in a 7:3 solvent system (DCM/DMF). Due to the high hydrophilicity of the PVA/CMC blend, the mats underwent a glutaraldehyde vapor cross-linking process to improve humidity stability. The parameters for co-electrospinning were: 16 kV; 15 cm between the needles and the collector; PCL/Ibu flow rate of 0.6 mL/h; PVA/CMC flow rate of 0.3 mL/h; both on 22G needles. Mats present nanofibers with diameters smaller than 400 nm. PVA/CMC and PCL/Ibu fibers showed distinct morphologies. The encapsulation efficiency (EE%) of ibu was 80%. Further analysis has been conducted to investigate the wound-healing capability of the hybrid mats.

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Titanium-Modified Mesoporous Silica Nanoparticles for Drug Delivery: Synthesis and Characterization

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Mesoporous silica nanoparticles (SiO_2) stand out as a significant innovation within the realms of nanotechnology and pharmaceuticals. Their substantial surface area, tunable pore , and biocompatibility render them an exceptional choice for drug delivery systems. These nanoparticles demonstrate efficient encapsulation of a wide range of therapeutic agents, from small molecules to proteins and nucleic acids, safeguarding them from degradation and enabling controlled release. Nevertheless, the detection of mesoporous silica nanoparticles in biological systems presents challenges, necessitating their combination with easily detectable chemical elements. To address this, SiO_2 nanoparticles have been modified with titanium to ensure or enhance specific functionalities. In this study, titanium-modified silica nanoparticles were synthed using the modified Stober method. Although we used a mixture of silicon and titanium alcoxides at different molar ratio, XRD patterns showed rutile structure despite the fact that EDX microanalysis spectroscopy confirmed the Si/Ti compositions. These combined nanoparticles showed 5 nm of average and enhanced absorption capacity when compared to pure TiO_2 nanoparticles and similar to pure SiO_2 and low citotoxicity, similar to the biocompatible silica nanoparticles commonly used as drug delivery sistems.

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Two-step electrodeposition of calcium phosphate on titanium substrate and its corrosion resistance

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Commercially pure titanium (CP-Ti) is widely utilized as a biomaterial, given its superior anticorrosive properties, attributed to the presence of oxide on the surface (TiO_2) [1]. However, in specific situations where elevated performance is desired, modifications to the surfaces become necessary [2]. This study aimed to investigate the anticorrosive properties of samples with a two-step electrodeposition process, comprising coatings of titanium dioxide with added magnesium and calcium phosphate (CaP). The TiO_2(Mg) electrodeposition process was conducted at a constant current of 1.0 mA/cm^2 for 600 s, while the CaP electrodeposition was performed using pulses of -1.5 V for 30 s and 0 V for 90 s in a cycle of 15 repetitions. The samples underwent characterization using scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDS), X-ray diffraction (XRD), and potentiodynamic polarization. SEM and EDS analyses revealed non-uniform morphologies and the identification of Ca and P. The diffractograms displayed the formation of specific elements in the coated samples. Electrochemical analyses indicated positive protective efficiency in CP-TiO_2(Mg) and negative efficiency in CP-Ti/TiO_2(Mg)/CaP. In conclusion, the addition of magnesium to TiO_2 undoubtedly enhances the anticorrosive capacity of CP-Ti, while the inclusion of CaP in the outermost layer exacerbates the corrosion resistance. Therefore, these findings may be valuable while designing biomaterials.

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Unlocking the antioxidant potential of coffee by-products

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Coffee, the second largest world commodity, generates significant by-products during processing [1]. These by-products have demonstrated diverse biological activities, including antibacterial, antioxidant, and anti-inflammatory properties [2]. The aim of this study was to determine the antioxidant capacity of coffee by-products and their bioactive compounds. Caffeine and chlorogenic acids were identified using HPLC, while antioxidant activity was assessed using DPPH and FRAP assays, along with phenolic compounds, flavonoids, and tannins. Arabica and robusta species exhibited 338.17 and 79.40 µg/ml of caffeine, 14.50 and 192.92 µg/ml of chlorogenic acid, 95.45 ± 0.10% and 89.81 ± 1.41% antioxidant activity via the DPPH method, and 8.93 ± 0.62 and 58.98 ± 2.88 via the FRAP method respectively. Total phenolic content was 19.46 ± 0.82 and 79.53 ± 5.61 mg gallic acid equivalents/g sample, flavonoids were 46.22 ± 13.85 and 46.22 ± 1.92 mg quercetin equivalents/g sample, and tannins were 44.47 ± 0.33 and 133.81 ± 3.56 mg tannic acid equivalents/liter. Robusta exhibited higher concentrations of chlorogenic acid and better results in FRAP, total phenolics, flavonoids, and tannin tests. This suggests that coffee by-products contain bioactive compounds with significant antioxidant activity, potentially suitable for pharmaceutical and cosmetic formulations in the future.

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Use of Agave Americana components for the production of biomembranes for controlled release of active components

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Agave Americana (AA) fibers can be applied in a viable and sustainable industry, as they are 100% biodegradable. Its leaves do not require agrochemicals for production and their processing generates organic waste that can be reused, as they have high mechanical resistance and flavonoid and phenolic substances that can be applied as drugs against various diseases [1]. Most living tissue has a negative charge, but chitosan is positively charged and attracted to tissues, skin, bones and hair. Therefore, the binding capacity of chitosan is an important property for living cells and biomedical applications [2]. This work describes the preparation of chitosan biomembranes containing AA fibers. Firstly, the ethanolic extract of AA was prepared by cutting, drying in an air circulation oven at 60 °C and stirring in 70% ethanol in a 1:10 ratio for 24h. Then, the membranes were prepared with the AA extract in a solution of chitosan in 1% lactic acid, via evaporation of the solvent at 40 °C, for 20 hours. They were characterized regarding their chemical composition, crystallinity, thermal and mechanical properties, morphology, wettability, ability to swell in a PBS solution pH = 6.4. The results were compared with those obtained for the biomembrane without AA and showed that the presence of AA promoted an increase in the hydrophobicity and mechanical resistance of the biomembranes and slightly reduced their water absorption capacity. Chitosan membranes with AA were, therefore, promising for application as dressings in the area of tissue regeneration, which could represent a new stage in the consolidation of natural extracts in medicine.

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Zn-based coordination polymer (Zn-MOF) is successfully synthed to determine dyes from fish samples

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Dyes are widely used in various industrial processes [1]. The disposal of dye waste into effluents results in a series of problems for flora and fauna, as well as human health, due to water body contamination [1]. This study describes the synthesis of a zinc-based metal-organic framework, Zn-MOF, for the removal of methylene blue and alizarin violet N from fish sample using the matrix solid-phase dispersion (MSPD) extraction technique. The material was synthed using the solvothermal method with ethylene glycol as the reaction medium, using 1,4-benzenedicarboxylic acid as the organic ligand and zinc nitrate hexahydrate (Zn(NO3)2.6H2O) as metal source. The prepared material was characterized using SEM, FT-IR, TGA, and BET. As a result, it was observed that material was successful synthed with high thermal stability and high surface area (2726 m^2/g). The dyes extraction process using was optimized using a multifactorial optimization approach, involving central composite design and full factorial design (22), to evaluate the optimal extraction conditions. The factors evaluated were: (i) fish/Zn-MOF mass ratio (1:1-1:10 w/w) and (ii) eluent strength (hexane, acetonitrile, and ethanol). As a result of the optimization, it was observed that the use of (i) 1:10 w/w and (ii) acetonitrile generated better extraction efficiency for methylene blue, while (i) 1:1 w/w and (ii) ethanol generated better extraction efficiency for alizarin violet N. Studies to evaluate (i) adsorption isotherms, (ii) adsorption kinetics, and (iii) adsorption thermodynamics are in progress and will be presented at the event.

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BS04 -2nd. Polysaccharide-based Materials

Advancing cellulose nanofiber production through integrated process engineering and machine learning strategies

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Cellulose nanofibers (CNFs) are produced through a hierarchical breakdown of lignocellulosic fibers, starting from macroscopic fibers and progressing to microfibrils and nano-d cellulose nanofibers. This process involves pretreatment and fibrillation stages, with the resulting properties of CNFs heavily influenced by both the inherent characteristics of the starting material and the specific pretreatment and fibrillation methods employed. Various strategies for pretreatment can be applied at different intensities, directly impacting the subsequent fibrillation stage. Similarly, fibrillation can be carried out using a variety of equipment and intensities, further complicating the production process. The successful industrial deployment of CNF production hinges on the effective linkage of fundamental aspects to process variables and parameters. However, this task is hindered by the lack of appropriate industrial instrumentation capable of real-time monitoring of materials transitioning from the micro to the nano domain. Additionally, most characterization techniques require experienced technicians and are time-consuming, leading to delays between the process and characterization stages.

The present work showcases recent advances focused on the implementation of machine learning, chemometrics, and process modeling for CNF production. These approaches enable the correlation of process parameters and variables with CNF properties, facilitating real-time monitoring and control strategies. Specifically, the study highlights the application of artificial neural networks (ANNs), random forests (RFs), and principal components analysis (PCA) with linear discriminant analysis (LDA) for predicting CNF properties. These techniques offer insights into the complex relationships between process parameters and CNF characteristics, empowering producers to optimize production processes and enhance the quality and consistency of CNF products.

Bio-based composites reinforced by lignocellulosic fibers: Potential of microwaves for the thermoforming

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Composites based on plant reinforcements and thermoplastics are considered alternative materials for several industrial sectors such as automotive, aviation, construction, textiles, etc. These natural reinforcements have several qualities compared to mineral reinforcements: low densitý, low cost and less abrasive. However, the thermo-formabilitý of these materials for thermoforming applications does not seem to be sufficiently elucidated. For this processś heating by infrared radiation, which is the most widely used technique, accounts for up to 50% of energy consumption, representing a significant economic cost. In addition, this infrared heating mode induces undesirable temperature distributions in the materials; what affects the quality of thermoformed products. To make thermoforming efficient in terms of heating time and qualitý the conference focuses, for a judicious choice of the of bio-sourced reinforcements, dielectric microwave heating. To illustrate this, a comparison is made between infrared and microwave heating modes on a family of virgin polypropylene (PP) sheets loaded with wood reinforcements of different s. The results show that the temperature distribution in the composite sheets is almost uniform with microwaves, and that the heating time, in some cases, can exceed that of infrared. This initiative may lead to a new niche in research into high-performance bio-composites for thermoforming, and bioplasturgy in general.

Chitosan Hydrogel with modified nanocellulose for the removal of toxic metal ions

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The presence of metal ions in contaminated water from industrial processes has led to great concern about their effects on human health, due to their toxicity. The search for alternatives is necessary and the adsorption process has the potential to treat ions in trace concentrations and guarantee water safety. Hydrogels, which have an interconnected three-dimensional structure with a high surface area presents potential for use in this area and the use chitosan offers a low-cost, non-toxic and biodegradable alternative, that stand out due to their reactive chemical surface with amines and hydroxyls. Additionally, the incorporation of modified nanocellulose structure have potential to enhance its sorption properties [1]. This study evaluated the production of chitosan hydrogels with the incorporation of cellulose nanostructures without and with modification using succinic anhydride. The nanocellulose was obtained from eucalyptus residue and treated to obtain the cellulose, then grinded and modified. The hydrogels were developed solubilizing chitosan in acetic acid solution and including glutaraldehyde as crosslinking agent. Infrared spectroscopy indicated the presence of new bands directly associated with the symmetrical and asymmetrical stretching of the COO- group, suggesting the success of the chemical modification process of the structure by the insertion of carboxylate groups on the cellulose surface, also impacting the zero-charge potential to a higher value [2]. For the hydrogels it was observed that it presents a natural potential to remove chromium, due to its surface amine groups. However, the pure hydrogels show a limited potential to remove cadmium and nickel. The inclusion of the modified nanocellulose significantly improved cadmium and nickel removal and showed a performance dependent on medium pH [3]. The results indicate the interesting potential of the materials developed in obtaining environmentally friendly alternatives for water decontamination.

Dialdehyde cellulose extracted from banana biomass as a key component in new biosuper absorbents for water stress controle in agriculture

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Superabsorbent polymers (SAPs) based on bio-sourced polymers are currently the subject of great interest as a biodegradable alternative to substitute synthetic , notably those based on petroleum sources such as the acrylics. In this context, we focus on synthetizing new hybrid and fully biosourced bioSAP based on dialdéhyde nanocellulose (DAC) extracted from banana agriculture by products.
For such purpose, chemical modification of bleached pulp extracted from banana biomass via periodate oxidation was performed to produce DAC of controlled properties (oxidation degree and particles), to be used for the preparation of the two families of BioSAP.
In the first family, the DAC was incorporated as a filler in a copolymer of acrylic acid and itaconic acid crosslinked by N, N’-methylenebisacrylamide (MBA) and initiated by potassium persulfate (KPS). BioSAPs from various compositions of DAC and monomers were prepared and analysed.
In the second family a fully biosourced bio-superabsorbent based on carboxymethylated β-chitin and DAC was prepared and studied. The crosslinking of this bioSAP was ensured by mean of the reaction between the amino groups of the developed Cm-chitin and the aldehyde functions of the DAC.
The elaborated hydrogels were studied and characterized using Fourier-transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), thermogravimetric analysis (TGA) and zeta potential. Indeed, the synthed Cm-chitin/DAC bioSAP showed high water absorption capacity, which could be an excellent alternative to synthetic superabsorbents commercially available.

New era of cellulose based films and coatings

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Society requires innovative sustainable solutions to address climate change, biodiversity loss, and chemical pollution. Nature-based technologies empower us, aiding the transition towards a fossil-free future. Cellulose-based solutions offer novel approaches. Our extensive knowledge in material and process development is crucial for utilizing cellulosic materials in high-value applications, such as barrier and 3D packaging, electronic and biomedical devices, optical films, and smart sensors. Future applications extend to membranes for filtration and energy storage. We've developed a unique pilot line to upscale regenerated cellulose films and coatings. Our formulation development and surface treatment options provide a broad spectrum of end-product performance enhancements. We demonstrate applications in dielectric and wearable electronic films, as well as cooling films and coatings for construction and automotive industries. Our packaging solutions, including multi-layer film structures, are designed to be recyclable/compostable, with biodegradability customizable to meet specific application requirements.

Polysaccharide and surfactant: A happy marriage

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The combination of polysaccharides and surfactants in the concentrate regime presents a unique opportunity to adjust their rheological properties and subsequently influence the characteristics of the resulting cryogels. This presentation focuses on exploring aqueous systems employing hydroxypropyl methylcellulose (HPMC), a cellulose ether, in conjunction with surfactants. Specifically, we examined the interaction between HPMC and two sodium negatively charged surfactants: SDS, characterized by a single C12 chain and sulfate head group, and AOT, featuring two C8 chains and a sulfosuccinate head group. SDS micelles bound to HPMC chains, forming structures resembling "bead necklaces," which led to a significant increase in both the storage modulus (G') values of the hydrogels and the compressive modulus (E) values of the corresponding cryogels [1]. Conversely, AOT micelles did not form such bead necklaces with HPMC chains; instead, they are likely embedded between them. The shorter double chains of AOT contribute to the softness and low friction observed in the cryogel cell walls [1,2]. Additionally, systems involving HPMC and CTAB, characterized by a single C16 chain and quaternary ammonium group, exhibit similarities to those containing SDS micelles. However, the rheological behavior of HPMC/CTAB systems across a temperature range of -5°C to +80°C reveals a notable impact on the crystallization of CTAB. The ion-dipole interaction effectively maintains viscosity constant over a wide temperature range, which is particularly advantageous for applications requiring stable viscosity during heating.

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Polysaccharides4life: Challenges, opportunities and future directions

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Polysaccharides are relevant for food, health and materials. They are common denominators for combining chemical engineering, chemistry, material science, bioscience, biotechnology and medicine to create a completely new generation of sustainable products and to enhance human and planet health. However, polysaccharides still face several challenges in sustainable processing, control and design of structure-property relationship and fabrication of functional biomaterials. Their potential to tackle great challenges remain locked and unexploited. In this talk, we will address challenges and opportunities of polysaccharides covering functional therapeutics, functional prevention, personal care and sustainable processes. Functional therapeutics involves the creation of new biomaterials for tissue engineering, implants, targeted drug delivery, diagnostics, purification and crystallization. Functional prevention involves the holistic of product design and formulation without health threatening additives or components for example in food and performance materials used in construction, energy storage and transportation. Personal care focuses on design of sustainable products such as cosmetics, personal hygiene and cleaning products. Sustainable processes involve the development of new processes combining chemical and biochemical processes using green solvents. Future directions and the importance of interdisciplinary and joint venture initiatives between polysaccharide scientists and technologists, policy makers and industry are presented and discussed.

Strategies for the adhesion of circulating tumor cells on 3D sensors coated with polysaccharide

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The performance of thin films deposited on electrochemical biosensors, produced by additive manufacturing, is under study. These sensors aim to detect cancer by capturing circulating tumor cells (CTCs). Surface functionalizations have been performed to improve the selectivity and sensitivity of this detection method. In fact, three-dimensional electrodes, with interconnected pores and smaller diameter, showed greater cell capture capacity compared to non-porous substrates. Pre-treatments carried out by deposition of an intermediate layer of metal nanoparticles and/or exposure to plasma changed the topography, altered the conductivity, providing differentiated tumor cell adhesion. On the organic part of the sensors, there are possible factors that influence the adhesion effect: biofunctional coatings with a increased number of bilayers and the attachment of recombinant proteins for the insertion of specific terminals in the films is underway to improve the specificity of biosensors, using biorecognition strategies.

3D printing chitin-based bilayer membranes for biomedical applications

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Direct ink writing (DIW) 3D printing was employed to produce bilayer membranes aimed at developing biomaterials potentially useful to be applied as: 1) wound dressing and 2) active drug delivery system for periodontal tissue regeneration. Beta-chitin (BCt) was subjected to acidolysis with concentrated HCl, and the resulting whiskers were characterized and then used for the preparation of both kind of biomaterials. Chitosan (CS) was synthed by employing a multistep ultrasound-assisted deacetylation process on beta-chitin, and subsequently subjected to a reaction with glycidyltrimethylammonium chloride, resulting in the production of cationized chitosan (CtCS), which was utilized for the development of a wound dressing. In this case, the ink was prepared by dissolving CtCS (2,9% w/v) in the beta-chitin whiskers aqueous suspension (10 mg/g), followed by the addition of genipin (0,5 mg/mL) to promote the crosslinking reaction. The ink used to the 3D printing of the other biomaterial was prepared by combining lipid nanoparticle-loaded grape seed extract and simvastastin, as well as beta-chitin whiskers, to result in a bilayer membrane that possesses antimicrobial properties and multi-scale porosity for periodontal tissue regeneration. Regardless of their compositions, both inks exhibited pseudoplasticity, thixotropy, and solid-like behavior under low oscillatory strain and liquid-like behavior under high oscillatory strain, which are considered ideal characteristics for DIW 3D printing. The 3D printing parameters were defined, in both cases, so that the membrane inner layer was porous and the outer layer was dense. Results show that the biomaterials produced in this study have a high potential to be applied as wound dressing and for periodontal tissue regeneration, both of which exhibited antimicrobial activity while the latter provided a sustained release of simvastastin and grape seed extract over 24 days. CNPq 311464/2022-0; FAPESP 2017/20973-4, 2018/22214-6, 2019/227

Beta-chitin nanocrystals as promising materials for dye removal from wastewater

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Wastewater treatment is a key subject related to some of the Sustainable Development Goals. Chitin nanofibers and nanocrystals have been studied for these applications, since they can interact with compounds such as metal ions and dyes, due to the presence of amino and N-acetyl groups in their structures [1]. In this work, beta-chitin flakes were submitted to acidic hydrolysis to produce chitin nanofibers (ChN) and then applied to remove Methylene Blue (MB) and Methyl Orange (MO) from aqueous solutions [2]. The acidolysis of beta-chitin was carried out with 3M HCl or 3M H_2SO_4 under reflux for 3h, and the resulting nanofibers were named as WHCl, WH_2SO_4 respectively. The stable nanofiber suspensions were diluted to 2,0mg/g and added to MO and MB solutions (with initial concentrations of 25mg/L and 50 mg/L). Adsorption assays were carried out at 25ºC, pH≈7. Kinetic assays were conducted from 5min to 120min, whereas samples at equilibrium (120min) were used for the thermodynamic assays. Due to the positive surface charge of ChN (ζ=+20mV), the interaction with MB was poor, and all ChN samples showed a MB removal efficiency (R%) lower than 1,0mg/g. On the other hand, WHCl showed R%≈70mg/g of MO in both concentrations (25 and 50mg/L). Kinetic assays indicated that the adsorption of MO follows a pseudo-second order model for both dye concentrations, leading to a removal capacity (qe) of 8,2 and 17,4 mg/g, respectively. According to the thermodynamic assays, the Langmuir model describes the adsorption mechanism. The maximum adsorption capacity (qm) of MO was calculated for WHCl (65,75 mg/g) and WH_2SO_4 (61,84 mg/g). These values are considerably higher than those found in the literature for adsorbents based on beta-chitin, indicating that these ChN are suitable for dye adsorption.

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Biopolymer functionalization for catalytic neutralization of agrochemicals

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Tackling agrochemicals´ toxicity is of increasing interest due to many threatening stockpiles and abusive use, especially for the class of toxic organophosphates. Particularly, their neutralization is important to guarantee their safe handling and elimination. and monitoring methods. Target functionalization of nucleophilic groups on biopolymeric templates allows the development of efficient and sustainable catalysts for organophosphates degradation. Our approach aims to green up the process through the rational mono- and bi-functionalization with imidazoles, hydroxamates and/or amidoximates in biocompatible and renewable supports: (i) gum arabic and Brazilian gum trees (commercial, tannin industry byproduct, cashew tree, Amazonic buxixão tree), (ii) cellulosic-materials (carboxymethylcellulose and nanocellulose-derivatives) and (iii) cellulosic-waste (rice and shrimp husk). The use of nucleophiles anchored in templates improve neutralization by catalysis and promote selective and recycle paths for detoxification. Furthermore, samples were obtained in different forms, such as solid, colloidal and gel, which showed high rate enhancements. Bifunctionalized catalysts also reveals some insights about neighboring group effects. We also developed neutralizing gels for intoxication prevention. In addition, some functionalized polymers showed scavenging effects (removes the toxic organophosphates) and artificial enzymatic activity (cleaves plasmid DNA). Overall, chemical security and safety can be successfully accomplished for highly toxic compounds relying on strategically designed sustainable catalysts based on biopolymers. These are optimized from playing with different polymeric supports, catalytic groups, synergy of the support, mechanism and processability (gel, colloidal, solid).

Cassava starch films containing quercetin: Analyzing the incorporation method and the physicochemical properties

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Traditional methods of drug intake usually release a high concentration of drug in a short period of time, as they cannot be released directly into the place of interest and must be administered in predetermined doses. Alternatively, there are controlled-release systems, which the drug can be released at the site of interest, thus increasing the effectiveness in treatment [1]. Starch- based films, which is a natural polymer found in abundance in sources like cassava and is recognized for being non-toxic, can be used as controlled release systems. Among the bioactive compounds with biological properties, quercetin can be highlighted, a well-known antioxidant molecule [2]. Therefore, the aim of this work was to produce a starch film incorporated with quercetin and evaluate its physicochemical properties. Quercetin was first subjected to a precipitation process with starch by the addition of acetone. The precipitate was then incorporated into the starch films, and characterized regarding their physicochemical properties.

The incorporation of quercetin on the starch film using the precipitation process showed significant advantages over other methods tested, and permitted the incorporation of high quercetin concentration (0.82 mg/cm 2 of film). The results demonstrate that the incorporation of quercetin by the precipitation method enhances the mechanical properties (Young modulus 82.54 MPa) and swelling (127.3%) of the film, while not negatively impacting the thermal stability and solubility, showing that the incorporation of quercetin brings physicochemical benefits to the starch film. The increase in mechanical properties, coupled with the well documented antioxidant properties of quercetin indicates that the incorporation of quercetin in starch films is of great biotechnological importance.

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Colorimetric sensor strips based on microfibrillated cellulose for digital and naked eye detection of total iron in water

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Microfibrillated cellulose (MFC), a sustainable material derived from biomass, stands out as an environmentally friendly alternative for developing chemical sensors substrates. Its advantageous features include low cost, abundant availability, facile degradability, renewability, and ability to form membranes of varied porosity [1,2]. In this study, we propose a simple and low-cost strategy for developing cellulose-based strips for the colorimetric detection of total iron in water. The strips were prepared by functionalizing MFC casting membranes with 1-(2-Thiazolylazo)-2-naphthol (TAN) and characterized by FTIR, SEM, and XPS. The sensing ability of the MFC@TAN strips for Fe(II) was evaluated under distinct reaction times (5 and 30 min) using digital image colorimetry. Under optimal conditions, the developed sensor afforded linear ranges of 0.1–1.5 ppm (R^2 = 0.996) and 0.1–3.0 ppm (R^2 = 0.998) and limits of detection of 0.05 and 0.14 ppm using the blue (5 min) and red (30 min) channels, respectively. Additionally, the sensor enabled detection of Fe(II) in tap water in the concentration range of 0.08 - 0.70 ppm, showing no significant difference (p = 0.05) against the standard method. When compared to commercial papers, the MFC@TAN strips showed enhanced sensing performance due to their porous and interpenetrating structure, which benefited the TAN immobilization and reaction with Fe(II) ions. Our sensor strips offer a compelling combination of simplicity in manufacturing and cost-effectiveness, underscoring their potential for routine water analysis.

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Combining and concentrating nanocelluloses for cryogels with remarkable strength and wet resilience

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The demand for environment-friendly products and processes according to the principles of green chemistry has highlighted the use of renewable feedstock instead of petroleum derivatives. In this context, cellulose cryogels are promising green materials that exhibit low density, high porosity, and renewability. However, the applications of these materials are limited by their lower mechanical and water resistance compared to petrochemical-based lightweight materials. In this work, charged cellulose nanofibrils (CNFs) were produced by oxidation with sodium hypochlorite mediated by the radical TEMPO and cationization with glycidyltrimethylammonium chloride (GTMAC), obtaining anionic CNFs (aCNF) and cationic CNFs (cCNF), respectively. To prepare the cryogels, aCNF and cCNF were produced at three different s and combined in various weight ratios, forming electrostatic complexes. The complex phase was concentrated by centrifugation and freeze-dried to generate lightweight materials. Porous and open cellular structures were assembled in all compositions tested (porosity >90 %), as revealed by scanning electron microscopy. Compressive testing showed that the mechanical properties of CNF cryogels were influenced by the charge ratio and the of CNFs. Moreover, the most resistant cryogels (1.7 MPa) were obtained by combining equal amounts of oppositely charged CNFs with an intermediate disintegration. The strength at this condition was achieved as CNF electrostatic complexes assembled in thick cells, as observed by synchrotron X-ray tomography. In addition to mechanical strength, electrostatic complexation provided remarkable structural stability in water for the CNF cryogels, without compromising their biodegradability. This route by electrostatic complexation is a versatile strategy to combine and concentrate nanocelluloses to tailor biodegradable lightweight materials with high strength and wet stability.

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Composite fertilizers produced from the alum sludge: combining a waste with a biodegradable material for agricultural application

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Composites produced from biodegradable matrices have been highlighted as a sustainable strategy to increase the fertilization efficiency and reducing nutrient losses. Thermoplastic starch (TPS) is a common polysaccharide biopolymer widely used to develop this type of material due to its low cost and high biodegradability. Combining TPS with fertilizer formulation promotes nutrient release through the degradation and dissolution of the fertilizer. Moreover, it increases the matrix's flexibility, allowing it to be molded into various shapes, which facilitates the production of granules. Water treatment plants (WTP) produce tons of alum sludge (AS) during the water treatment process. The chemical composition of this waste makes it a promising raw material for the development of zeolite materials. In this work, we developed a composite fertilizer using TPS, urea (as a plasticizer and also as N source) and zeolite synthed from AS using alkaline medium and autoclave treatment. Alum sludge from Hortolândia – SP WTP was used as Si and Al source. Sodium silicate was added to improve cristalization process. The obtained zeolite material, sodalite (SOD-Na), underwent a cation exchange procedure to become SOD-K. This process enriches it with K^+ ions, contributing to the nutritional value of the material. SOD-K was then used to prepare composites with the final composition of 70% solids (50g SOD-K, 40g TPS and 12g urea) and 30% desionized water. After mixing to obtain a homogeneous material, the formulation was processed in a silicone mold, dried at room temperature, and then characterized using various techniques. The fertilizer composite was evaluated for its potential to achieve controlled-release of K^+ ions and to control nitrogen losses related to ammonia volatilization. Additionally, it was assessed for its potential to control plant pathogens through the addition of microorganisms.

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Contribution to the protection of forest heritage: towards a preventive tool for phytosanitary microwave treatment of industrial wooden packaging

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The trafficking and transportation of products, using wooden packaging (pallets), across the world is one of the causes that have facilitated the migration of pathogens and insects between countries. These biological invasions have led to the destruction of plant species, causing major economic and ecological losses in many parts of the world. To this end, in 2003, the World Trade Organization, through the expert groups of the International Plant Protection Convention, established the Standards for Phytosanitary Measures (ISPM 15), which require wooden pallets to be heat-treated or fumigated with methyl bromide. In 2013, microwave treatment was approved. In 2016, Brazil decided to strictly apply International Standard for Phytosanitary Measures No. 15 (ISPM 15) relating to the regulation of wood-based packaging materials. Therefore, any goods entering Brazilian soil must be accompanied by a declaration.

Given the diversity of commercial wood-based products, how can we be sure that pathogens and insects will be destroyed by microwaves when applying ISPM 15? This is a very complex problem, and the optimum time for microwave treatment depends on several factors: wood type and its thermophysical and dielectric properties (non-linear, anisotropic); the initial state of the wood packaging (frozen or not); the packaging design; the characteristics of the microwave oven, and so on. The aim of this conference is to develop a preventive tool to determine the optimum time for microwave phytosanitary treatment of wood packaging. By way of application, three Canadian wood species will be studied.

Controlled release of curcumin encapsulated in κ-carrageenan beads loaded within sponge matrix

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This study introduces an innovative investigation aimed at developing and characterizing a sponge containing κ-carrageenan (κ-CRG) beads loaded with curcumin. The κ-CRG was evaluated for viscosity, Gel Permeation Chromatography (GPC), and Fourier Transform Infrared (FTIR) characteristics [1]. Beads were prepared using three different concentrations of κ-CRG and examined using an inverted phase-contrast microscope, Scanning Electron Microscopy (SEM), FTIR, swelling degree assessment, mass uniformity analysis, encapsulation efficiency measurement, and drug release evaluation [2]. Beads formulated with the κ-CRG concentration that produced the most favorable outcomes were integrated into a sponge and subjected to the same tests. The beads exhibited spherical morphology, around 146% swelling degree, high mass uniformity, and encapsulation efficiency of 90.9±2.5%, 92.4±2.3%, and 92.9±2.2% for 2.5%, 3.0%, and 3.5% κ-CRG, respectively, with a drug release exceeding 70%. The sponge also demonstrated satisfactory drug release at 67.9±0.6%. These findings highlight the potential of both the beads and the sponge in facilitating the controlled release of curcumin, indicating their suitability for pharmaceutical applications across various fields.

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Developing bagasse-based composites bonded with natural rubber latex/lignin adhesive

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The urgent need for sustainable and environmentally friendly materials in various industries, including construction and manufacturing, has led to the exploration of renewable resources for the development of new composite materials [1]. In response to this demand, we have developed bagasse-based composites utilizing natural rubber latex /lignin adhesive as the formaldehyde-free binding agent [2], focusing on sustainability and cost-effectiveness. Our study aimed to optimize the composite formulation by adjusting the proportions of bagasse fibers, an agricultural byproduct, with latex/lignin adhesive. We assessed their compatibility with coating applications, considering factors such as adherence, protective properties, thermal and gas barrier performance, hydrophobicity, biocompatibility, and decorative aspects. The findings reveal that the refined composite formulations boosted superior mechanical strengths, enhanced resistance to water, and remarkable thermal stability, rendering them suitable for coating applications. The fabrication of such sustainable composites not only repurposes agricultural byproducts but also introduces a more eco-conscious option to the coatings market. This innovation may decrease the dependency on petrochemical-derived materials, fostering a more sustainable approach within the construction industry. Acknowledgements:

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Edible biopolymeric films for fine cheese coating: a sustainable approach using chitosan, guar gum and quercetin

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Cheese is a widely appreciated dairy food. Some types of cheese, such as Tomme, Gouda and Edam, are known for their coated exterior. Coating is used for protection against contaminants, moisture regulation, flavor development and visual appeal. Coating compositions include wax, paraffin and polyvinyl acetate (PVA) resin. In this study, films based on chitosan (CS), guar gum (GG) and different amounts of quercetin (Q) [1] were produced and characterized aiming application as cheese coating as an alternative to PVA. Solutions of 1% CS and 1% GG were crosslinked with 5% to 20% quercetin (percentages related to the polymer mass), and films were obtained by casting at 40ºC. The viscosity of the mixtures increased with quercetin amount, varying from 3370 - 54540 cPs, while commercial PVA is 8240 cPs. Films with 0% and 5% quercetin were water soluble. Increasing quercetin from 10 to 20% decreased water swelling from 1717% to 387%, and changed mass loss from 23% to 28%. PVA swelling and mass loss were 3.5% and 14.5%, respectively. Swollen films were softer than PVA, a desired characteristic for an edible coating. Thickness decreased from 104 to 73 µm, with increasing quercetin amounts. Cheese moisture regulation was associated with films water vapor transmission rate (WVTR), measured in a cheese ripening chamber. The WVTR values varied between 100 and 139 g/day·m2, while PVA displayed 107 g/day·m2. Samples of Tomme cheese (1x2cm2) were coated, resulting in good adhesiveness, especially for the 15% and 20% quercetin formulations. In summary, films crosslinked with 15 and 20 % quercetin are promising to produce edible cheese coatings with properties similar to PVA. Further studies on cheese ripening will be performed.

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Enhancing Sustainable Packaging: Nanocellulose-Based Multilayer Films treated with Cold Plasma

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Nanocellulose-based films offer promising properties for sustainable packaging. In this work, a multilayer matrix was produced consisting of nanocellulose, followed by tannin and nano-chitosan/CNC layers. To improve adhesion between layers, a surface treatment was conducted using dielectric barrier discharge (cold plasma), with nitrogen as carrier gas. The resulting multilayer system were evaluated in terms of barrier properties (liquid water, water vapor, and oxygen permeability), and their efficacy in preserving strawberries exposed to the environment. The findings revealed enhanced hydrophilicity of the nanocellulose matrix after plasma treatment, transitioning to hydrophobicity with the addition of tannin and nano-chitosan/CNC layers. The analysis demonstrated a significant decrease in water vapor permeability with the addition of the last layer, attributed to the specific properties of each added layer acting as additional barriers. Plasma treatment induced surface roughness, reducing water vapor permeability. Thickness, weight, and density measurements indicated increased thickness and weight with additional layers, resulting in lower densities. The multilayer system, especially with plasma treatment, exhibited significantly lower oxygen permeability, attributed to a possible polymer chain crosslinking and surface roughness induced by plasma treatment. The multilayer system, particularly with plasma treatment, demonstrated superior efficacy in preserving strawberry quality, highlighting its potential for sustainable packaging of perishable food items. This research underscores the importance of developing innovative packaging materials to prolong food shelf life, contributing to sustainable practices in the packaging industry.

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High-bulk papermaking fibres designed by green surface modification

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High bulk is an appealing feature for paper products that allows the design of lightweight materials for applications in packaging, tissue, and filters. However, chemical and mechanical refining often involves a trade-off between bulk and tensile index, where prioritizing one property can compromise the other.[1,2] To prepare high-bulk fibres, in this work, we explored the application of hydroxypropyl methylcellulose (HPMC), a bio-based and low-surface tension polymer, to mechanical pulps. Two application methods were investigated: (I) pre-treatment by adding HPMC to the pulp dispersion and (II) post-treatment by spraying HPMC solution onto handsheet. Both methods efficiently improved tensile index and bulk simultaneously, representing an exceptional performance. The increased bulk can be attributed to the attenuation of capillary forces during drying, with HPMC acting as a surface de-bonder. At the same time, the enhancement in the tensile index was promoted by reinforcement in fibre-fibre bonding by physical cross-links (i.e. mechanical interlocking). X-ray tomography showed that HPMC promoted open fibres and symmetric structures, indicating that the surface modification improved the cell wall strength. These findings point to the use of HPMC as a green approach to valorizing paper products, offering an alternative to oxidizing agents and overcoming the typical deal between tensile index and bulk in pulp refining.

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Hydrogel beads formed from the sisal lignocellulosic fibers' deconstruction: applications in the purification of water polluted with heavy metals

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Hydrogels made from sisal biomass, which consists of cellulose, hemicelluloses, and lignin, were produced, and assessed for their ability to sorb toxic metals. The process of creating hydrogel beads from sisal fibers involved the following steps: (i) fibers deconstruction using bis(ethylenediamine)copper(II) hydroxide solution (CUEN, 1M); (ii) dropping the resulting gel in calcium chloride solution at 80ºC ($CaCl_2$-80) and 120ºC ($CaCl_2$-120); (iii) crosslinking with citric acid (CA) at 80ºC ($CaCl_2$-CA-80) and 120ºC ($CaCl_2$-CA-120). The beads were characterized by sorption capacity, scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FTIR), and compressive properties. The beads' sorption capacity (q/mmol/g), total and for each metal, was obtained by putting them in contact with simulated wastewater containing several toxic metals for 24 h under agitation and analyzed via ion chromatography. The FTIR spectra of $CaCl_2$-CA-80 and $CaCl_2$-CA-120 indicated the esterification of the hydroxyl groups (band at 1724 cm^{-1}). CA crosslinked beads presented smoother surfaces than their counterparts, $CaCl_2$ crosslinked ones. The crosslinking process with CA was expected to increase Young’s modulus of the spheres. However, the reaction at 80°C barely affected the beads’ modulus, while the one at 120°C resulted in beads with a lower modulus than those not crosslinked. These findings suggest that CA caused partial hydrolysis of the bead components. On the contrary, CA crosslinking positively impacted the sorption capacity of Cu(II) and Cr(VI), while the sorption of Ni(II), Zn(II), Mn(II) and Cd(II) was not significantly affected. This is ongoing research, and the initial outcomes indicated a potential application of hydrogels derived from the sisal´s fibers deconstruction for removing heavy metals from wastewater.

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Influence of the degree of deacetylation of chitosan on the surface properties of layer-by-layer films

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Here, we assessed the influence of the chitosan degree of deacetylation (DD) on the surface properties of alginate(ALG)/chitosan(CHI) films developed via the Layer-by-layer (LbL) technique. The CHI solutions were prepared under different DD conditions (40, 75 and 95%). LbL films were produced by alternating immersions of glass substrates in ALG and CHI solutions at pH 3.0 for 15 min each, followed by three rinsing steps with ultrapure water (2 min, 1 min, and 1 min, respectively) between each polyelectrolyte immersion. The ALG/CHI films were characterized by Water Contact Angle and Atomic Force Microscopy (AFM) to evaluate the effect of the chitosan DD on the hydrophilicity and roughness of the coatings, respectively. Water contact angle and AFM results indicated that the increase of the chitosan degree of deacetylation led to less hydrophilic and rougher ALG/CHI films. The wettability properties of the films are a direct consequence of the presence of functional groups in the CHI chain since CHI samples tend to be more hydrophobic with a lower amount of amino groups in their structures [1]. Since the film assembly occurs in the isolated islets growth regime, a higher DD condition requires a smaller amount of CHI for charge compensation, which hampers the assembly of a large number of isolated islets, increasing film roughness as reported in the literature [2]. In summary, we suggest DD as a key factor in controlling the properties of chitosan-based materials for a wide range of biotechnological applications.

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Modulating charge density and size of cationic cellulose nanofibrils to increase flocculation performance

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The search for environmentally friendly routes for wastewater treatment is crucial to address the increase in freshwater contamination. Flocculation is one of the most used processes in wastewater treatment since it is cheap and highly efficient.[1] Although the coagulation/flocculation process is well established, using inorganic salts and synthetic polymers raises environmental concerns. In this context, cellulose-based compounds emerge as a sustainable alternative, offering renewability, biodegradability, and significant capacity for chemical modification.

Herein, we evaluated the efficacy of employing cationic (positively charged) cellulose fibers with different charge densities and s as a flocculant for purifying water contaminated with model kaolin particles (negatively charged). Flocculation efficiency was evaluated by visual inspection and transmittance measurements in UV-visible spectroscopy at 750 nm.

The results demonstrated that all cationic celluloses interact with the negative surface of the kaolin. However, the colloidal stability and phase separation of the systems proved to be dependent on the and charge density of the fibers: smaller and highly charged fibers have greater efficiency in floc formation. The high flocculation capacity (%T > 80%) was attained with only 2 mg L-1 of the cellulose possessing the highest charge density and smallest.

These findings demonstrated the potential of tailoring fiber properties to develop flocculants that facilitate direct flocculation with high efficiency, enhancing the environmental friendliness of effluent treatment processes.

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Plasma at atmospheric pressure in the production of starch nanoparticles in water

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Plasma at atmospheric pressure in the production of starch nanoparticles in water

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This study proposes a production route for nanoparticles from larger granules in a top-down approach. This study is motivated by the need to understand how oxygen plasma, produced at atmospheric pressure by a plasma pen, interacts with starch granules immersed in water and leads to their degradation and, therefore, production of nanoparticles in an extremely fine distribution. 5 mg of starch was added to 100 ml of ultra-pure water and exposed to oxygen plasma for 5, 10, 15, and 20 minutes. The liquid temperature, as well as its pH, were monitored. After plasma treatment, the liquid was let to decant. The water was analyzed via DLS, AFM, SEM, and UV-Vis after filtration through a 220 nm filter. The presence of nanoscale particles was observed. The starch granules were dried in a kiln and stored for subsequent analysis by SEM and AFM, and degradation of the protective hydrophobic layer of the granules was observed. With these results, it is possible to infer the model of plasma action on starch and how nanoparticles are formed.

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Preparation and characterization of edible nanocomposite films based on a matrix of carrageenan and thermoplastic starch blends, reinforced with cellulose nanofibers.

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Edible films are of great interest for replacing synthetic packaging [1], however, using natural polymers for this purpose, the properties of these films need to be improved due to the poor properties of the natural polymers. The way to improve the properties of it is by working with blends and composites [2]. In this work, edible composite films made from carrageenan and arrowroot starch, reinforced with cellulose nanofibers (CNF), were developed. In addition to the CNF that were used to improve the mechanical properties of the film, additives were also added such as glycerol that acted as a plasticizer for the starch, aloe and vera gel to generate antibacterial properties, sesame oil as an antioxidant, myristic acid as a surfactant and compatibilizer, and hibiscus flower extract as a pH indicator. A central composite design was employed to study the compositions of the carrageenan/starch blends and CNF content. The films were prepared via casting. The composite films were evaluated by SEM, UV-Vis, moisture absorption, water contact angle, water vapor permeability, TGA and tensile testing. The films had reasonable transparency in the visible region and low transmission in the UV region, making them interesting for applications in packaging with barrier properties to UV radiation. From the SEM microphotographs, it was shown that the films were very homogeneous with good CNF dispersions. Higher starch and CNF contents lead to films with greater thermal stability. Films with lower carrageenan content, regardless of CNF content, showed lower water vapor permeability and moisture absorption. The films with the best mechanical properties were those with the highest CNF content.

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Preparation of Erlotinib amorphous particles of pullulan-based matrix via dialysis nanoprecipitation

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Erlotinib (ERL) is a chemotherapeutic agent that belongs to tyrosine kinase inhibitor (TKI) compound class, mainly applied to pancreatic and non small cell lung cancer treatment (NSCLC) [1]. However, this drug has a low solubility under neutral pH, which can result in a poor gastrointestinal absorption. Different formulation types have been applied to improve the drug's physical properties and, consequently, its biosorption, such as, the development of amorphous nanoparticles, which improve drug solubility by modifying their crystalline form. Therefore, amorphous ERL nanoparticles were prepared based on previously synthed [2] cationic amphiphilic pullulan copolymer, using nanoprecipitation via dialysis method. To do so, pullulan copolymer and ERL were dissolved in dimethyl sulfoxide (DMSO) at a specific concentration and polymer:drug proportion. The mixture was dialysed against water solutions with acidic and neutral pHs for 48h. After precipitation, the particles were analyzed in terms of particle and polydispersity. The solution was freeze dryied, and the encapsulated amount of ERL was determined by UV/Vis photometry. The change in ERL crystallinity was evaluated using a X-ray diffractometer (XRD) and the morphology was evaluated using Atomic Force Microscope (AFM) technique. The results demonstrated that lower pH values with higher polymer concentrations represented a better ERL encapsulation, around 45% w/w with an inhibitited the recrystallization of ERL, resulting in an amorphous form of the drug. Therefore, ERL nanoencapsulation in the PULL matrix demonstrated a potential system to improve ERL solubility and biodisponibility.

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Production and characterization of potential 3D printed bone scaffold based on modified potato and hydroxyapatite

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Bone scaffolds can provide a model for reconstructing defects, promoting cell fixation, proliferation, and generation of extracellular matrix. It can be produced by 3D printing, which allows personalization of the material and processability involving a wide range of composition possibilities. In this sense, modified starches have shown one interesting potential for this application, mainly considering its rheological properties. Among the various modification methods, dry heating treatment (DHT) is a simple, safe, and environmentally friendly method to improve starch properties [1]. Within this context, this work produced bone scaffolds based on modified potato starch by DHT added with hydroxyapatite (HA), one active compound present in the bones. HA were synthed following an adapted methodology from Nassif et al. (2019) [2]. The potato starch was modified by DHT for 1 h at 130 oC [1]. The formulations (inks) were based on hydrogels based on native (N) and modified (M) potato starch by DHT (10% w/w, d.b.) added of HA (5% w/w starch, d.b.). The scaffolds (N, M, N_HA, and M_HA) were printed using a 3D printing extrusion (BioedPrinterV4, BioEdTech - Brazil). The inks were characterized concerning rheology and printability. The printed scaffolds were characterized in relation to biodegradability (7 and 14 days), mechanical properties, and morphology (Micro-CT and SEM). The M_HA inks showed more adequate rheological properties which can be confirmed by its superior printability. The scaffolds M_HA presented higher rigidity and lower biodegradability, and the HA was well dispersed in both matrix (N or M), and it was visible that the scaffolds M and M_HA showed higher porosity than the N and N_HA. Finally, these materials showed great potential as bone scaffolds.

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Starch-based biomaterial cross-linked with citric acid for enhanced properties

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Starch-based hydrogel is unsuitable for tissue engineering due to its fast degradation [1], making its application challenging. To overcome this, citric acid (CA) cross-linker is an interesting option. Therefore, this study proposes improving starch-based hydrogel stability using citric acid (CA) cross-linker. Wheat starch (10%, control) was mixed with CA (5%), gelatinizated at 85°C/20 min followed by gelification at 5°C/24h and water removal by freeze-drying. Dried samples were then heated at 180°C for 10, 20, and 30 min and washed with phosphate buffer for 24h to release the unreacted CA. Compared to the control, the CA-starch hydrogels were more stable in the cell culture medium ($> 80\%$, $p<0.05$) and in the presence of amyloglucosidase ($>45\%$, $p<0.05$), suggesting the presence of covalent bonds between CA and hydroxyl groups of starch [2]. Surprisingly, the CA-starch hydrogels had a greater swelling capacity ($>40\%$, $p<0.05$) and a greater blood coagulation index than starch hydrogel. These results suggest the potential application of CA-starch hydrogel as a hemostatic material since its behavior is better than the gelatispon®. In addition to the hemocompatibility (absence of hemolysis), the CA-starch hydrogels did not show a cytotoxic effect on dermal fibroblasts. Finally, when cultured in the presence of macrophages, in contrast to the starch hydrogels, the CA-starch hydrogels did not induce an overproduction of proinflammatory TNF-α and IL-1β. To sum up, CA-starch hydrogel showed good features for tissue healing and subsequently will be evaluated for its osteo-biocompatibility and potential application in bone tissue engineering.

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Thermal treatment of metal ion adsorbed functionalized nanocellulose fibers in order to synthesize hybrid inorganic-carbon material for generation of asymmetric supercapacitor

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Ever-increasing demand for environment-friendly, high-performance and renewable energy storage devices gave rise to supercapacitors. Asymmetric or hybrid supercapacitor can be prepared by combining carbon material with metal oxide nanostructures, where the charge can be stored both by Faradaic (redox reactions) and non-Faradaic processes (electrochemical double layer formation). One of the many advantages of carbon-based supercapacitor is it can be derived from renewable bio-sources, such as cellulose. Nanocellulose fibers can be obtained from cellulose and after adequate surface functionalization it can adsorb a huge quantity of metal ions from their aqueous solutions. After the completion of such an adsorption process, the precipitate (metal ion adsorbed onto functionalized nanocellulose fibers) can be filtered and it can be submitted to heat treatment in a tubular furnace under inert atmosphere varying temperature and time of the thermal treatments. The resultant hybrid material (metal/metal oxide nanoparticle embedded in a carbonaceous matrix) can be characterized thoroughly. The atmosphere of the calcination environment as well as the initial metal ion to nanocellulose ratio can be changed in order to vary this hybrid nanostructure. These materials can be a good candidate for supercapacitor application as it contains nanoparticles of metal/metal oxides of varying composition and stoichiometry, in a porous carbon matrix, thereby allowing both Faradaic and non-Faradaic processes in the electrochemical evaluation. Interestingly, in this scheme, more than one application related to the environment and energy can be chained with one another as the starting material of the second process (carbon-metal oxide hybrid material generation for supercapacitor application) is actually the waste generated in the first process (metal ion adsorption on nanocellulose fiber).

The Role of Cellulose and Other Components from Biomasses in Sustainable Materials Formation

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Sustainable materials require raw materials that, in addition to being renewable, have the potential for long-term availability while maintaining their properties. Creating materials from biosources should be environmentally sound and, ideally, scalable. Brazil has been a major producer of raw materials from biological sources, such as fruit, lignocellulosic, and oilseed biomass, which can be used alone or combined to create materials. Polysaccharides are essential in this context as their long chains provide structural support during the material formation process, and their functional groups can be modified to achieve specific goals. Different sustainable materials can be produced from lignocellulosic biomass and other renewable raw materials, such as those from oleaginous biomass and citrus fruits, through synthesis or blends. Cellulose, hemicelluloses, and lignin have a chemical structure rich in hydroxyl groups, making them useful for various syntheses. The "Macromolecular Materials and Lignocellulosic Fibers Group" strives to employ non-complex and clean methodologies on a laboratory scale that can eventually be scaled up. In this scenario, synthetic procedures free of solvent have been used, resulting in the simultaneous formation of film-forming or thick and robust materials, composites reinforced by plant fibers, such as sisal or coconut. Cellulose plays an essential role in these syntheses. It is complemented by other reagents from biomass, such as ricinoleic acid triglyceride (the main component of castor oil), epoxidized soybean oil, or citric acid. Films have been formed from aqueous solutions of cellulose derivatives with quaternary ammonium groups, mixed or not with lignosulfonate and zinc oxide nanoparticles, aiming for antibacterial properties. All materials have been thoroughly investigated, and the results suggest they hold promise for various applications.

Triblock copolymers in hydrogel particles of anionic oxidized cellulose nanofibers and cationic polymers for encapsulation

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Hydrogel microspheres with a core-shell configuration were obtained via charge-induced interfacial complexation, providing enduring stability within water-based environments [1]. The preparation method consisted of drip-dispensing a dispersion of anionic cellulose nanofibril (OCNF) into a solution of positively charged cationic polymer, poly(diallyldimethylammonium chloride) (PDADMAC) and a triblock copolymer (poloxamer). The resulting hydrogel microspheres possess a solid OCNF-PDADMAC outer shell, serving as a selectively permeable barrier. The core is comprised of a liquid mixture of OCNF and poloxamer in water. Visual observation revealed a shrinking/swelling behavior of the microspheres in different mediums, showing less shrinkage in the presence of NaCl due to osmotic pressure. The presence of triblock copolymers in the core enhanced the encapsulation of hydrophobic actives with no alteration on the structure of the microspheres. These results demonstrate the potential use of these microspheres for a controlled delivery of actives.

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use of plant biomass to design lightweight materials

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This work seeks to redirect the biomasses sugarcane bagasse and eucalyptus bark, currently obtained as agro-industrial waste, to the production of lightweight, biodegradable and renewable foams to replace plastic foams. These materials have expanded three-dimensional structures, with high porosity and low density (0.10 to 0.49 g cm-3) that promote good capacity for thermal insulation and mechanical energy absorption [1,2]. For the production of foams, the biomasses were milled, obtaining fibers in a wide distribution, ranging from 0.026 to 2.866 mm for eucalyptus, and 0.017 and 1.867 mm for sugarcane bagasse. Then, aqueous dispersions of plant fibers were prepared with surfactant (sodium dodecyl sulfate, SDS) and thickeners. The fiber dispersions were foamed through mechanical agitation, obtaining foamability, observing a good stability condition, in 70% (from its initial volume), and then oven-dried (60 ºC) [3]. The dry foams underwent a compression test for mechanical strength testing and showed a performance compatible with cellular materials Moreover, the foams exhibited low density, ranging from 0.10 to 0.26 g/cm3. The impact of the morphology and chemical composition of the biomasses on the structure and mechanical properties of the materials was evaluated in order to create foams for applications intended in packaging and civil construction [1,3].

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3D PRINTED OSTEOGENIC SCAFFOLDS BASED ON POTATO STARCH ENRICHED WITH BIOACTIVE GLASSES AND LANTHANIDES BIOMARKING

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Recent developments in the field of additive manufacturing have led to the possibility of creating complex-structured porous scaffolds [1] with polysaccharides, which show great biocompatibility and biodegradability, such as starch. Similarly, bioactive glasses (BG) accelerate healing in bone tissue due to their oxide composition [2]. Therefore, this study seeks to produce 3D printed scaffolds based on potato starch enriched with 45S5 BG and europium and dysprosium biomarking for an enhanced healing process while providing a method of measuring the biodegradation of the implant. The BG were synthed via melt-quench and characterized by SEM, XRD, and luminescence. The BG were added (5-10% w/w starch, d.b.) in the hydrogels based on the potato starches (10-15% w/w solution, d.b.). The scaffolds were printed (BioedPrinterV4, BioEdTech-Brazil), freeze-dried, and characterized by biodegradability rate, swelling power, and mechanical properties. The BG showed non-uniformed in and morphology, diffractogram profile compatible with 45S5, and luminescent character when doped. The increase of the BG content in the hydrogels resulted in higher viscosity and elasticity in hydrogels and resulted in scaffolds with lower biodegradability rate and swelling power, and superior mechanical properties. Considering the processability in 3D printing, the optimum formulation was 5% (w/w starch) of BG added in the starch hydrogels 10% (w/w solution). Biomarkers displayed a luminescence profile, being europium an effective biomarker in dry conditions while the dysprosium compound in dry and wet conditions. Finally, this work shows the preliminary positive effects of the inclusion of BG with biomarkers in the properties of potential starch-based bone scaffolds.

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A Chitosan active film incorporating Amazon bioactive compounds to obtain a sustainable dermatological mask

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Dermatological products are daily treatment routines for slowing aging and maintaining skin health. In general, these products are based on synthetic polymers that present a long biodegradation period, promoting an enormous environmental concern. Environmental-friendly cosmetics formulations using natural ingredients from renewable raw materials are demanded by conscious consumers that promote skin health, balancing effectiveness with environmental responsibility. Chitosan is a natural polysaccharide that can form flexible biofilms and act as a matrix for the incorporation of bioactive compounds. Its properties show promising potential for partially replacing synthetic polymers as ingredients in skincare product formulations. Murumuru butter (*Astrocaryum murumuru* Mart.) and white breu essential oil (*Protium heptaphyllum* Aubl.) are found in the Amazon region. The murumuru exhibits moisturizing ability and antimicrobial properties. White breu essential oil presents antioxidant, anti-inflammatory, relaxing, and healing activities. The chitosan-based films (1% w/w) incorporating white breu essential oil (0.3% w/w) and murumuru butter (0.2%, 0.6%, and 1% w/w) were developed using the casting method. The average thickness, moisture content, and release of active compounds (diffusion) were analyzed. The diffusion of bioactive compounds was conducted at 37°C, simulating the corporal temperature and calculated according to Fick's Law. The active chitosan films showed an increase in thickness and a decrease in moisture content as the concentrations of murumuru increased. Chitosan films incorporating murumuru butter and white breu essential oil represent a promising alternative for use as an environmentally friendly daily dermatological treatment mask.

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ACTIVE HYDROGEL FILMS WITH ROSEWOOD ESSENTIAL OIL

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Hydrogels are among the main subjects of interest to researchers due to their potential applications, including tissue engineering such as dressings, packaging films, sensors, and bioactive transport and delivery of bioactives. This work aims to evaluate the carboxymethylcellulose (CMC, 2.0 wt.%) hydrogels crosslinked by acetic acid (AA3 % and 5 %) and active with rosewood oil nanoemulsion (ROE) encapsulated, prepared by casting. The majority component identified in RO was the linalool (96 %). The ROE showed high stability, with an average capsule of 122 nm and IP of 1.452, determined by DLS. In the release test (24 h), the ROE rate was 12.54 mL/L, and the hydrogel film's rate was 84.67 mL/L.

The RO released (in 24h) was enough to promote the 17 mm and 15 mm inhibin zone on P. aeruginosa, 35 mm e 41 mm on E. coli, and 32 mm e 35 mm on S. aureus, respectively. The minimum inhibition concentration (MIC) and minimum bactericidal concentration (MBC) values were on P. aeruginosa 0.38 % and 0.75 %, E. coli 3.0 % and 1.5 %, and S. aureus were 0.38 %and 0.75 %, respectively. Then, excellent inhibition properties against the bacteria tested were observed. The thermal analyses confirmed the stability maintenance in the pure CMC and CMC/ROE hydrogel films. The pure CMC hydrogel film demonstrated thermal stability with a 36 – 46 % mass loss at around 250-320 oC. Similarly, the CMC/ROE hydrogel films (AA3 % and 5 %) maintained thermal stability at around 250 – 320 oC, with a 34 – 35% mass loss. The first peak of the most significant 44 % mass loss at the maximum temperature (270 oC), at which the cellulose degradation was maintained constant. These findings underscore the potential of active hydrogel films in the medical field, particularly in developing active healing dressings. The applications of this research extend beyond medicine to the food industry, where these films can be used for packaging, extending shelf life, and transporting food products.

ASH from green coconut shells coupled with a hydrogel based on cassava gum as a corrective and soil conditioning

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Brazil is one of the countries with large agricultural productions, including the production of green coconut in its species varieties, with the northeast one of the largest producers of this cultivation and planting; among them are the states of Bahia, Sergipe, Ceará, and Pará. The production of green coconut is a profitable and economical activity for residents, being one of the tools for technological advancement in the coming years. This work aims to produce ash from green coconut shells, develop a hydrogel based on cassava gum coupled with green coconut ash, and then characterize the chemical compounds present in the ash used in soil conditioning [1]. The characterization techniques used for this research will be XRF, FTIR, TG, and XRD. Green coconut ash was obtained to compare the chemical compounds of rice, sugar cane, and cashew nut ashes. The expected results of this research will be the chemical compounds K2O, CaO, MgO, P2O5, SiO2, Fe2O3, MnO, and potassium and phosphorus, considered essential macronutrients in the soil fertilization process. The ash from green coconut shells, coupled with hydrogels, can benefit agriculture and contribute to future advances in materials science and technologies.

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Assessment of galactomannan extraction methods from *Dimorphandra gardineriana* seeds

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Galactomannan, extracted from the endosperm of legume seeds, is a natural, cost-effective, and innocuous polysaccharide. This study evaluated five distinct extraction methods for *Dimorphandra gardineriana* seeds, employing various process conditions, including the use of an autoclave, medium pH, and ethanol proportion during precipitation. Due to its edibility and biodegradability, this polymer holds significant potential as an alternative material for edible films in fruit coatings, substantially prolonging the shelf life of products. The results indicate that the method involving autoclave usage yielded superior results (33%) compared to alkaline extraction methods (10.69%). This variance suggests that alkaline treatment likely compromised yield due to its inefficacy in inducing seed swelling. Characterization techniques such as FTIR and TGA were utilized to analyze the properties of the gums. These analyses revealed that gums extracted with a lower proportion of ethanol demonstrated enhanced thermal stability, suggesting possible alterations in the composition of the extracted polymer. Furthermore, FTIR spectra indicated structural similarity among the five gums, displaying characteristic bands of galactomannans. Thus, the selection of the optimal extraction method should balance yield requirements and thermal stability demands for the final application of galactomannan.

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Bentonite@gelatin as adsorbent for Copper (II)

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The presence of toxic metals in water is a risk to health [1] and metal removal processes have been proposed, among them, adsorption. Raw and modified clay minerals behaved as good adsorbents for toxic metals [2]. In this work, gelatin@bentonite nanocomposites were prepared in 10 and 20% mass proportions and applied as adsorbents for copper from aqueous solution. The solids were characterized by X-ray diffractometry (XRD), Fourier transform infrared spectroscopy (FTIR), thermogravimetry (TG), and scanning electron microscopy (SEM). XRD patterns suggested the formation of intercalation hybrids, considering that the basal space increased by 0.48 nm after the reaction between clay and gelatin. FTIR spectra showed a band at 3632 cm-1, which was assigned to M-OH stretching (M = Al3+, Mg2+ ou Fe3+). Bands at 1115 cm-1 and 1042 cm-1 were attributed to Si-O antisymmetric and symmetric stretching, respectively. A new band at 1541 cm-1 in the nancocomposites was assigned to vibrations of amide present in the gelatin structure, demonstrating the interaction of the precursor material with the protein. The effectiveness of the solids for Cu(II) adsorption was evaluated by varying the pH, the adsorbent dosage, the time, and the initial Cu(II) concentration. Better adsorption occurred at pH 6 for raw clay and pH 5 for both nanocomposites. The adsorbed amounts were 0.19; 0.26 and 0.28 mmol g-1 for sodium bentonite and the solids Bent@Gel10% and Bent@Gel20%, respectively, at 0.02 mol L-1 Cu(II) initial concentration.

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Carboxymethyl cellulose hydrogels modified by vitamin D loaded cellulose nanocrystals for drug delivery applications

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Cellulose and its derivatives have been widely used as a natural compound in the preparation of hydrogels. Hydrogels are three-dimensional structures formed by polymeric networks, which adsorb large amounts of water or fluid of interest [1]. These hydrogels can incorporate nanoparticles, such as cellulose nanocrystals (CNC), improving their properties, such as biodegradability, biocompatibility, mechanical resistance and increased crystallinity. Furthermore, CNCs have some characteristics related to high strength and high specific surface area, which can improve the applications of hydrogels, such as drug release [2]. In this sense, considering the improvements resulting from the incorporation of CNC in hydrogels for drug release, vitamin D becomes a promising treatment agent for several diseases, and can be incorporated into the matrix of hydrogels [3]. In this approach, the present research carried out the synthesis of hydrogels using carboxymethyl cellulose (CMC) chemically cross-linked with citric acid, modified with vitamin D and incorporating CNC. These hydrogels and CNC were characterized by FTIR, UV-Vis, XRD, SEM, TEM, XPS, cytotoxicity assay, vitamin D release kinetics, swelling and gel-fraction. The results demonstrated that the formation of the cross-linked structure occurred mainly due to the reaction of the hydroxyl groups of CMC with the hydroxyls of citric acid. The morphology of the hydrogels presented a smooth and homogeneous surface, while the CNC presented morphologies forming nanocrystals and nanofibrils, depending on the route. Furthermore, CNC did not show cytotoxicity at different concentrations. Then, these hydrogels with compatible characteristics were developed for use as biomaterials.

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Carboxymethyl celulose hydrogels loaded Morinda citrifolia extract for biomaterials applications.

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The species Morinda citrifolia (M. citrifolia) is a native plant from Asia and French Polynesia, introduced in Brazil because its various therapeutic purposes. This plant presents regional variations and is popularly known as Indian mulberry, cheese fruit and noni in Brazil, where it is well present in the semi-arid region. The therapeutic potential of M. citrifolia is widely documented in the literature, with its properties attributed to the phytoconstituents present in its composition. In this context, this study aimed to produce carboxymethylcellulose (CMC) hydrogels cross-linked with citric acid incorporated the natural extract of leaf of M. citrifolia for biomaterials application with antimicrobial activity. Thus, characterizations using techniques such as UV-vis (Ultraviolet-Visible Spectroscopy), DLS (Dynamic Light Scattering), Zeta Potential and Raman Spectroscopy were carried out. Furthermore, extract release kinetic assays were conducted and antimicrobial evaluation with the bacteria Escherichia coli (ATCC 1597) and the fungus Candida albicans (ATCC 90029) were carried out. The results showed that the formation of the cross-linked structure in hydrogels occurred mainly due to the reaction of the hydroxyl groups of CMC with the hydroxyls of citric acid, confirmed by Raman. The zeta potential indicated a negative surface charge of the extract, as well as a chain in the range of 100 to 150 nm by DLS. In the case of extract release kinetics, the greatest release occurred in the initial 30 minutes. The antimicrobial evaluation indicated good antimicrobial activity with the microorganisms evaluated. Then, in this work, hydrogels presenting compatible characteristics were developed for use as biomaterials, showing their great potential and the possibility of intensifying the social and economic development of the Brazilian semi-arid region.

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Cashew Gum-Based Aerogel for Organic Dye Removal

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Aerogels are polymeric materials with a remarkable water retention capacity due to their three-dimensional structure and hydrophilic groups [1]. These materials have demonstrated broad utility in various areas, such as water and soil treatment [2]. This study aims to synthe aerogels produced from cashew tree gum (Anacardium occidentale), targeting potential applications in the adsorption processes of organic dyes. The aerogels were characterized by Fourier transform infrared spectroscopy (FTIR) and evaluated for their water absorption capacity, toxicity analysis, and organic dye adsorption capacity. Through FTIR, the band at 1675 cm^{-1} was observed, indicating the conversion of amide groups into carboxylates, which favors the adsorption process. The aerogels showed a high water absorption capacity, with values exceeding 215 g g^{-1}.Moreover, the aerogels did not exhibit toxicity against Artemia salina. Remarkably, the aerogels demonstrated an adsorption capacity of approximately 950 mg g^{-1}, highlighting them as materials with great potential for adsorption. Thus, the developed aerogel proved to be effective in removing cationic dyes. It also had a high water absorption index and lack of toxicity, making it applicable in various areas.

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Cashew tree gum superabsorbent polymers with phosphates for environmental remediation

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Superabsorbent polymers can be produced from polysaccharides, such as cashew tree gum, obtained from the exudate of the species Anacardium occidentale L., widely found in Northeast Brazil [1]. These materials have the most diverse applications and can be used in environmental remediation and agriculture [2]. Furthermore, its efficiency can be improved with the addition of hydroxyapatite, a calcium phosphate, which has been used in wastewater treatment. The objective of this work was the synthesis of superabsorbent polymers from cashew tree gum containing phosphates with and without modification for application in the adsorption of methylene blue dye. The materials were characterized by FTIR, SEM, phPcz, swelling test and in the adsorption tests parameters such as time and pH were evaluated. The characterizations indicated that the bands observed in the FTIR suggest the formation of the materials, according to the SEM images it was observed that the materials presented a rough surface with pores of irregular s and the pHpcz was between 8.5 and 9.6. Water retention for the materials was best in the pH range of 4 to 10, with swelling ranging from 20,000 to 30,000%. The superabsorbent polymers showed excellent adsorption capacity for the cationic dye methylene blue, whose adsorption rates were around 628 to 900 mg g^{-1} in the equilibrium time determined in 360 minutes and the optimum pH was 10, whose rates were in around 780 to 1020 mg g^{-1}. Superabsorbent polymers developed from cashew tree gum have proven effective in removing methylene blue, making them promising in environmental applications.

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Cassava gum hydrogel with oxide addition for organic dye removal

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The synthesis of hydrogels from polysaccharides of renewable sources has garnered significant interest in scientific research [1]. The combination of the adsorptive properties of these hydrogels with the photocatalytic properties of oxides, such as titanium dioxide (TiO_2), emerges as a promising alternative in the production of new photocatalysts [2-3]. This study focuses on developing a composite material based on the synthesis of cassava gum hydrogel with the addition of TiO_2 synthed by the sol-gel method, aiming at removing methylene blue dye (MB). The materials developed were characterized by X-ray Diffraction (XRD), UV-Vis Diffuse Reflectance Spectroscopy (DRS-UV-Vis), and Scanning Electron Microscopy (SEM). XRD results indicated the presence of peaks corresponding to the anatase crystalline phase of TiO_2. A slight reduction in the bandgap energy of the composite compared to pure TiO2 was observed. SEM images revealed an adequate dispersion of TiO_2 nanoparticles in the polymeric matrix. Adsorption and photocatalytic tests showed that the composite exhibited a better capacity for MB removal than pure materials. The composite demonstrated efficiency in methylene blue dye removal, presenting a viable alternative for contaminated water treatment.

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Cellulose acetate from Pinus elliottii barks

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In recent decades, polymer consumption has grown considerably, representing a significant environmental liability. A significant portion of these polymers originates from petrochemical sources [1]. However, there is growing concern about the future scarcity of this raw material, as well as economic and environmental regulations for fossil-based products. This has led the scientific community to seek alternatives based on renewable resources [2]. In this context, biorefineries demonstrate great potential for supplying raw materials for polymer production. This study focuses on a biorefinery that uses Pinus elliottii bark as raw material to produce lignin tannins and cellulose pulp. The obtained pulp was used to produce cellulose acetate through cellulose acetylation. Acetic acid was used to dissolve the pulp, sulfuric acid acted as the protonating agent for the hydroxyl groups, and acetic anhydride was used as the source of carbonyl groups. After 24 hours of reaction, cellulose acetate was precipitated through phase inversion by adding deionized water to the suspension [3]. Preliminary Fourier-transform infrared spectroscopy (FTIR) analyses indicate that the OH band between 3600 and 3000 cm-1 present in the cellulose pulp spectrum was replaced by a peak at 1750 cm-1. characteristic of carbonyl group. This suggests that the OH groups were replaced by carbonyl-type functional groups, demonstrating the feasibility of producing cellulose acetate from bioresources obtained in a biorefinery.

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Cellulose acetate/polylactic acid blends plasticized with triethyl citrate obtained by twin-screw extrusion

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This study aims obtain Cellulose Acetate (CA)/Polylactic Acid (PLA) blends using a twin-screw extrusion, to improve processability of the blends triethyl citrate (TEC) was used as plasticizer. Different proportions of CA, PLA and TEC were prepared. Thermal characterization by differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA) were carrying out. The effect of TEC on CA/PLA blends was investigated regarding glass transition temperature (Tg), melting temperature (Tm), thermal stability, and morphological characteristics. Preliminary results indicate that addition of TEC caused significant changes in thermal and morphological properties of the blends, resulting in decrease on glass transition temperature. Additionally, morphological analysis revealed changes in the blend structure according to component proportions. This study contributes to advancing the development of customizable polymeric blends, highlighting the potential of PLA, CA, and TEC in formulating materials for various applications, especially in the field of biodegradable packaging and products.

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Cellulose-based filters: functionalization for pesticide removal from water and SERS quantification

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Nowadays, to produce more food and faster harvests, farmers are using large quantities of pesticides in their daily practices. Unfortunately, these pesticides can end up sticking around in food, soil, and water, causing concerns for our health and the environment.[1]. In this sense, different processes and techniques have been developed to increase the efficiency of removing these chemicals. In this sense, adsorptive membranes have emerged as an alternative for removing pesticides from water, adsorbing contaminants on its surface [2]. Seeking a more complete procedure, it is possible to combine the removal method and the quantification. Thus, surface-enhanced Raman scattering (SERS) has emerged as an alternative to detect and quantify pesticides in different matrices, exhibiting reproducibility and signal accuracy [3] Herein, we propose the production of cellulose filters, functionalized with positive and negative charges, and their application in removing pesticides from the aqueous medium through gravity filtration. Subsequently, assisted by silver nanoparticles (AgNPs), quantify the contaminant via SERS. Cellulose microfibers were obtained from sugarcane bagasse through chemical isolation and subsequent functionalization. The membrane was used to filter different pesticides. To quantify the contaminant, AgNPs were deposited on the membrane, and spectra were obtained by a Renishaw MicroRaman (InVia). Characterizations were carried out on the membranes seeking to understand the adsorptive behavior. In this way, we present membranes for water decontamination combined with Raman spectroscopy for the quantification of the pesticide present.

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Characterization of Chitosan Physical Hydrogels: Insights into Structure and Performance

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Hydrogels, known by their ability to absorb water and form macromolecular networks, represent a versatile class of materials with widespread applications. Their unique properties make them particularly intriguing for diverse fields, notably in biomedicine where they excel in drug delivery, tissue engineering, and beyond. This study underscores the importance of hydrogels as potential drug carriers, aligning with the broader objectives of this research. Among natural polymers, chitosan stands out for its exceptional qualities as a drug carrier. This polysaccharide boasts attributes such as biodegradability, non-toxicity, and remarkable biocompatibility, making it an attractive candidate for various biomedical applications. To optimize chitosan hydrogels, incorporating cellulose nanocrystals (CNCs) is a promising strategy. CNCs enhance mechanical strength, thermal stability, and barrier performance due to their rod-like shape, high mechanical strength, and biodegradability. By integrating these nanomaterials into the polymeric matrix, it becomes possible to elevate essential properties such as mechanical strength, thermal stability, and barrier performance, thus expanding the potential applications of chitosan hydrogels. The aim of this study was to examine how the origin (bacterial or vegetal) of nanocrystals affects the properties of chitosan hydrogels. CNCs concentrations and chitosan concentrations were varied to explore their impact on hydrogel characteristics. Through spectroscopic, rheological, thermal, and structural analyses, we assessed how the inclusion, source and amount of CNCs influenced. Nanocellulose load increases thermal stability linearly, with vegetable-origin nanocellulose being more effective. CNCs inclusion alters optimal pH for loading. Vegetable-origin CNC improves 1% hydrogel loading, while bacterial-origin CNC is better for 2% hydrogels.

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Characterizations of xylan:chitosan films using xylan from different extraction conditions.

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The pursuit of replacing petroleum-based plastics with renewable alternatives has been a focal point of research for several years. Xylans sourced from agro-industrial residues offer a promising opportunity to produce films from a renewable, abundant, and cost-effective source. However, isolating xylan in a pure form proves challenging, as it often contains varying degrees of contamination from other biomass components. This study assesses the film-forming capacity of xylan extracted from industrial eucalyptus residues, using chitosan as a copolymer. Two extraction methods were evaluated for xylan extraction. In the first method (Xylan A), eucalyptus wood underwent treatment with 17% NaOH (based on oven-dry wood) at 105°C for 45 minutes. The second method (Xylan B) involved an extraction step with 23% NaOH (based on o.d.w) at 155°C for 45 minutes, following removal of wood extractives with a NaOH/Na2SO3 solution. The resulting xylan-rich fractions were precipitated with ethanol, washed, and chemically characterized.

Subsequently, xylan/chitosan films were prepared using different mass ratios (80/20, 70/30, 56/44, and 44/56). Xylan A precipitate consisted of approximately 30% glucuronoxylans, 35% lignin fragments and wood extractives, and 30% ash. In contrast, Xylan B precipitate comprised around 56% glucuronoxylans, 18% lignin fragments, and 25% ash.

Films prepared with Xylan A exhibited a consistent tensile strength of about 30 MPa across all xylan ratios tested. Films prepared with Xylan B showed an increase in tensile strength with increasing chitosan content, ranging from 20.6 to 54.9 MPa. However, the elongation at break was uniformly low, around 3-4% for all films tested. The water vapor transmission rate ranged from 676-695 g m-2d-1 for films with a xylan ratio of 56:44, increasing to 717-760 g m-2d-1 for films with a ratio of 44:56, reflecting the hydrophilic nature of the polymers used.

Chemically modified babassu mesocarp and bacterial cellulose hydrogels and their performance in Ibuprofen release

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Alternative methods of disease treatment, such as drug delivery systems, provide the administration of specific medications at controlled rates over the long term, minimizing side effects resulting from toxicity and increasing therapy effectiveness[1]. In this regard, polysaccharide-based hydrogels have been extensively investigated for use in such systems[2,3]. The main objective of this research was to prepare hydrogels based on babassu mesocarp and bacterial cellulose that were chemically modified through a copolymerization reaction of polyacrylamide for use in the controlled release of the drug Ibuprofen. The results of the hydrogels loaded with Ibuprofen showed that the samples exhibited toxicity only at a concentration of 5 mg mL-1. All hydrogel samples were considered non-cytotoxic. Regarding Ibuprofen release, there was rapid drug release within the first 12 hours in PBS, and the release in gastric fluid was slower and more prolonged, but all hydrogels tended to stabilize at 100%, making these hydrogels promising for drug release applications.

Chemically modified pullulan-based nanoparticles via nanoprecipitation: the effect of pH medium and polymer concentration on particles diameter a polydispersity

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Nanoparticles have been extensively researched as an alternative to improve the pharmacokinetic and targeting properties of poorly water-soluble drugs, increasing their efficacy and reducing side effects [1]. Pullulan (PULL) is a hydrophilic and biodegradable microbial polysaccharide that is a promising candidate for development of nanoparticles systems, due to its biocompatibility, specific interactions in the body and possibility of chemical modifications [2]. PULL can be easily modified to obtain amphiphilic and cationic properties, capable of self-assembling into nanoparticles suitable for drug encapsulation [2]. Since pH medium and polymer concentration in particle's preparation via nanoprecipitation have influence in the particle's and polydispersity, this work reports the preparation of PULL-DEAE-g-PZLL (PDPL)-based particles varying its concentration and pH medium. The appropriate concentration of PDPL, from 2 to 20 mg/mL, was dissolved in dimethyl sulfoxide (DMSO), and submitted to dialysis against water solutions with acidic and neutral pHs for 72h. After nanoprecipitation, the particles were analyzed in terms of particle, distribution, and stability over 30 days. Morphology of dry particles was also evaluated using AFM technique. The results demonstrated that lower pH values have a significant effect on the particle's. Besides it, intermediated concentration values present a better particle size and distribution, and the association between lower pH medium with lower polymer concentration can result in a polymer hydrolysis. Therefore, the optimized conditions will be further applied to prepare nanosystems to encapsulate drugs and improve their delivery. Acknowledgements: FAPESP (2019/12940-4 and 2023/11796-2). References: [1] P.K.Aktas, I.Baysal, S.Yabanoglu-Ciftci,A.Lamprecht, B.Arica, v. 650, p. 123703, 2024.[2] L.T.Carvalho, A.J.R.M.Teixeira, R.M.Moraes, R.F.S.Barbosa, R.C.Queiroz d, D.B.Tada, D.R.Mulinari, D.Rosa, M.I.Ré, S.F.Medeiros, v. 181, 10544

CHITOSAN/BENTONITE/GELATINE BEADS AS ADSORBENTS FOR COPPER(II)

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The contamination of water bodies by toxic metals is currently one of the greatest risks to human health. In this sense, adsorption has been a versatile strategy in the treatment of water containing organic and inorganic pollutants [1]. Among adsorbents, chitosan is widely used due to its biocompatibility and biodegradability [2], and can be applied in the form of beads and films, which facilitates the separation process. Chitosan can also be combined with inorganic matrices originating hybrid materials with higher reactivity for use in adsorption. In this work, chitosan beads were synthed by reacting sodium bentonite (NaBent) or sodium bentonite with 10% by weight of gelatin (NaBent@GEL10), reticulated with sodium tripolyphosphate. The obtained solids were applied in the adsorption of copper (II) in aqueous solution. The X-ray diffractograms of the solids modified with clay mineral presented the 001 reflection of the montmorillonite phase and the basal spacing increased 0,24 nm, which confirmed the modification. The infrared (FT-IR) spectrum of the chitosan beads showed a broad band at around 3376 cm-1 associated with the overlap of O-H and N-H stretchings, two characteristic bands in 2941 and 2878 cm-1, that were assigned to the asymmetrical and symmetrical C-H stretchings, respectively. The band at 1661 cm-1 was associated with C=O stretching of amide groups of the biopolymer. In the nanocomposites, the FT-IR spectra presented two new bands at 518 and 469 cm-1, referring to the Si-O-Si and Si-O-Al bendings, respectively, indicating the formation of the composites. In the copper (II) adsorption evaluation, all materials had the best adsorption at pH 6.

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Chitosan films containing white breu essential oil and murumuru butter for potential cosmetic application

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Eco-friendly products play a key role in building a more conscientious world. At the same time, the growing awareness of skincare is making personal care a common habit. In this context, the natural bioactive compounds incorporated into the biopolymers matrix could be a favorable alternative to produce facial treatment masks, combining environmental consumption consciousness and personal care. Chitosan is a biopolymer that presents the characteristics of antimicrobial activity, low toxicity, biocompatibility, and a matrix for bioactive compounds. Murumuru (*Astrocaryum murumuru* Mart.) and white breu resin essential oil (*Protium heptaphyllum* Aubl.) are bioactive compounds from the Amazon region, used in the cosmetic and perfume industries respectively, presenting properties such as hydration, skin protection, antioxidant, antimicrobial, and anti-inflammatory. The chitosan-based films (1% w/w) incorporating murumuru butter (0.2%, 0.6%, and 1% w/w) and white breu resin essential oil (0.3%, w/w) were developed with potential cosmetic applications targeting hydration, anti-aging, and antimicrobial effects. Parameters such as average thickness, microstructure, water vapor permeability, and water solubility of the films were determined. Films containing murumuru butter and white breu resin essential oil were characterized by easy handling and uniformity. The film-forming matrix in the presence of bioactives indicated the presence of pores which influenced the reduction of barrier properties, modifying the characteristic compact, cohesive, and barrier structure of chitosan films. The observed differences showed significant positive results compared to the chitosan control film. The developed material can be considered a sustainable and biodegradable skincare alternative, considering that the differences caused by the presence of bioactive demonstrate advantageous properties for their use as a facial mask.
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Chitosan Functionalized with Photosensitizers: Study of Bacterial Photoinactivation in Solution and in Films

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Photodynamic Inactivation of microorganisms (PDI) emerges as an important bactericidal approach to overcome the development of multiresistent drug microorganisms (MRD) due excessive or incorrect uses of antibiotics [1]. Furthermore, biofilm formation considerably increase resistance to drugs. In the present study chitosan (CS) was functionalized with porphyrinic (aminophenyl porphyrin (P1) and the corresponding Zn(II) complex (ZnP1)) and phenothiazinium (Toluidine Blue - TOB) photosensitizers by a convenient linker, resulting in the corresponding functionalized CS polymers (FunCS): CS-P1, CS-ZnP1 and CS-TOB. The FunCS have been tested in PDI systems in cell suspensions of S. aureus and E. coli and in films for P. aeruginosa. Experiments with cell suspensions were irradiated with commercial diode lasers and with white light irradiation provided by a quartz-halogen lamp in agar plates. Films of FunCS were immersed in cell suspensions of P. aeruginosa and submitted to periods of dark-ligth or light-dark regimes using white light. Results in cell suspensions can be summarized: i) S. aureus (1E8 CFU/mL): All FunCS were effective in the complete photoinactivation of this microorganism in solution or in agar plates; ii) E. coli (1E8 CFU/mL): in solution were obtained a drastic decrease of 6-7 log; CS-ZnP1 required the shortest irradiation time (3 min), followed by CS-TOB (4 min) and CS-P1 (4,5 min) and in agar plates complete photoinactivation was observed for a standard irradiation time of 30 min for all FunCS.
P. aeruginosa biofilms: A slight decrease of 1log was observed to all FunCS films that were just immersed in P. aeruginosa compared to cells collected from biofilm formed in glass slide (control). Light-dark regimes were more effective than dark-light ones with 4 log decrease compared to 2 log decrease indicating the PDI process is more effective in the cell adhesion process.
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CO_2 adsorption by graphene oxide-chitosan sustainable filter elements

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Innovations in the field of nanotechnology provide opportunities and applications in different segments. Chitosan foams can be used as filter elements due to their adsorptive characteristics, but they have limited mechanical strength and flexibility. Graphene oxide (GO) nanoparticles can be incorporated into polymer matrices to enhance filtration properties and mechanical resistance. This work incorporated GO into chitosan-based polymer matrices structured in the form of low-density foams. The foams were produced according to patent number BR1020150292597 [1]. Chitosan was obtained from shrimp shells processed at the Federal University of Paraná (UFPR) and presented a deacetylation degree of 85% and a molar mass of 75 kDa. For the carbon dioxide (CO2) adsorption tests, a gas mixture of methane (CH4) and CO2 in the ratio of 50:50 was used. The samples of chitosan foam and chitosan foam with GO were placed in a bed of a high-pressure reactor and subjected to the adsorption test at atmospheric pressure and 2 bar. The flow rate of the gas mixture at the column inlet was 5 mL/s. After the test, the chitosan foam showed an adsorption capacity of 110 mg CO2/g foam, while the chitosan foam with GO showed an increase in adsorption capacity of 530 mg CO2/g foam, about 5 times higher than the control foam. This result demonstrates the better adsorption capacity of the GO-containing foams and may also be related to the greater mechanical strength of the material, since less foam was needed in the reactor to fill the bed.

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Composites of nanocellulose and chitosan in the development of concentrated emulsions for food systems

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Colloidal particles based on biopolymers, which come from renewable, clean, and ecological sources, are acceptable as food-grade materials, and their use as high internal phase emulsions (HIPEs) stabilizers has been stimulated due to consumer demand for more natural foods. HIPEs present internal phase concentration superior to 74% (v/v), resulting in a semisolid texture [1,2]. When stabilized by solid colloidal particles, they are called Pickering HIPEs [1], presenting increased resistance to coalescence due to particles' irreversible adsorption at the interface [2]. The use of hybrid particles compared to single component particles has been suggested as one better way to improve the Pickering HIPEs performance and stability. Cellulose nanocrystals (CNC) and chitosan (CS) are candidates with great potential for use in food. CNC can be modified with negative charges, whereas CS becomes positively charged at low pH. Therefore, they present a strong electrostatic attraction due to their opposite surface charges forming new composites [3]. This work aims to obtain CNC/CS composites in different ratios with cross-linking with glutaraldehyde and explore their use as HIPES stabilizers. The CNC/CS composites obtained will be characterized in terms of distribution, zeta potential, and wettability. With this study, is expected to obtain composite materials with characteristics suitable for use as stabilizers in Pickering HIPEs and subsequently investigate the use of natural cross-linking agents.

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Comprehensive study of Macro and micromechanical assessment of polyssacharide based scaffolds

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The mechanical properties of scaffolds play a crucial role in the phenomenon of cellular mechanotransduction[1]. One of the most important physical parameters related to any material's mechanical property is its Young’s modulus (E), which is a measurement of the material's elasticity. There are several techniques to quantify E, each with its unique approach[2]. E values can be determined from the slope of stress-strain curves in the elastic deformation regime of the material under tension or compression, for example, which are macroscopic measurements. Microscopic measurements, like nanoindentation AFM, use nano to micrometric tips to locally “poke” the material surface at extremely low forces, generating the so-called force curves. This study uses macroscopic and nanoindentation approaches in order to mimic cellular stiffness perception to determine E values of hydrogels in their swollen state. E values obtained via compressive tests were up to three orders of magnitude smaller than those from nanoindentation in the case of Alginate/Polyvinyl alcohol scaffolds. Conversely, for chitosan/PDMS composite films the tensile modulus was generally higher than EAFM. These disparities may stem from various factors. Local interactions between the AFM tip and composite layers could influence micromechanical experiments , while water squeeze-out effects might affect macromechanical results. Nonetheless, further experiments are warranted to comprehensively grasp the dynamics governing E values of swollen hydrogels across different scales.

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Conductive, flexible and sustainable films using lignin nanocarbon coating on starch films

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The energy generation from photovoltaic sources has been consolidated as one of the most promising initiatives in order to provide a renewable energy generation and with reduced levels of CO_2 emissions [1]. Although in the last decades the photovoltaic technology has achieved an enormous progress in terms of efficiency and durability, as well as in terms of reducing production costs, continued efforts are still needed in different areas, such as the development of new flexible substrates. Therefore, this work aims to produce new flexible, transparent and conductive electrodes to be used in photovoltaic devices. This innovative technology is based on the synthesis of graphene nanoplatelets (GNP's) from biomass such as lignin and rice husk [2], which leads to use of graphene properties as a promising possibility to replace ITO (indium tin oxide) and FTO (fluorine-doped tin oxide) as transparent electrodes in photovoltaic devices. This methodology includes exposing the biomass to a sequence of pre-treatments, such as UV irradiation, polycondensation of aromatic rings in autoclave, degassing in a vacuum oven, pyrolysis in inert atmosphere and sonication. In the sequence, the GNP's was deposited by blade coating onto a flexible starch substrate and, posteriorly, the GNP coated starch films were electrically characterized in order to determine their resistivity. The first visual inspection of the fabricated films showed a homogeneous distribution of GNP's on starch surface, keeping the transparence of the film up to 90 %, allowing its application as substrate for organic photovoltaic devices.

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Cytotoxic and antileishmanial effect of silver nanoparticle stabilized with angico gum

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Leishmaniasis constitutes a group of prominent neglected infectious diseases globally, manifesting in various clinical forms [1]. In this context, cutaneous leishmaniasis, caused by the species *Leishmania amazonensis* [2], is characterized by distinctive lesions varying in severity and clinical appearance. Therefore, the aim of the study was to evaluate the activity of silver nanoparticles stabilized with Quaternized Angico Gum (AgNP-GAQ) against promastigote forms of *L. amazonensis* and cytotoxicity against RAW macrophages. The AgNP-GAQ was synthed and characterized using UV-visible spectroscopy, atomic force microscopy, and zeta potential analysis. The nanomaterial exhibited a plasmonic band at 410 nm, with a spherical shape and an average of 19.74 nm as determined by microscopy, and a zeta potential of +40 mV. AgNP-GAQ demonstrated an IC_{50} of 24 µM in promastigotes and a CC_{50} greater than 250 µM in macrophage cells, resulting in a selectivity index of 10.41. Thus, the biomaterial showed greater selectivity towards the parasite than the tested cells. These results indicate that AgNP-GAQ is a promising biomaterial for potential application as an alternative treatment against this parasite.

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Design of electrically conductive foams based on cationic cellulose and carbon black for antistatic packaging

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Electrically conductive foams are used as antistatic packaging to protect electronic items sensitive to electrostatic discharge. Commercial antistatic foams are usually composed of conductive particles dispersed in petroleum-derived polymers, combining high energy demands and large dust generation on production processes, poor fire resistance, and low degradation rates [1]. As an alternative, cellulose is a biodegradable biopolymer that can be used to assemble greener foams [2]. Thus, this study proposes a more sustainable system composed of cationic cellulose (CC) and carbon black (CB). Cellulose was isolated from sugarcane bagasse, and CC was obtained by cationization reaction with GTMAC. CB was added to CC suspension, producing stable colloidal dispersions due to electrostatic interactions between positive surface charges ($–N(CH_3)_3^+$) of CC and polarized π electrons in aromatic structure of CB. CC/CB foams were obtained by freeze-drying the dispersions. CC/CB foams showed low densities (<54 mg/cm^3), high porosities ($>91\%$), and a robust network structure with high specific compression moduli (11−21 MPa.cm^3/g). Two ranges of behavior in electrical properties were observed: foams with (i) 1−5 wt% of CB showed resistivity around 10^8 Ω.cm (static-dissipative), and (ii) ≥10 wt% of CB presented values between 10^3 and 10^1 Ω.cm due to the formation of an interconnected network (conductive). CC/CB foams showed great resistance to the initiation and spread of fire, being less flammable than a commercial antistatic foam. In conclusion, the interactions between CC/CB produced stable dispersions and foams with good mechanical/electrical properties, exhibiting considerable promise for electrical applications and potentially replacing commercial plastic-based antistatic foams.

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Developing gelling ingredients to produce 3D-printed milk gels with tailored properties

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3D printing technology is an interesting approach to producing gels with customized textures. This strategy can produce food products for special needs, such as with a specific texture for dysphagia – but new ingredients are needed to ensure it. This study developed 3D-printed milk gels for dysphagic diets combining two biopolymers as structuring agents: native or Dry Heating Treatment (DHT)-modified cassava starch and kappa-carrageenan (κC). Starch was DHT-modified (130 °C for 2 and 4 h) and the gels were prepared with reconstituted skim milk with 5% of gelling agents: starch (100, 99.7, 99.4, 99.1, 98.8 and 98.5%) and κC (0, 0.3, 0.6, 0.9, 1.2 and 1.5%), by gelatinization and gelification. The milk gels were then 3D-printed in different geometries and evaluated in relation to shape and texture. The results showed that κC had a dominant effect compared to the DHT-modified starch on gel texture and 3D printing performance, while the DHT-modification had no significant difference to native starch. In addition, a small κC concentration is enough to improve the milk gel properties, whereas, as the κC concentration is increased, the printing quality decreases. The gels obtained by molding or 3D printing resulted in different texture behaviors, which was associated with the gel extrusion process that breaks down their initial structure. Some conditions were able to suit the dysphagic diet needs. In conclusion, this study demonstrated an approach to modify the milk gel texture by adding two different gelling agents, and that these agents act in different ways on the formation of gels and final textural properties, just like 3D printing technology.

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Development of cross-linked hydrogels based on cassava gum coupled with rice ash and urea.

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Agriculture has a huge economic activity with the characteristic of planting and growing food in society, an important factor for the great advancement of technology in the coming years. The objective of this work was to develop hydrogels based on cassava gum coupled with rice ash and urea for soil conditioning [1]. The characterization techniques used were XRF, FTIR, SEM, and XRD. A synthesis was carried out with cassava gum and another combining rice ash and urea. This could be verified in the presence of ash with a content of 80 to 95% of SiO2, NPK, and urea. The results for the XRF technique were the presence of the chemical compounds Si, O, N, P, K, C, H, Ca, and Fe in the hydrogel. In FTIR, stretching of the OH bond is expected in the 3382 cm -1 band and CH stretching in the 2935 cm -1 and 2890 cm -1 bands. The NH group could be observed in the absorption bands at 3426 cm -1 and 3326 cm -1. In the SEM analysis, the incorporation of urea due to porosity was be observed. In XRD, the change in the crystalline structure of the hydrogels was verified respectively at 2Θ= 23.5 and 39 [2]. Hydrogels coupled with rice ash and urea can enhance productivity growth in agriculture and contribute to future advances in materials science and technologies.Acknowledgment:

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Effect of hybridization on impact strength of recycled acrylonitrile-butadiene-styrene (ABS) composites reinforced with jute and recycled carbon fibers

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Interest in hybrid composites has increased due to the possibility of synergistic effects [1]. The aim of this work was to mold and evaluate the impact properties of composites using recycled acrylonitrile-butadiene-styrene copolymer (rABS) as matrix, and three types of jute fiber fabrics (bidirectional) as dispersed phase: T1 (Jute, 365 g.m-2); T2 (Jute, 445 g.m-2); and T3 (Jute/Cotton, 360 g.m-2). Furthermore, recycled carbon fiber fabrics (rFC) obtained from prepregs subjected to heat treatment at 500°C for 2h were used to recover bidirectional carbon fiber fabrics. Nine combinations were molded by hot compression process. Izod impact tests (ASTM D256) were carried out with a 1J pendulum and notched specimens measuring 63.5x12.7x4mm3. The results obtained after analysis of variance and Tukey's test showed that the incorporation of only jute fiber fabrics did not result in increase in the impact strength of rABS/1T1 (105.54±12.56 J/m), rABS /1T2 (106.00±27.00 J/m), rABS/1T3 (96.35±12.85 J/m) compared to rABS (91.15±8.17 J/m). Similar situation occurred in composites containing only one layer of recycled carbon fiber fabric (rABS/1rFC), that achieved an impact strength of 110.87±7.69 J/m. But the hybridization caused a percentage increase ranging from 32-38% in the impact strength of rABS/1rFC/1T1 (120.28±15.67 J/m), rABS/1rFC/1T2 (121.24±10.31 J/m) and rABS/1rFC/1T3 (126.03±16.00J/m). The best result was obtained for the composite containing two layers of recycled carbon fiber fabric (rABS/2rFC) with impact strength of 158.80±53.00 J/m, an increase of 74% compared to rABS. Thus, the remanufacturing process of these materials is an alternative for reusing high added value solid waste and reinserting it into the production chain, promoting the circular economy.
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EFFECTS OF CELLULOSE NANOCRYSTAL DIMENSIONS ON THE MECHANICAL PERFORMANCE OF POLYMERIC FILMS

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Cellulose nanocrystals (CNCs) are nanostructured particles derived from cellulose, an abundant and renewable resource, that have achieved extensive research attention due to their sustainability and unique mechanical performance when they are used as reinforcing agents in polymer composites. These nanocrystals are typically rod-like in shape and are characterized by their high crystallinity, large surface area, and low density. CNCs are obtained through processes that remove amorphous regions from cellulose, leaving crystalline structures with higher aspect ratios (L/d). The longer nanocrystals (L) with relatively small diameters (d) can interact more effectively with the polymer matrix, providing improved mechanical strength and stiffness. In the present work, CNCs and their efficiency in acting as a mechanical reinforcement in polymeric films were investigated, motivated by the number of cellulosic resources and availability of biomass in Brazil, mainly in the Northeast region, and also for the opportunity to provide insights for developing advanced materials with tailored properties for various applications, from packaging to electronics, and biomedical engineering. Thus, a systematic review was performed including all papers published until 2024, regarding the terms: cellulose AND (nanocrystals OR nanowhiskers) AND reinforcement AND polymeric films, through a search of three articles databases (Scopus, Web Science and MDPI). Overall, the findings reported that the addition of properly dispersed CNCs leads to an enhanced toughness in polymer matrices, representing an eco-friendly reinforcement with superior properties. However, excessive CNCs or poor dispersion in polymer films can lead to brittleness by creating stress points and reducing ductility. Finding the right balance of CNC concentration and dispersion is key to maximizing toughness while minimizing brittleness.

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Enhanced stability of Pickering emulsions promoted by cellulose nanofibrils electrostatic complexes

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Pickering emulsions are a type of emulsion stabilized by solid particles adsorbed at the oil-water interface. For the design of more sustainable products, cellulose nanofibrils (CNFs) are attractive candidates for Pickering emulsions, as they are renewable and biodegradable1,2. However, ensuring long-term stability against variations in pH and ionic strength remains a challenge, hindering widespread production and application. This study explored the electrostatic complexation of anionic and cationic CNFs to stabilize almond oil-in-water emulsions. Systems with different proportions of oppositely charged CNFs were prepared to evaluate the effect of charge balance on the colloidal stability, which was examined by optical and confocal microscopies. The results revealed that higher levels of cationic CNFs exhibited superior efficiency in stabilizing oil-in-water emulsions, maintaining droplet morphology and distribution for over three months under ambient conditions. The stabilization mechanism involves (1) interaction between the positive groups of CNFs and the negatively charged droplet surface and (2) the enhanced viscosity due to entangled nanofibers in the aqueous continuous phase. Remarkably, this stability was maintained with a remarkable tolerance to pH and ionic strength changes, revealing its suitability for practical applications in multi-component systems. Therefore, CNF complexes offer an environmentally friendly solution for developing highly stable emulsions with significant utility in food, pharmaceutical, and cosmetic formulations. Acknowledgments São Paulo Research Foundation (FAPESP, grant # 20/07794-6)

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Enhancement of Hydrophobicity of PET Membranes Using Plant Polysaccharides

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Considering the global context of exponent growth of solid waste generation, scarcity, water resources and increased pollution of water bodies as a consequence of anthropic actions, polymeric membrane technologies applied to water purification becomes important tools that assist in the environmental remediation process [1]. However, hydrophobicity of polymeric membranes is one of the main problems in its application as it leads to less efficiency and membrane performance during the separation process [2]. From the perspective of solid waste generation, it is estimated that the global population produces about 381 million tons of plastic waste per year. This study focuses on the development of a polymeric membrane composed of PET polymer recycled with the Karaya Gum Polysaccharide as an additive, with the objective of decreasing the hydrophobicity of the material. The membranes were developed by the phase inversion technique and characterized by measurements of contact angles and permeability. Contact angle results for samples with the additive indicated a 30.3% decrease compared to membranes produced only from the PET polymer. The measurement of permeability was only possible in materials produced with additives, indicating the lack of permeability in the pure pet membranes. The materials therefore demonstrate the reduction of hydrophobicity satisfactorily, presenting a viable alternative for membrane production for the treatment of water bodies, in addition to the great sustainable approach with the use of residual material.

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Evaluation of the antibacterial activity of bacterial cellulose films incorporated with silver nanoparticles stabilized with natural polymers

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Bacterial cellulose (BC) is a biopolymer secreted mainly by bacteria of the genus Gluconacetobacter [1]. In this study, bacterial cellulose (BC) functionalized with silver nanoparticle stabilized with collagen and agar (AgNPcolAG) is evaluated as an antibacterial film against antibiotic-resistant bacteria. The films were synthed and characterized by FTIR, AFM, SEM - EDX. The antibacterial evaluation was investigated by the agar diffusion method, against: Staphylococcus aureus ATCC 43300 - MRSA (Gram positive), Escherichia coli ATCC 35218 (Gram-negative) and Enterococcus faecalis ATCC 51299 – VANB (Gram-positive). The FTIR results showed typical CB bands. In the images obtained by SEM, it is possible to observe that the nanoparticles were uniformly dispersed and adhered to the 3D CB fibers, and that they have a spherical morphology. The EDX results confirm the homogeneous distribution of particles on the surface, indicating the presence of silver. The synthed film showed antibacterial activity against the tested strains, presenting an inhibition halo between 10.0 and 11.0 mm in diameter. Therefore, the use of NPsAg in the functionalization of films in the healthcare sector is viable, including in future applications, such as antimicrobial dressings.

EXPLORING THE RELEASE OF ACYCLOVIR FROM CHITOSAN-BASED MICROSTRUCTURED SYSTEMS

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Herpes simplex virus (HSV) infections is endemic worldwide and a frequent public health concern [1], configuring one of the most prevalent in the world with 640,000 new cases/year in Brazil [2]. Acyclovir, the drug which acts inhibiting its viral DNA polymerase, requires frequent application to achieve the desired efficacy, due to its low permeation. In this context, the use of biomaterials such as chitosan as a carrier is an alternative, once can improve permeation and avoid toxic effects [3]. In this work, chitosan-based membranes, capsules, and membrane/capsule microstructures were produced, characterized, and used for Acyclovir encapsulation/release. The membranes and capsules were produced using the casting and ionotropic crosslinking techniques, respectively. The physicochemical and mechanical microstructures properties were obtained, and release tests were performed. The better stability in drug encapsulation were observed for capsules and membrane/capsules systems. Regarding to release assay, the membrane/capsules system modulates the acyclovir release in 1 hour and 20 minutes, with peak concentration at 2 hours, meanwhile, the membrane and capsule systems, presented a conventional release profile with all drug concentration being released in 15 - 20 minutes. All obtained structures are promising to act as conventional and controlled release systems. The differential of these microstructures is the combination of healing properties, tissue repair, biocompatibility, biodegradability, and physicochemical and mechanical properties evaluated, associated with the selective action of the Acyclovir in the treatment of lesions caused by the HSV.

Films based on quaternized hydroxyethylcellulose: Formation and characterization

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Despite the great availability of cellulose and its considerable characteristics and properties, its quaternized ethoxylated hydroxyethylcellulose (CELqeh) derivative has practically not been used in film production. The films in this study have been effectively produced using a significant proportion of renewable and water-soluble raw materials. Different concentrations of CELqeh were considered, as well as the use of glycerol as a plasticizer. Lignosulfonate (LS), also soluble in water, was used as an additive to evaluate the impact on the properties of the films. Zinc oxide nanoparticles with an average of 19.7±1.4 nm were synthed, and incorporated into films to confer them with antimicrobial properties. The films were characterized using various methods including dynamic mechanical analysis, thermogravimetry, tensile testing, scanning electron microscopy, contact angle measurements, electrochemical impedance spectroscopy, and water vapor barrier measurements. All films investigated exhibited hydrophilicity, transparency, and good homogeneity with the incorporation of the selected additives, besides thermal stability up to approximately 200 °C. Compared to the control (CELqeh), the electrical conductivity of the films increased with the presence of glycerol and decreased with the presence of ZnO and LS, indicating the interference of the additives in the transport of electrical charges. The CELqeh film presented tensile strength, Young's modulus, and elongation at break of approximately 13 MPa, 23 MPa, and 47%, respectively, varying to higher or lower values, depending on the additive and their concentration. Water vapor permeability was approximately 6.5 10-10gm-1s-1Pa-1 for CELqeh, and only decreased when LS, rich in hydrophobic aromatic rings, was present. The current findings are quite promising and the study is still in progress. Funding: Foundation Coordination for the Improvement of Higher Education Personnel, CAPES, Code 88887756608.

Films of chitosan/gelatin blends with mucoadhesive properties

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Films of natural polymers with mucoadhesive properties represent an alternative for biomedical and pharmaceutical applications. The use of biopolymers to produce the films has the advantages of being biocompatible, biodegradable, often hydrophilic and enabling a wide range of applications [1]. Furthermore, biopolymers can be combined to form mixtures with improved properties over individual biopolymers, providing the desired properties to the system, which can improve application and be used as a carrier for bioactive compounds [2]. Therefore, the objective of this study was to develop blend films of natural polymers with mucoadhesive properties to be used as a carrier of bioactive compounds [3]. Different biopolymers chitosan (Ch) and gelatin (G) and their blends were explored to produce the films (100Ch:0G, 75Ch:25G, 50Ch:50G, 25Ch:75G and 0Ch:100G). The films were produced by the casting technique using glycerol as a plasticizer and characterized in relation to structural, morphological, mechanical, thermal and physical-chemical properties, in addition to mucoadhesive properties. The blends did not show macroscopic phase separation and formed homogeneous films. The results indicated that the addition of Ch caused a significant increase in tensile strength and young's modulus, leading to stronger films compared to gelatin film (0Ch:100G). Increasing the G content in the blends did not show a significant difference in the mucoadhesion strength of the films. Moreover, the film of pure chitosan (100Ch:0G) showed greater mucoadhesion and solubility when compared to the blends. Therefore, chitosan films were chosen regarding their mucoadhesive properties for the next steps of the project, for the incorporation and release of bioactive compounds.

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Formulation of 3D-Printed Hydrogels Based on Biopolymers for Bone Regeneration

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Biopolymer hydrogels like alginate aid bone regeneration via 3D printing, serving as cell regeneration matrices.[1] They accommodate additives like calcium phosphates and chitosan without altering the polymer matrix.[1] The use of calcium phosphate nanoparticles from the bones of the Nile Tilapia fish (*Oreochromis niloticuls*) offers improved mechanical properties and bone remineralization,[1] and is a low-cost material. In this study, alginate hydrogels with varied concentrations of chitosan and calcium phosphates were prepared. The gel was extruded through a glass syringe for 3D printing and cross-linked with $CaCl_2$. The biocomposites were characterized by Scanning Electron Microscopy (SEM) and Fourier Transform Infrared Spectroscopy (FTIR). SEM images showed the formation of hydroxyapatite aggregates in the polymer structure with good dispersion in the matrix. FITR spectra showed the interaction between the gel and the bioceramics. Preliminary in vitro bioactivity tests showed that the hydrogels are potential candidates to act as bioinks for the 3D printing of biomaterials for bone repair.

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Galactomannan from Fava D'anta as a Polymeric Additive in water-based drilling fluid

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Recent studies have demonstrated that the application of natural polymers in drilling fluids has led to significant advancements in the search for more effective solutions [1].This study aimed to extract and evaluate galactomannan (Gal) from *Dimorphandra gardineriana*, which has applications in biodegradable materials such as coatings and films, as well as acting as a viscosifying agent and filtrate reducer in water-based drilling fluids (WBDFs). The isolated Gal was characterized by FTIR and GPC. Three fluids were prepared containing bentonite, barite, calcite, hydroxypropylamide, and varying proportions of Gal with or without xanthan gum (GX). Their rheological and filtration properties were evaluated. The yield was 16.5%, and the FTIR results displayed bands at 814 and 869 cm-1, which are assigned to α-D-galactopyranose and β-D-mannopyranose units, respectively. The molar mass estimation revealed a unimodal distribution with Mw 2.38 × 10^6 g/mol and Mn 1.24 × 10^6 g/mol, with a PDI of 1.92. Another parameter, the apparent viscosity, varied from 32.5 to 46 cP, while the plastic viscosity ranged from 10 to 23.5 cP, and the yield point was between 45 and 52 lbf/100ft², all in compliance with the Petrobras standard 2604. The Herschel-Bulkley parameters indicated that WBFs with a higher concentration of Gal exhibited a higher yield point. The fluid with the highest proportion of Gal showed a reduced filtrate volume. The results suggest that Gal can be considered an innovative and renewable alternative to partially or completely replace GX in WBFs.

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High fibrillated sugarcane bagasse-derived lignin containing cellulose nanofibrils: combining minimal chemical treatment and mechanical fibrillation

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Bionanocomposites obtained through the incorporation of lignin-containing cellulose nanofibrils (LCNF) into biodegradable thermoplastic matrices are emerging as promising candidates for petroleum-derived polymers for the development of innovative biopolymeric materials. This work aimed to produce LCNF by employing a combination of minimal chemical reagents and high-shear mechanical processes, ultimately serving as a reinforcing filler in thermoplastic matrices. LCNF was pre-treated with 1-2 wt.% sodium hydroxide followed by mechanical fibrillation in Masuko grinder. Atomic Force Microscopy (AFM) images revealed fibrils with average diameter reaching 20 nm, accompanied by spherical particles lesser than 20 nm in , likely representing lignin particles that precipitated after the alkaline treatment. Moreover, Zeta potential indicated a stable dispersion (-31 mV), and LCNF presented high inherent viscosity, as a result of fibril entanglements and pseudoplastic behavior, which facilitates its processability. These findings indicated the efficiency of the developed protocol for LCNF production, establishing a foundation for its subsequent addition into biodegradable matrices, which is anticipated to not only enhance the mechanical and barrier properties of the polymer matrices but also introduce UV-blocking and antioxidant functionalities.

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HYBRID HYDROGELS BASED ON CASHEW GUM AND LAPONITE: A STUDY ON WATER ABSORPTION AND ITS REUSE CAPACITY, FOR APPLICATION AS SOIL CONDITIONERS

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The increase in water consumption due to the expansion of agricultural areas, driven by population growth and soil desertification processes due to climate variations, raises questions and concerns about the possible economic and social impacts of the water scarcity scenario [1] [2]. Hydrogels stand out in the search for sustainable water use practices, especially hybrids, which combine synthetic and natural materials, presenting good degradability and non-toxicity and enabling reuse due to the reinforcement promoted by chemical cross-linking between monomers [3]. Thus, this study focuses on synthesizing a cashew gum-based copolymer through a chain grafting reaction, incorporating laponite to evaluate water absorption and reuse. The hydrogels were analyzed by techniques such as Fourier Transform Infrared Spectroscopy (FTIR), X-ray Diffraction (XRD), and Thermogravimetry (TGA), as well as tests related to water absorption capacity, comparing their swelling behavior with pH variation, their reuse capacity, and finally, their toxicity. Successful synthesis was achieved, with consistent properties and absence of toxicity. The presence of laponite influenced water absorption capacity. It showed stability in cycles of use and reuse, suggesting application as soil conditioners with economic potential and promoting a sustainable bias regarding water use.

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Influence of cellulose microfibers/silver nanoparticles (Ag-CMF) on the interaction of PA microplastic and phthalocyanine: a removal study

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Studies involving microplastics (MPs, 1 – 5000 μm), have grown exponentially in recent years, however their effects as polluting agents on the environment are still poorly understood [1]. The presence of MPs in the environment occurs due to the processes of physical, chemical, or biological degradation of plastic waste [2]. Additionally, MPs can interact with diverse emerging contaminants (ECs), acting as a "Trojan horse", carrying such ECs to humans [3]. This work aims to study the interaction of polyamide (PA) MPs with nickel phthalocyanine dye (NiTsPc) and cellulose microfibers/silver nanoparticles (Ag-CMF), which will promote the adsorption of contaminants (MPs+NiTsPc) on their surface. The Ag present on the cellulose surface shows plasmonic properties that may help in the future identification of contaminants through surface-enhanced Raman scattering. UV-Vis and Raman scattering were used to study the adsorption mechanism. Two concentrations of MPs (1 and 5 mg/mL) have interacted with a 10^{-5} mol/L NiTsPc solution to evaluate the adsorption capacity of MPs. The results showed the adsorption of NiTsPc on surface of PA 5 of 58%, and PA 1 about 12%. On the other hand, under cellulose microfiber/AgNPs presence (PA+NiTsPc+Ag-CMF), the concentration of dye decreases 92% (PA 5) and 64% (PA 1). Additionally, the Ag-CMF increases the Raman signal to detect the contaminants. In this sense, in the PA+NiTsPc+Ag-CMF system, was possible to observe the spectra of both contaminants without spectral change; due to the physical interactions between PA and NiTsPc. Thus, the results showed the adsorption of NiTsPc on the PA surface, then the Ag-CMF act as a substrate for the removal and detection by Raman of pollutants.

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Influence of Chitosan Molecular Weight in Films containing Hyaluronic Acid

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Chitosan (CHI) is a versatile well-known polysaccharide, whose molecular weight may vary depending on the process of preparation. CHI has been widely used in biomaterial applications due to its effective film-forming ability, biocompatibility, and low toxicity [1]. Layer-by-layer thin films of CHI and hyaluronic acid (HA) have shown potential applications in cancer cell detection [2]. In this study, we investigated the influence CHI molecular weight (low and high) and salt concentrations (0 and 0.1 M NaCl) for detecting prostate cancer cells (PC3) in multilayer films with HA. Assays for capturing PC3 cells were performed to verify the effect of the CHI. Results showed similar cell adhesion behavior in the presence of ionic strength, regardless the molecular weight of CHI, which was a tendency also seen for HA so far. In this condition, film characterization indicated similar film roughness and surface charge density by carboxylate group availability, based on AFM and UV-vis absorbance measurements. However, in the absence of salt, films containing CHI of low molecular weight demonstrated a 1.6-fold improvement in cell adhesion. This study provides valuable insights into the factors that influence cell adhesion, highlighting the ionic strength as a factor in the design and optimization of chitosan-based thin films for biomedical applications, particularly in cancer detection and tissue engineering.

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Influence of crosslinking on the structure of Polysaccharide-based Hydrogels

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Polysaccharides are interesting for the synthesis of adsorbent hydrogels due to their biodegradability properties and low cost [1]. This study aimed to synthe hydrogels based on polysaccharides: cellulose (CEL) and alginate (AL), carboxymethylcellulose (CMC) and alginate (AL) with and without the addition of epichlorohydrin (ECH) in order to understand the interactions involved in the formation of these hydrogels. The hydrogels were produced from solutions (3% w/v) of CEL and AL, (1% w/v) of CMC, with 50/50 proportions (w/w) of the polymers and gelled in a calcium chloride solution. (1% w/v). Swelling index (I%), crystallinity (X-ray diffraction – XRD) and molecular interactions (FTIR-ATR transform infrared spectroscopy) were verified. The CEL/AL and CEL/AL/ECH hydrogels showed crystalline peaks characteristic of CEL while the CMC/AL and CMC/ALG/ECH hydrogels did not show diffraction peaks, being characterized as amorphous. The crystalline regions are impermeable to water, reflecting the lower I% of the CEL/AL (194%) and CEL/ALG/ECH (360%) hydrogel compared to the CMC/AL (1999%) and CMC/ALG/ECH (3170%). Crosslinking contributed to the resistance to dissolution of the hydrogels, resulting in higher I% values. In the FTIR spectra, it was observed that asymmetric and symmetric stretching bands of carboxylate groups (COO^-) moved to higher wave numbers with the addition of ECH, indicating that the carboxylate group is responsible for the crosslinking interaction of the polymers. These observations suggest interactions between polymers in the formation of the analyzed hydrogels.

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Innovations in Cassava Starch Processing: Dual Thermal Modification for Enhanced 3D Printing Capabilities and Potential in Bone Scaffold Fabrication

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The 3D printing process can be applied to develop precisely shaped biomaterials such as bone tissue regeneration. Starch as raw material, for example, can be used in tissue engineering to mimic bone tissue, facilitating osteoinductive cell growth. However, native starch hydrogels have limitations in terms of their mechanical and functional properties [1]. Intending to overcome these deficiencies, thermal modifications (dry heating treatment – DHT, and heat moist treatment – HMT) were applied, combined in different orders, for modifying cassava starch. The native starch was modified through DHMT and HMDT, with DHT step at 130 °C for 4 h, and the heat moist step conducted with adjusted moisture (27%) at 100 °C for 4 h. The modified starches were characterized by FTIR spectroscopy, and the granules morphology was analyzed by SEM. The starch hydrogels (inks) were prepared by the gelatinization of 10 % (w/w, d.b.) of starch at 85 °C for 30 min, and then stored (24 h, 4 °C). The viscosity of starch hydrogels was characterized by RVA, firmness by penetration assay using a texturometer (TA.XT Plus Instruments), and printability by image analysis of the printed samples using Image J software. Scaffolds based on these hydrogels were printed (BioedPrinterV4, BioEdTech - Brazil), freeze-dried, and characterized by XRD. Their mechanical properties were evaluated by compression tests, and the morphology and porosity by SEM. In general, the dual modifications (DHMT and HMDT) promoted oxidation and fractures in the granules, resulting in firmer hydrogels and porous materials. Finally, the combined methodology improved hydrogel printability and the final properties of the starch-based scaffolds, enhancing the potential of these source to be used in the production of bone scaffolds by 3D printing.

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In-situ growth of metal oxide nanoparticles on nanocellulose-based cryogel for biomedical applications

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In situ of metal oxide nanoparticles (NPs) rise as a valuable strategy to prevent aggregation, while ensuring well dispersibility and the production of functional hybrid polymeric nanocomposites with both compounds' properties [1,2]. This work investigated the potential generation of functional hybrid nanocomposite through the *in situ* synthesis of copper oxide (CuO) NPs on a cellulose nanofibrils (CNF)/natural rubber latex (NR) cryogel [3], using a wet chemical technique on a template-mediated synthesis. These substrates were incubated in $Cu(NO_3)_2$ under ambient conditions, and then subjected to reduction in an alkaline hydroxide sodium solution at 70°C for the same duration. The obtained hybrid nanocomposite (CuO20) presented well-dispersed particles throughout the matrix, as well as exhibited mechanically rigid characteristics and higher resilience in water. Its functionality was also evaluated in terms of antimicrobial activity. The viability assay and cell culture of sensitive (AmpS) and ampicillin-resistant (AmpR) *Escherichia coli* strains showed that only CuO20 inhibited the growth of both strains of *E. coli*, compared to the CNF/NR control. Therefore, we developed a functional hybrid material derived from renewable sources with promising applications in the biomedical field.

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INTERMOLECULAR INTERACTIONS INVOLVED IN THE STRUCTURING OF CELLULOSE AND ALGINATE BEADS WITH MAGNETITE NANOPARTICLES

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Attenuated Total Reflectance Fourier Transform Infrared Spectroscopy (FTIR-ATR) applied in Materials Science allows the recognition of functional groups and the observation of intermolecular interactions involved in the structuring of materials. This work compared experimental and summed FTIR-ATR spectra obtained from cellulose (CEL) and alginate (ALG) beads with magnetite nanoparticles (MAG) in order to seek relationships between band shifts and the intermolecular interactions involved. The MAG obtained by co-precipitation was dispersed (30% w/w) in the 3% (w/v) polymer solutions. CEL and CEL/MAG beads were prepared by dripping in sulfuric acid (H_2SO_4) (10% v/v) and ALG; ALG/MAG; CEL/ALG; CEL/ALG/MAG in calcium chloride ($CaCl_2$) (3% w/v). The FTIR-ATR spectra were obtained in the spectral range of 4000 to 400 cm^{-1}, resolution of 4 cm^{-1} with 16 scans and the sums were obtained by combining the spectra of pure materials. When adding MAG to the polymer matrix, shifts of the O-H bands to higher wavenumbers (between 3292-3331 cm^{-1}) were observed, when compared with the summed spectra (between 3222-3320 cm^{-1}), indicating that the interactions (hydrogen bonds) between polymer/polymer have weakened. These changes suggest that the functional groups of the polymers are involved in the interaction with the added MAG. Therefore, based on the functional groups present in the structure of the polymers and MAG and the displacements of the O-H stretches observed in the spheres' spectra, it is suggested that the materials are interacting via hydrogen bonds [1].

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Lignocellulosic hydrogel from the deconstruction of sisal fibers by bis(ethylenediamine)copper(II) hydroxide

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Bis(ethylenediamine)copper(II) hydroxide solution (CUEN) was used to deconstruct sisal fibers and create hydrogels from their macromolecular components. The deconstruction of sisal fiber in CUEN 1M was done by mixing 1 or 2 g of ground sisal fiber in 25 mL of distilled water and then adding 25 mL of CUEN. The solvent could dissolve cellulose and hemicelluloses, while lignin remained suspended in the medium. The viscous solutions were added to cylindrical templates immersed in a distilled water bath until the complete hydrogel formation by phase inversion. The hydrogels were named Sisal_{1hydro} or Sisal_{2hydro} according to the initial biomass amount. The hydrogels were characterized by scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FTIR), compressive properties, and swellability. FTIR analysis confirmed the presence of functional groups typical of cellulose, hemicelluloses, and lignin in both hydrogels. SEM images show that the lower biomass amount (Sisal_{1hydro}) generates smaller pores and higher porosity in the hydrogels. Young's modulus of the hydrogels was 30 KPa and 62 KPa for Sisal1hydro and Sisal_{2hydro}, respectively, indicating the direct effect of the hydrogel density in the compression properties. Sisal_{2hydro}'s superior performance can be attributed to its higher amount of lignin acting as a reinforcement than Sisal_{1hydro}. The water sorption content was 5076 % and 2686 % for Sisal_{1hydro} and Sisal_{2hydro}, respectively, indicating that the presence of a greater amount of the hydrophobic lignin in Sisal_{2hydro} negatively impacted this property. The hydrogels derived from the disintegration of lignocellulosic sisal fibers exhibited high water absorption and showed great potential as sustainable alternatives to petroleum-based hydrogels in various applications. They can offer a promising solution for the development of materials that are both cost-effective and performance-efficient.

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Modification of orange bagasse by reactive extrusion process

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The chemical and functional modifications caused by reactive extrusion, an eco-friendly process that generates little or no effluent, can adapt agro-industrial waste into raw materials for various applications. The aim of this study was to evaluate how the reactive extrusion process can modify orange bagasse (OB). For this purpose, raw OB and depectinized OB were processed in a single-screw extruder (initial moisture content 40% w/w); the modified materials obtained, named OB_E and OB_EP, respectively, were analyzed for cellulose, hemicellulose (by Van Soest method [1]) and lignin content and swelling capacity (SC) (Yoshimura et al. [2]). OB_E had 30.56% insoluble dietary fiber (6.28% cellulose, 9.08% hemicellulose, 15.20% lignin); the prior extraction of pectin in OB_EP facilitated the rupture of the lignocellulosic structure, leading to increases in cellulose (14.12%) and hemicellulose (12.36%) content. The SC values, which indicate changes in the polymer network, were 16 and 15 (mL water/g solid) for OB_E and OB_EP, respectively. SC is induced by physical forces drawing liquid into the polymeric matrix; materials with high SC can be used as sources of dietary fiber. According to the results, the extrusion process was considered an efficient method for modifying the lignocellulosic materials.

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Nanocomposites of thermoplastic starch reinforced with nanofibrillated cellulose: plasticization with glycerol in the presence of water as process plasticizer

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The use of nanocellulose fibers (NFC) [1] to reinforce thermoplastic starch (TPS) has been subject of research. However, the incorporation poses challenges due to the formation of aggregates when NFC dries and irreversible hornification[2]. Here we propose employing a combination of glycerol as a plasticizer for TPS and wet NFC, utilizing water as a process plasticizer in synergy with glycerol. The residual water in partially dried NFC acts as a process plasticizer and can be eliminated in the final product. The samples were prepared with a TPS matrix (corn starch/glycerol) in 70:30% and 80:20% ratios, using wet NFC with 15% and 25% residual water to achieve final dry concentrations of 2.5%, 5%, 7.5%, and 10%. Samples were processing utilizing a single-screw extruder (16 mm, L/D26) with a temperature profile set at 115°C, 120°C, and 110°C, from feeding to matrix. Extruded compounds were then hot-pressed into 2 mm films. Characterization included TGA for water content, tensile testing at 53% RH, and moisture absorption analysis. The results indicated that higher NFC content led to increased Young's modulus and tensile strength, but decreased elongation, as well as reduced moisture absorption in samples. The elasticity modulus of samples 70/30% and 80/20% with NFC concentrations of 0% to 10% were 20 MPa, 30 MPa, 29 MPa, 32 MPa, 65 MPa, and 28 MPa, 44 MPa, 76 MPa, 335 MPa, and 1000 MPa. Samples containing 15% and 25% residual water visually exhibited homogeneity without signs of agglomerates, mechanical properties satisfactorily demonstrated the reinforcing effect of the fibers.

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Obtention of cellulose-rich materials from orange bagasse

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Orange bagasse (OB), an agro-industrial waste, is a renewable raw material that has been little exploited for cellulose extraction. The present research aimed to obtain cellulose-rich materials from OB using two different combinations of chemical and physical treatments. The OB was dried, ground and treated with NaOH 2% w/v or HCl 2% w/v combined with an autoclaving process 121°C for 30 min in the OB:liquid ratio (1:15 w/v). From the solid fraction obtained, cellulose, hemicellulose (Van Soest method [1]) and lignin were measured. The relative crystallinity index (CI) was based on the method of Segal *et al.* [2]. The raw OB presented 28.8% insoluble dietary fiber content (12.4% cellulose, 7.5% hemicellulose, 8.9% lignin). After the alkaline and acid treatments, the cellulose content increased significantly to 53 and 42% respectively. Alkaline extraction breaks the ester and hydrogen bonds between the components of the lignocellulosic matrix. Higher hemicellulose (10.2%) and lignin (17.3%) contents are also observed, due to the elimination of the non-lignocellulosic fraction. The CI evaluates the removal of amorphous components; raw OB had a CI of 18%, which increased to 49 and 40% with alkaline and acid treatment, respectively. The treatments used in one-step were effective in obtaining cellulose-rich materials, reducing the environmental impact and overall costs of the process.

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Optical and barrier properties of films based on carrageenan (kappa) and beeswax.

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The widespread production of conventional plastics and their use in different commercial applications, such as the manufacture of packaging, represent a threat to the environment since the plastic waste generated is not easily degraded and accumulates in planetary systems. Marine macroalgae appear in this context as a renewable natural resource and a sustainable source of raw materials that can be used to make biodegradable films and packaging for food preservation, largely due to the availability of polysaccharides in their structures. Carrageenan is a sulfated anionic polysaccharide derived from red marine algae (*Rhodophyceae*). It has a high molecular weight, with an average molecular mass of 100 and 1000 kDa. This study aimed to develop and characterize biopolymeric films based on kappa carrageenan and beeswax, using a simplex-centroid quaternary experimental design (carrageenan, beeswax, glycerol, and tween 80) in different proportions, divided into 17 treatments, calculated as 2% dry mass and 98% solvent (carrageenan, ranging from 45-90%; beeswax, from 0 to 50%; glycerol from 5 to 25% and tween 80, from 5 to 25%). The optical and barrier properties of the films were analyzed. The water-related properties of the carrageenan-based films (water vapor permeability rate and solubility) were improved with the introduction of beeswax. The water vapor permeability rate was reduced with the addition of beeswax, making the film more hydrophobic and consequently reducing solubility. Adding 25 and 50% beeswax to the biopolymer matrix resulted in a lower water vapor permeability rate and solubility of the films, making it a valuable resource for use as a coating in preserving fruit and vegetables.

Optimization of ZnO Properties through Temperature Variation and Modification with Natural Polymer

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The application of photocatalytic technology emerges as a promising solution to address environmental challenges [1,2]. This study focuses on the sustainable enhancement of ZnO properties. ZnO was functionalized with a natural polymer through the co-precipitation method, varying temperatures during synthesis. We investigated the effect of these temperatures on the morphology, optical properties, and photocatalytic performance of the material. Morphology was characterized by scanning electron microscopy (SEM), while optical properties were evaluated by diffuse reflectance spectroscopy (DRS), with emphasis on calculating the bandgap. Additionally, photocatalytic tests were conducted to assess the degradation of a model pollutant under ultraviolet irradiation. The results revealed an optimal temperature that maximizes photodegradation efficiency, highlighting the promising potential of modified ZnO as a photocatalyst. These findings significantly contribute to the advancement of wastewater treatment techniques, providing a more sustainable and effective approach.

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Optoelectronic noses based on starch films for food spoilage monitoring in smart packaging

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The optoelectronic nose, also known as a colorimetric sensor array, is made up of chemosensitive dyes embedded in a solid substrate. This setup allows the contact of device with the volatile compounds in the sample's headspace. Traditionally, substrates such as polymeric membranes or paper-based materials have been used, but they require time-consuming preparation steps, the use of toxic solvents, and are limited to single-use applications. We present a reversible optoelectronic nose prepared with ten acid-base indicators embedded in a starch-based film that covers a wide pH range. The starch substrate has several advantages, including odorlessness, biocompatibility, flexibility, and high tensile strength. We used this optical artificial olfaction system to detect the early stages of decomposition in three different food products: beef, chicken, and pork. The system recorded color changes caused by intermolecular interactions between each dye and the emitted volatiles over time, using a smartphone. These digital images were then processed to generate a differential color map, which resulted in a unique signature for each food product based on observed color changes. To improve discrimination between different samples and exposure times, we used chemometric tools like hierarchical cluster analysis (HCA) and principal component analysis (PCA). This analytical approach for detecting food deterioration is practical, cost-effective, and user-friendly, making it ideal for smart packaging applications. Furthermore, the use of starch-based films in the food industry is favored due to their biocompatibility and biodegradability properties. These features make it a promising candidate for developing efficient and reusable optoelectronic noses for volatile compound analysis.

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Orange Essential Oil Encapsulation in Chitosan Nanoparticles

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Orange essential oils (OEO) have antioxidant, antimicrobial, and anti-inflammatory characteristics, which can benefit well-being [1]. OEO nanoencapsulation may protect and enhance the characteristics of essential oil due to its volatility and sensitivity to environmental factors. Here we investigate the encapsulation of commercial OEO in chitosan nanoparticles (Cs). Chitosan was obtained by fermentation of molasses, and its bioextraction process was developed in collaboration with the LAMAN laboratory at CCA/UFSCar [2]. Chitosan nanoparticles were obtained by ionic gelation method [2]. Dynamic Light Scattering (DLS) data showed Cs nanoparticles ranging between 437-529 nm and zeta potential (ZP) value in -25.2 mV that present reasonable stability and a low tendency to form agglomerates [3]. OEO-Cs encapsulation was also obtained using the ionic gelation method. OEO 3% (w/v) was mixed with 10 mL of Cs 5% (w/v) suspension in an aqueous medium, stirred overnight, and dried in an oven at 50 °C for 24 h [2]. DLS results showed OES-Cs particles ranging from 194 to 455 nm and ZP of -3.54 mV., indicating that the nanoparticles have a strong tendency to agglomerate, verified by FEG [3]. FTIR data showed that the chitosan nanoparticles are impregnated with OES, as the intensity of the bands increased in a region between 2920 cm-1 to 2871 cm-1, indicating the aliphatic part of these oils, as well as a change in the bands in the amide region, which changed from 1640 cm-1 to 1654 cm-1, indicating interactions with OES. More experiments will be in processing. Essential oils extracted by different citrus cultivars will be tested with chitosan nanoparticles.

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Pectin as a cement additive

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The use of materials derived from plant waste has emerged as a promising alternative for the sustainable development of the cement industry[1, 2]. In this context, biopolymers have stood out; pectin, for example, is one of the main components of plant cell walls, which makes them an abundant material that can be extracted from a wide variety of plant products, allowing their use in different locations as well as low-cost[1, 2]. As it is a polysaccharide, pectin is a polyelectrolyte that interacts strongly with water, making it an attractive additive. This interaction changes the conventional hydration routes and curing kinetics of cement pastes, thus affecting the properties of the final composites. The interaction also occurs with other substances present in the cement, such as calcium ions. This study evaluated the impact of different concentrations of additives (1% and 3% w/w) on the behavior of high initial strength Portland cement pastes. The additive initially improved the paste's workability, while oscillatory tests showed an increase in storage modulus compared to the unadditivated paste. The additive modified the classic cement hydration pathways by altering the rheology of the added paste. Associated with these changes, the low cost of pectin makes it a promising option for adjusting the properties of cement pastes, highlighting its potential as an effective and environmentally friendly additive.

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Pharmacokinetic study of the controlled drug release system composed of curcumin encapsulated in chitosan biopolymer/polysaccharide and carried by "green" iron oxide (Fe_3O_4) nanoparticles

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Problem: Curcumin comes from turmeric (*Curcuma longa*) and is antioxidant, anti-inflammatory, antitumor, antimicrobial and antiparasitic, has a low cost and no side effects, making it a potential drug [1]. However, curcumin is unstable and insoluble in water [1]; **Solution:** A controlled drug release system can improve the properties of curcumin [1,2]. Fe_3O_4 nanoparticles are biocompatible and interact with magnetic fields and chitosan is a biopolymer and polysaccharide that can encapsulate curcumin, increasing its stability and solubility and improving the dispersion and oxidation of Fe_3O_4 [1,2]. Thus, this work aims to produce a curcumin release system encapsulated in chitosan and carried by “green” Fe_3O_4; **Methodology:** “Green” Fe_3O_4 was synthed by Green Chemistry, with Fe^{+2}, english potato peel (*Solanum tuberosum*) and sodium carbonate [3]. The system was produced from chitosan in acetic acid, Fe_3O_4 “green”, curcumin in acetone, EDC and NHS [2]. The characterization techniques were: XRD, SEM, FTIR, TG/DTA, PZ/DLS and RAMAN [2]. The controlled release was carried out over 27h with 25mg of the system and 2mL of PBS, 1mL aliquots were collected in 1h-1h and replaced with 1mL of PBS and the concentration of curcumin released was determined by UV-vis [2]. Pharmacokinetics was performed with the models: zero and first order, Korsmeyer-Peppas and Hixson-Crowell [2]; **Results and discussion:** The characterization techniques confirmed the production of the system. Pharmacokinetics determined that in the first six hours most of the curcumin was released, reaching an equilibrium at 0.20 g L-1, thus, Korsmeyer-Peppas was the model that best fit, characterized by diffusion [2]; **Conclusion:** The system has the potential to be applied in the treatment and prevention of diseases.

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Poly (butylene adipate-co-terephthalate)-based nanocomposites reinforced with functionalized renewable materials

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The growing concern over the environmental ramifications of petroleum-based plastic packaging has increased the exploration of sustainable and cost-effective bionanocomposites. Despite this, challenges persist, notably due to the divergent processing behavior and mechanical-physical characteristics of some biopolymers when compared to traditional polyolefins.1 In an effort to overcome these hurdles, this study explored the incorporation of natural rubber latex (NR) compounded with cellulose nanocrystals (CNCs) into poly (butylene adipate-co-terephthalate) (PBAT) matrix.2 The PBAT matrix containing nanofiller demonstrated good processing scalability in the co-extruder, producing continuous, planar, and transparent films without the need for any organic solvents. These films exhibited enhanced physical barrier properties against water vapor and improved mechanical behavior, becoming less anisotropic in terms of the orientation of PBAT chains during film formation. Preliminary biodegradation tests of the films indicated that the NR-CNCs fillers do not interfere in the biodegradation of the PBAT, thereby maintaining the nature characteristics of the biopolymeric matrix. Such findings underscore the potential of these nanocomposites for food packaging applications, aiming to develop materials distinguished by their superior physico-mechanical properties, biodegradability and commercial feasibility.

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Potato and cassava starches modified by green technology ozonation to improve processability in additive manufacturing; production of potential bone scaffolds

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The additive manufacturing of bone scaffolds from this modified polysaccharide is innovative, combining sustainable approaches with its well-known biocompatibility and better processability [1,2]. Ozonation, a green technology, improves the functionality of native starches through chemical and structural modifications [3]. Against this backdrop, this study sought to assess the potential for applying ozonation to potato and cassava starches to improve 3D printing processability and final properties of potential bone scaffolds. The starches were modified by ozonation (30 min, 10 % m/m, 50.8 g/m^3 O_3 (g)) and characterized by SEM, XRD, and FTIR-ATR. The hydrogels based on the native and modified starches (10% w/w, d.b.) were evaluated in rheology and printability (ImageJ analysis). The scaffolds were printed (3D extrusion printing BioedPrinterV4, BioEdTech - Brazil), freeze-dried and its mechanical properties (compression tests by texturometer) were characterized. The results showed that the ozone-modified potato and cassava starches showed no change in morphology, a reduction in relative crystallinity, and FTIR bands corresponding to oxidation signals. The hydrogels based on the modified starches showed a predominantly elastic rheological character which resulted in inks with better printability. In addition, the bone scaffolds based on the modified starches had a higher compressive strength. Finally, it was noted that potato starch had greater potential for application in 3D printing than cassava starch. In addition, this work shows that the process of modifying starch by ozonation is an interesting alternative for functionalizing these biopolymers, improving their potential for use in bone tissue engineering.

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Potential active CMC/NPQ biofilm with rosewood for packaging

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Significant quantities of food are discarded due to microbiological deterioration. This problem can be mitigated through adequate packaging, extending the shelf life of food, and reducing product waste. Growing environmental concerns associated with plastic waste highlight the need for innovative, biodegradable polymers. In this context, our research proposes the study of carboxymethylcellulose (CMC)/chitosan biofilms, enhanced with rosewood oil nanoemulsion (RO), as a potential solution for food packaging, offering a promising avenue to combat food waste. The chitosan nanoparticles (QNP) were successfully synthesized using the ionotropic gelation technique in acid acetic solution and TPP (sodium tripolyphosphate, crosslinking agent). The casting technique prepared the resulting CMC/QNP/RO biofilms in different concentrations. DLS analysis revealed the nanoparticles to be within the electrical stability value, with particle s (134nm to 215nm) and zeta potential (29 mV and 44 mV). As detected by FTIR peaks, crosslinking of chitosan chains with phosphate bridges was successfully carried out. Chemical compounds were identified and quantified in RO, and its majority component was the linalool (96%). In a previous study, RO presented active action against P. aeruginosa, E. coli, and S. aureus. The films FTIR indicated the formation of bonds between the polymer chains, as evidenced by a decrease in the intensity of the absorption peaks. The thermal analysis results demonstrated the films' thermal stability up to around 300ºC. This high thermal stability is a significant advantage for active packaging, as it ensures the biofilms can withstand the heat during food processing and storage. The mechanical tests revealed results concerning maximum stress (38MPa to 42MPa), elongation at break (7% to 12%), and elasticity modulus (869MPa to 1165MPa). These results indicate the biofilms' potential to maintain their integrity and protect the packaged food from physical damage.

PREPARATION BLEND CHITOSAN/POLI-(N-VINYLCAPROLACTAM) FILMS

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Poli(N-vynilcaprolactam) is a polymer derived from an available commercial monomer, N-vynilcaprolactam, obtained by radical polymerization, biodegradable and bioabsorbable, and an example of a thermosensitive polymer with a lower critical solubility temperature (LCST) in water close to human body temperature, between 32 and 36°. Due to this biofunctional behaviour, PNVCLs find numerous biomedical applications, similar to chitosan (CS) ((1,4)-2-amino-2-deoxy-β-D-glucan), a biopolymer widely used as a pH-sensitive carrier for drug delivery in the pharmaceutical and biomedical fields due to its biocompatibility, biodegradability and non-toxicity. Copolymers of these materials have already been investigated for the formation of dual-stimulus responsive materials for controlled drug delivery. However, another strategy in materials science is the preparation of polymer blends. In this work, films of CS/PNVCL were prepared to obtain a biocompatible material with better mechanical properties and a dual-stimuli-responsive that can be explored in biomedical applications. For this purpose, PNVCL was synthesised by radical polymerisation in DMSO from the NVCL monomer, in an inert atmosphere, for 4 h at 70°C, using AIBN as initiator. The blends were prepared by mixing (1:1) aqueous solutions of PNVCL and CS in acetic acid with stirring for 24 hours. This mixture was dried in a polypropylene Petri dish for 7 days at room temperature to form films. The films were analysed and tested to determine their morphological, structural and physicochemical properties. Blended CS/PNVCL films were obtained with better mechanical properties, such as less brittleness and better toughness than pure PNVCL. In addition, CS/PNVCL retained temperature and pH-responsive properties important for biomaterial applications.

PRODUCTION OF CELLULOSE/PVOH AND CHONDROITIN SULFATE MEMBRANES BY ELECTROSPINNING

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Electrospinning is a promising technique for producing biocurative membranes, utilizing cellulose (cel), polyvinyl alcohol (PVOH), and chondroitin sulfate (SC) 1. The aim of this study was to develop a method for producing fibers through electrospinning from a solution of cel/PVOH/SC subjected to different aging times in 98% trifluoroacetic acid (TFA). Initially, aging was studied at 1 h, 24 h, 48 h, 7 days, and 10 days for a 5% (w/v) cellulose solution. The viscosity of the cellulose solution was determined, and Fourier-transform infrared spectroscopy (FT-IR) of the regenerated cellulose was performed. The viscosity of the cellulose solution decreased as time increased; however, even with the viscosity reduction, it was not possible to form fibers with the pure cellulose solution in TFA. Infrared results showed that the cellulose membranes did not contain residual trifluoroacetylated cellulose. Solutions of cel/PVOH/CS (40/40/20 (w/w)%) at 5% (w/v) were prepared and aged for 24 h, 7 days, and 10 days. All cel/PVOH/SC solutions were suitable for electrospinning. The fibers were analyzed by scanning electron microscopy (SEM) and FT-IR spectroscopy. Fiber formation with diameters of 0.66 µm, 1.02 µm, and 0.73 µm was observed with increasing aging time. Infrared technique demonstrated that the presence of PVOH hindered the regeneration of trifluoroacetylated cellulose into cellulose. This study paves the way for the development of new methodologies for producing electrospun materials based on cel/PVOH/SC.

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Removal of synthetic dye by cellulose microfibers/copper nanoparticles: the adsorption investigation

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Synthetic dyes are widely used in the food industry to enhance the attractiveness of foods. However, their use has been linked with carcinogenesis, fetal abnormalities, and fertility problems[1]. Also, improper disposal can cause environmental damage, as in the Santa Cruz stream[2]. Aiming to remove dyes from aqueous media, a new substrate based on cellulose microfibers and copper nanoparticles (CMF/CuNPs) is being studied. Cellulose microfibers were obtained from sugarcane bagasse, and then copper was reduced *in situ* to form the CMF/CuNPs hybrid material[3]. The nickel tetrasulfonated phthalocyanine (NiTsPc) probe molecule was chosen for the adsorption study. Its anionic character represents a facilitator for adsorption on CMF/CuNPs, with a positive Zeta potential (+11.5±0.2 mV). For removal tests, CMF/CuNPs was added into NiTsPc solution in different concentrations. After 10 minutes, the suspension was centrifuged for 10 min and 10^4 rpm. UV-Vis absorption was used to evaluate the removal efficiency (%R). At initial concentration of 10^{-4} and 10^{-5}mol/L of NiTsPc, the removal efficiency was 61.7±0.4 and 100%, respectively. The adsorption isotherm fits in a Freudlich model, which describes a multilayer adsorption. At the higher tested concentration the adsorption capacity was Q=66.01±0.4 mg/g. Raman spectroscopy by SERS effect allowed to confirm the adsorption by the NiTsPc detection until 10^{-7} mol/L, showing the characteristic peaks at 755, 1341 and 1559cm^{-1} , presenting only electrostatic interaction. In conclusion, the CMF/CuNPs substrate shows high removal efficiency of NiTsPc at lower concentrations in aqueous media.

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Silk Fibroin Aerogels with Shape Memory through Freeze-thaw Cycles

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Fibroin is used in several applications, such as hydrogels and aerogels [1]. Aerogels, produced by controlled freezer-thaw cycles, improve the physical properties of polymeric materials, serving as physical crosslinking [2]. Kolahreez and Morshed [1] produced shape memory sponges, indicating the need to investigate the material's behavior under freeze-thaw cycles. Therefore, this work evaluates the impact of freezing and drying methods on sponge stability. The fibroin solution was molded into a cylindrical mold and subjected to freezing cycles for 24 hours, at -20°C and -80°C, followed by thawing at 4°C for 24 hours. The number of freeze-thaw cycles (1, 2 and 3) was investigated. Freeze-drying and supercritical drying with CO_2 were performed to evaluate structure preservation. They were characterized by evaluating their properties. They exhibited shape memory and were able to return to their original shape and after several compression cycles when fully hydrated. Moreover, water absorption was the key mechanism for shape memory. Detailed analysis provides a comprehensive understanding of its mechanical strength properties and material morphology as it covers numerous areas [2][3]. The versatility of the shape memory of the developed gels expands knowledge in the area and can find several applications.

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STRUCTURE AND MECHANICAL PROPERTIES OF HYDROXYPROPYLATED STARCH FILMS

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Hydroxypropylation has been widely studied as a form of chemical modification of carbohydrates and to obtain lignocellulosic biomass-based polyols. In this work, we study the formation of hydroxypropylated starch films in order to decrease moisture absorption and delay its retrogradation, due to the graftization of bulky hydroxypropyl groups in the starch chain [1,2]. Gelatinized cassava starch was obtained through the hydroxypropylation reaction performed in an autoclave reactor, varying temperatures of 115 and 135 °C and molar ratios of 0.4 and 0.8 [PO/OHstarch]. X-ray diffraction analysis (XRD) was performed in a PANalytical X'Pert Pro MPD, from 5 to 50°, with a wavelength of 1.5418 Angströms by the CTMC – CERMAV-CNRS laboratory. The tensile tests of films were carried out in an Instron model 5165 equipment, at a speed of 5 mm/min in the LGP2 laboratory – PAGORA. Previous results showed that the starch was gelatinized during the reaction related to heating and the presence of propylene oxide, which acted as a plasticizer for the starch chains. XRD results showed that the hydroxypropylated starch films started to retrograde before the control sample showed the native starch control. In addition, the mechanical properties obtained demonstrate that the modification promoted greater plasticization of the material, through significantly higher elongation values at break, emphasizing that the presence of polyol molecules are playing a role in starch’s structure.

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Study of Properties of PLA Filaments with Oxide Modified and a Natural Polymer for 3D Printing

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The 3D printing technology has emerged as an innovative approach for manufacturing materials with antimicrobial properties. In this study, Polylactic Acid (PLA) filaments were synthed by combining PLA with a modified oxide produced by co-precipitation with the addition of a natural polymer [1–3]. Characterization of the filaments using techniques such as thermal analysis (TG/DTG) revealed increased thermal stability with the addition of the oxide, while scanning electron microscopy (SEM) showed alterations in the morphology of the samples. Furthermore, antimicrobial activity tests demonstrated a proportional increase in incorporated oxide. These results confirm the viability of these filaments for use in 3D printing of materials with antimicrobial properties and highlight their potential impact on the industry, thereby contributing to the advancement of technology in this emerging field.

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Study of the chemical composition of agricultural waste ash from the perspective of a source of nutrients for agriculture

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Using biomass to generate energy in plants produces ash that tends to be discarded inappropriately, thus losing valuable components that could be returned to the environment and used to fertilize plants and/or enrich the soil in nutrients [1]. Using biomass ash as fertilizer is considered one of the most sustainable means of disposal [2]. Examples of organic waste include rice grain husks, sugar cane, and cashew nut husks. This study aims to analyze the chemical composition of ash and its use as a source of nutrients. Fluorescence analysis was used to study the ash. Data obtained from the literature demonstrated an average of 1.276% P2O5 and 2.268 of K2O5 for rice husk ash, 1.172% P2O5 and 2.176% K2O5 for sugar cane bagasse ash; 3.480% P2O5 and 12.918% K2O5 for cashew nut shell ash. The results after fluorescence analysis of this study were 0.869% P2O5 and 1.135% K2O5 for rice husk ash; 1.098% P2O5 and 1.498% K2O5 ash from sugar cane bagasse; 3.168% P2O5 and 75.059% K2O5 for cashew nutshell ash. Thus, it is inferred that the ash fluorescence results obtained in this study are within the estimable range and suitable for use as a source of nutrients.

Study of water sorption on porous vegetable cellulose membranes prepared by the salt leaching method

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Porous biomaterials cover a range of materials, whether they are natural, synthetic, or hybrid, all with the potential to demonstrate biological functionality [1]. With this in mind, the study aims to develop sustainable and porous biomaterials from vegetable cellulose (CEL) using the salt leaching method. CEL membranes were dissolved (5% w/w) in copper(II) bis(ethylenediamine) hydroxide and calcium carbonate (CaCO3) (Vaterite) was added to obtain samples (w/w): 1:4 (CEL/CaCO31:4) and 1:6 (CEL/CaCO31:6). The mixture was stirred for 1 hour, spread on a petri dish and then dried for 24 hours at room temperature. After this time, the membranes were regenerated in 5% sulfuric acid for 50 minutes, washed 4 times with distilled water (until pH ~ 5) and then dried for 24 hours. The membranes were characterized using infrared spectroscopy (FTIR) and water sorption kinetics. The interaction of water with cellulose and the effect of salt proportion on cellulose structure were evaluated using FTIR. The swelling kinetics data of all membranes are fitted to the nonlinear pseudo-first-order model, in which the swelling speed is proportional to the number of active sites. Using the parameter n of the Korsmeyer-Peppas equation it was found that the diffusion of water in membranes follows a quasi-Fickian behavior. Quantitative evaluation of the models was carried out by comparing the correlation coefficients (R2), experimental qe with the qe obtained by modeling and root mean square error (RMSE).

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Synthesis of bio-based polyurethanes using cellulose and lignin as polyols with simultaneous film formation: incorporation of SiO_2 nanoparticles for antibacterial properties

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In the past few decades, there has been a growing interest in using lignocellulosic biomass to develop sustainable materials that can replace those made from fossil sources. Under this scenario, this study aimed to synthesize bio-based polyurethanes with simultaneous formation of films with SiO_2 nanoparticles incorporated, looking for antibacterial properties[1]. Renewable polyols sources such as castor oil, microcrystalline cellulose[2], and kraft lignin[3] were used along with an isocyanate resin. SiO_2 nanoparticles formed from a biotechnological route were incorporated into the films by adding them to the reaction mixture while stirring or using an airbrush right after the reaction mixture was spread on a glass plate. Neat films were formed for comparison purposes. The films were characterized via infrared spectroscopy, thermogravimetric analysis, tensile properties, contact angle, and antibacterial properties. This study is in progress, and preliminary findings have demonstrated good properties and identified the direction to be pursued to enhance antibacterial activity.

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Synthesis of bio-based polyurethanes with simultaneous formation of composites reinforced by coconut and sisal fiber mats

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The present study aims to contribute to replacing fossil sources with renewable ones in forming polymer matrix composites. Bio-based polyurethanes were synthed, in the absence of solvents and catalysts, using as polyols ricinoleic acid triglyceride (the main component of castor oil) and lignosulfonate (obtained from wood) in addition to an aliphatic source of isocyanate groups. Mats composed of sisal or coconut lignocellulosic fibers were used as reinforcement. Mats and reagents were inserted into molds and the synthesis and formation of composites co-occurred under heating and compression. For comparison purposes, an unreinforced polymer was obtained under conditions similar to those of the composites. The results indicate that the syntheses were completed successfully, as demonstrated by the materials formed and the excellent thermal stability of the neat bio-based polyurethane and composites, as shown by thermogravimetric analysis. The study is ongoing, with the perspective that materials with good resistance to impact and flexion were formed, meeting the expectations of creating sustainable and environmentally sound materials.

Thermoplastic starch reinforced with short sisal fibers

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Thermoplastic starch (TPS) is a renewable and biodegradable material that aligns with the current sustainable trend. However, it is crucial to enhance the mechanical properties of TPS-based materials to replace materials derived from fossil sources with TPS [1]. The present study aims to investigate the impact of reinforcing TPS (Mater-Bi EI51NO) using short sisal fibers (2mm) on its properties. To achieve this, TPS mixed with sisal fibers was processed using a Gelimat machine at 130-150°C temperature and then through an injector. The injector was operated at various temperatures (120, 125, 130, 135, and 145°C) with a flow of 8.0 cm3/s and a pressure range of 300-500 bars. Here, results of flexural properties are reported specifically. The study found that adding fibers to TPS increased its flexural strength. Specifically, the strength increased by approximately 63%, 83%, and 106% when 20wt%, 30wt%, and 40wt% of fibers were added, respectively. However, when 50wt% of fiber was used, the strength decreased compared to 40wt% fiber, from 106% to 71%. From 50% onwards, the dispersion of fibers within the material will probably become more difficult, favoring agglomerations, which can negatively impact flexural strength. Adding 20wt%, 30wt%, 40wt%, and 50wt% of fibers increased the flexural modulus; at 50wt%, there was no significant change compared to 40wt%. The deformation decreased as the fiber percentage increased, with a reduction of about 180% at 40wt% and 50wt%. The addition of fibers increased the material's stiffness, resulting in greater resistance to deformation. Highly renewable TPS matrix composites were successfully produced, exhibiting good flexural properties. This is an ongoing study. Following the flexural tests, impact and tensile strength tests will be carried out.

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Treating atopic-dermatitis-like skin lesions in mice with gelatin-alginate films containing 1,4-anhydro-4-seleno-d-talitol (SeTal)

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This study investigated the encapsulation of 1,4-anhydro-4-seleno-d-thalitol (SeTal), a bioactive seleno-organic compound, in gelatin and alginate (Gel-Alg) polymeric films as a strategy for improving the treatment and attenuation of atopic dermatitis (AD) like symptoms in a mouse model [1]. Hydrocortisone or vitamin C were encapsulated with SeTal in the Gel-Alg films, and their synergy was investigated. All the prepared film samples were able to encapsulate and release SeTal in a controlled manner. A series of in-vivo/ex-vivo experiments were performed using mice sensitized with dinitrochlorobenzene, which induces AD-like symptoms [2]. The long-term topical application of the loaded Gel-Alg films was found to be highly effective in attenuating disease symptoms and pruritus, suppressing the levels of inflammatory markers, oxidative damage, and skin lesions associated with AD [3]. Moreover, the loaded films demonstrated superior efficiency in attenuating the symptoms analyzed compared to hydrocortisone cream, a traditional AD treatment.

Keywords: Skin diseases; 1,4-anhydro-4-seleno-D-talitol; hydrocortisone; vitamin C; biomaterials.

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Utilization of Cassava Gum to Produce Microcapsules for Agricultural Applications

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Sustainable agricultural practices emerge as alternatives to address environmental issues[1]. Some plant-associated microorganisms promote plant health and growth using various mechanisms[2,3]. This study aimed to synthe cassava gum-based hydrogels for the microencapsulation of microorganisms. The technique of ionotropic gelation and Spray dryer were employed to form microspheres. Microscopic analysis of the spheres produced by ionotropic gelation revealed a spherical morphology with some cracks and porosity. Meanwhile, particles produced by the Spray dryer exhibited high roughness due to the drying process. The production of microcapsules with cassava gum proved effective, offering a promising alternative for agricultural applications in microorganism encapsulation.

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BS05-Nanomaterials for Medicine Application and Nanotoxicology

Nano-bio Interface Probed by Synchrotron Radiation

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The field of nanotechnology has opened up new frontiers in our understanding of biological systems, offering unprecedented opportunities for biomedical research and materials science applications. This new field called nano-bio interface considers nanomaterials interacting with biological entities, ranging from individual biomolecules to complex cellular structures. This seminar will explore the interplay between nanotechnology and biology, primarily focusing on elucidating nano-bio interactions using synchrotron radiation techniques as powerful probes for investigating this complex dynamic. For example, nano-tomography enables three-dimensional imaging of nanostructures within biological samples (specifically mammalian cells), providing invaluable insights into their spatial organization and morphology. Also, nano-infrared spectroscopy, which can probe molecular vibrations at the nanoscale, offers a unique window into the chemical composition and dynamics of nanomaterials interacting with biomolecules (in the specific case, Gram-negative bacteria) [1]. Additionally, small-angle X-ray scattering (SAXS) provides crucial information on nano-bio complexes' structural arrangement and conformational changes. For this latter case, the SAXS technique can selectively investigate unspecific protein adsorption on nanoparticles [2,3]. It will be shown how these advanced synchrotron techniques can be used to unravel the mysteries of the nano-bio interface. This deeper understanding holds immense promise for advancing various biomedical applications, such as drug delivery systems, biosensors, and tissue engineering. Acknowledgements:

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Theranostics combined hyperthermia treatment and micro-CT imaging in osteosarcoma 3D models

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Superparamagnetic Iron Oxide Nanoparticles (SPIONs) hold immense potential in theranostic medicine, seamlessly blending diagnostic and therapeutic capabilities within a single adaptable framework. In this study, aminosilane-functionalized SPIONs were employed to examine the impact of magnetic hyperthermia on SAOS2 osteosarcoma cells cultivated within a 3D spheroid model. The distribution and behavior of iron nanosystems were examined using micro-CT imaging techniques. The osteosarcoma 3D models were exposed to varying SPION concentrations, followed by multiple cycles of magnetic field application to assess the cumulative effects of hyperthermia on the tumor. The results revealed a substantial uptake of iron nanoparticles by the tumor cells, accompanied by a progressive reduction in tumor after consecutive cycles of magnetic hyperthermia, with notably more pronounced effects observed at a concentration of 300 µg/mL. Micro-CT analysis indicated that after the initial application of the magnetic field, there was an increase in the volume occupied by nanoparticles within the spheroid. However, this increase was not observed in subsequent cycles, indicating potential particle movement that may complement the effects of magnetic hyperthermia. These findings underscore the potential of aminosilane-functionalized SPIONs in therapeutic applications, showing the SPIONs' capability to reduce tumor through magnetic hyperthermia, while also demonstrating a dynamic behavior within the tumor microenvironment. Such insights hold promise for advancing theranostic approaches, harnessing SPIONs for precise therapy and diagnostic imaging in oncology.

Thermoluminescent nanosensor for real-time monitoring of thermal therapy

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Thermal therapy is well established in the clinic when combined with radiotherapy/chemotherapy and has potential for immunotherapy. One of the great challenges for the success of the therapy is monitoring the heat delivery (non-invasively and in real-time). In the clinic, the gold standard protocol is the proton resonance frequency shift (PRF) MRI thermometry method, but not all thermal therapy modalities are MRI compatible, like magnetic nanoparticle hyperthermia (MNH). Luminescent thermometry has been suggested as a possible alternative. Here we developed a thermoluminescent liposome and demonstrate its application as a near infrared luminescent thermometer. The liposome contains the theranostic lipophilic heptamethine dye IR780. Dynamic light scattering revealed a hydrodynamic diameter on the range of 80 to 120 nm (depending on the preparation) with a PDI around 0.3. IR-780 was incorporated through two processes, pre-insertion, or post-insertion. The amount of the dye tuned the zeta potential of the nanoparticle. The functionality of the nanothermometer is proved for two thermal nanomedicine cases, photothermal therapy (PTT) and MNH. For PTT the sensor is also the heat agent, while for MNH magnetic NPs are generating heat while the thermoluminescent liposomes are detecting the environment temperature variation in real-time. Thermal sensitivities around 4% per degree are reported, while repeatability values close to 0.95 are found. Samples with different ratio of the lipid to the IR-780 dye are investigated. We found a mean photothermal conversion efficiency of 15%, estimated using Roper's method. We also show that the multifunctional nanocarrier has application for in vivo fluorescence molecular tomography and as a photothermal agent. In addition, we report PTT inside a pre-clinical 1T MRI equipment, that is monitored in quasi real-time using the PRF-MRI thermometry. The results demonstrate the theragnostic applications of the lipid-based nanoparticle.

Attenuating *in vitro* keratinocyte inflammation through Quinizarin-loaded nanocapsules with Photodynamic Therapy and analysis of permeation in a 3D bioprinted skin equivalent

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Keratinocytes contribute directly to the immunopathogenesis of skin inflammation, triggering a range of immunological responses. Chronic skin diseases, such as psoriasis, are characterized by the hyperproliferation of keratinocytes, which are responsible for the development of the characteristic skin lesions [1,2]. Still, there aren't any highly targeted medicines, being ideal for the development of more specific therapies in this field. In this project, nanocapsules containing Quinizarin (NC/QZ) were developed, evaluating their action in a model of the keratinocytes inflammatory process in vitro with the action of Photodynamic Therapy, as well as analyzing the permeation in a 3D skin model as a substitute for the use of 2D and animal models. Physicochemical analysis, stability, cytotoxicity assays, internalization and permeation in a 3D skin model were carried out. The quantification of cytokines was also executed, evaluating the joint action of nanotechnology and PDT. Promising results were obtained, where the nanocapsules showed desirable physicochemical characteristics and were stable during the analysis period, with a high degree of quinizarin into the system, without spectroscopical modifications in UV-Vis. The cell viability assay was carried out with NIH/3T3 and HaCaT cell lines, showing cytotoxicity only in the highest concentrations. The nanocapsules in their empty form (NC/unloaded) and free QZ showed no cytotoxicity at the tested concentrations. The permeation and cellular uptake studies showed the permeation of NC/QZ in 3D skin models and the intracellular incorporation and internalization of the drug, respectively, enhancing its action in the drug delivery technique. The in vitro inflammatory process was developed, with subsequent application of PDT and immuno-enzymatic analysis, in which it was possible to observe representative effects of PDT, presenting highly favorable results in the use of the model developed for induction of the inflammatory process in vitro and the use of the synthed nanomaterial with PDT, representing a possible new therapeutic approach for several inflammatory skin diseases.

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Bacterial inactivation by propolis-based nanomaterials as an alternative solution to the problem of antimicrobial resistance.

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The revolution in medicine caused by Alexander Fleming's discovery of penicillin in 1928 is threatened by the acceleration of drug resistance by many pathogens, culminating in the antimicrobial resistance (AMR) crisis. This crisis has hampered treatments and caused millions of new infections and thousands of deaths around the world. In combating MR, the biggest challenge, according to the WHO, has been the search for alternative approaches, since the new antibiotics currently in clinical development (only 43) are insufficient and inefficient to combat AMR. Today we face the threat of entering an Era in which simple medical procedures and minor injuries can easily kill, similar to what we experienced in medieval times before the discovery of penicillin. This threat has led us to the urgent need to develop innovative antimicrobials, looking for alternative materials and approaches for inactivating microorganisms. In this scenario, natural products such as propolis, a resinous material produced by bees, can be considered as a new candidate for this perspective, due to its already known antibiotic properties, and the diversity of composition. Furthermore, the action of these natural materials can be enhanced when associated with biomaterials, such as micelles, microspheres, nanoparticles and, in the case of this work, nanoclays. We are going to show propolis extracts from stingless bees (*Meliponini* tribe), and their composites with halloysite nanotubes (HNT) and kaolinite (KAO) nanoclays, fully characterized by several physio-chemical and spectroscopic methods, and tested against *E. coli* and *S. aureus* bacteria. The efficiency of the propolis extracts and of the nanocomposites will be discussed and new routes for antimicrobial activity will be proposed.
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Bismuth sulfide nanoparticles as radiosensitizers for cancer treatment

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Cancer is one of the main threats to human health due to the large number of cases and high mortality rates. Although radiotherapy is the main course of treatment, it is not specific for tumor cells, affecting also healthy tissues. Radiosensitizers provide a novel and simple solution to this problem, since they increase the amount of radiation that a cell can absorb. This study investigates the use of biocompatible bismuth sulfide (Bi_2S_3) nanoparticles as radiosensitizers and their potential advantage over cell death. Using a hot injection method and oleylamine as ligand, we synthed Bi_2S_3 nanorods measuring on average 4.1 nm in width and 20.4 nm in length. Next, the ligand of the nanoparticles was successfully exchanged to polyvinylpirrolidone (PVP) to improve their biocompatibility. We also examined the effect of PVP-coated Bi_2S_3 nanoparticles on the response of breast and lung cancer cell line (MCF7 and A549) to a dose of 2 Gy Co-60 gamma radiation or 6 MeV linear source. Their effectiveness raised up to 38% more cell death in comparison to only irradiated cells. We have also performed a comprehensive study of the mechanism of cell death using the triple-stain assay, which employs three fluorescent days: Hoechst, propidium iodide and fluorescein acetate. This assay revealed the importance of the synergy between nanoparticles and irradiation in enhancing the effect of radiotherapy, resulting in a significant increase in the percentage of cell death by necrosis when cells are irradiated in the presence of nanoparticles. Additionally, we examined DNA damage using the micronucleus assay, which revealed chromosomal aberrations. We observed an increase in the number of micronuclei generated when cells were irradiated, particularly in the presence of nanoparticles. In conclusion, we have observed a more efficient radiotherapy treatment as a result of the use of nanoparticles as radiosensitizers, resulting in a greater amount of cell death, particularly by necrosis.

Coaxial nanofibers with electromechanical properties for Tissue Engineering

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Electroactive polymers (EAPs) are a special class of materials that can modify their morphology upon application of an external stimulus. In particular, electromechanical stimulation is of great interest for the field of tissue engineering, since it has been demonstrated that cyclic mechanical deformation promotes cell regeneration [1]. In this study, we will fabricate EAP-based scaffolds for myoblast cell culture. The advantage of using this type of scaffolds is that they are able to mimic the microenvironment where muscle cells grow. Furthermore, mechanical stimulation of the scaffold induces cell alignment and increases the elongation of the cells. These advantages have led to the development of heart patches and nerve tissue. Here, we developed a core-shell nanofiber, using an EAP as the core material and a shell composed of a blend of salmon gelatin (SG), chitosan (Ch), and poly(vinyl alcohol) (PVA) [2]. The blended shell improves cell adhesion with SG and enhances mechanical stability with Ch. Once we have our biomaterial, we measure its mechanical properties using Atomic Force Microscopy (AFM). The AFM will allow us to study nanoscale mechanics both in dry and liquid medium.

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Comparative study of electrospun nanofibers incorporating PVA- Salmon Gelatin- Chitosan with different alignment methods: Assessing muscle cell alignment for tissue engineering applications

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Electrospun nanofiber scaffolds are suitable for tissue engineering due to their use of **biocompatible and biodegradable materials** allowing cell growth. They offer **manipulable nanofiber orientation** (Jin et al., 2018). Aligned nanofiber scaffolds show promise for muscle cell applications by guiding cell alignment and emulating extracellular matrix properties, like stiffness (Choi et al., 2008). In this study, scaffolds were made from polyvinyl alcohol, salmon gelatin, and chitosan blends. Aligned nanofibers were produced using **two electrospinning collectors: microstructured static and rotating collector**. Nanofiber alignment was assessed via scanning electron microscopy, and its impact on cell development was evaluated by epifluorescence microscopy and cytotoxicity test WST-1. Young's modulus was measured using AFM with colloidal probe technique (Kappl & Butt, 2002). **Scaffold stiffness closely matched muscle tissue**. Both scaffold types showed nanofiber alignment, but only the **scaffold fabricated with rotating collector influenced muscle cell alignment**. This study introduces a promising scaffold for muscle tissue engineering applications as it is biocompatible, has adequate stiffness and allows cell alignment.

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Detection of IgG antibody against COVID-19 N-protein by a Hybrid Graphene-Nanorod sensor

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COVID-19 pandemic disclosed the global necessity to develop fast, affordable, and user-friendly diagnostic alternatives. Alongside recognized tests such as PCR and ELISA, nanotechnologies have since been explored for direct and indirect diagnosis of SARS-CoV-2, the etiological agent of COVID-19 [1]. Accordingly, in this work, we report a method to detect antibodies anti-SARS-CoV-2 based on the graphene transistor effect (GFET), using a nanostructured platform of graphene added of gold nanorods (GNR) and a specific viral protein.

To detect anti-N-protein IgG antibodies for COVID-19 in human sera, gold nanorods were functionalized with the nucleocapsid (N) protein of SARS-CoV-2 and subsequently deposited onto graphene. Our test results demonstrate that the sensor is highly sensitive, capable of detecting antibody concentrations as low as 100 pg/mL. Testing human sera, previously diagnosed with ELISA, showed an 90% accuracy rate compared to ELISA results, with the test completed in under 15 minutes. The integration of graphene and nanorods eliminates the need for a blocker, thereby simplifying sensor fabrication. This hybrid sensor holds robust potential to serve as a simple and efficient point-of-care platform.

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Development of an Erythrosine nanoemulsion obtained by low-energy and solvent-free method for Photodynamic Therapy applications

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Gliomas are the most common type of tumor of the central nervous system and all the types, glioblastoma multiforme (GBM) is the most common and aggressive brain cancer. Although this is the case, the treatments currently available are not highly effective in combating the disease. Photodynamic therapy is therefore a complementary alternative to traditional treatments [1]. Erythrosine is a natural dye from the xanthenes class, widely used in the food and cosmetics industries, and which has enormous potential for application in PDT as a photosensitizing substance [2]. Although it has this potential, its low stability in water is a limiting factor in its use. In this context, the development of nanoemulsion systems containing Erythrosine is an excellent strategy to solve this problem. Therefore, this work aimed to develop and characterize nanoemulsion systems containing Erythrosine for application in photodynamic therapy in the treatment of glioblastoma multiforme. To this end, nanoemulsions were synthed; the influence of different surfactant processes was evaluated; the region of nanoemulsion formation in the pseudo ternary phase diagram was determined; and the best nanoemulsions were characterized. At the end of the tests, it was possible to develop a nanoemulsion (Size: 127.4 nm; PdI: 0.156; PZ: -34.6 mV) containing Erythrosine, without the use of heating, organic solvents through a low-energy method.

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Enhanced stability of triangular silver nanoparticles with N-doped graphene oxide quantum dots

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This study aims to investigate the stabilization of triangular silver nanoparticles (tAgNPs) using N-doped graphene oxide quantum dots (N-GOQDs). While tAgNPs hold promise for medical applications and offer advantages like easy tunability and low-cost synthesis, their instability arises from high surface energy and specific crystallographic facets, particularly vulnerable to rounding in the presence of halide anions such as Cl–, commonly used in biological tests in high concentrations of NaCl and KCl salts.1 The solution proposed to address this issue involves impregnating tAgNPs onto N-GOQD surfaces through electrostatic interactions. Due to low toxicity, water solubility, and good affinity to AgNPs,2 N-GOQDs can act as stabilizers. The acquired hybrid nanocomposite (tAgNP/N-GOQD) was synthesized through a direct reaction between the nanoparticles. Scanning electron microscopy confirms the retention of the triangular shape of tAgNP in the composite, while dynamic light scattering reveals an increased hydrodynamic radius compared to bare tAgNPs. UV-Vis spectroscopy of bare tAgNPs with NaCl 154 mM shows an immediate degradation of tAgNPs, indicated by a high blue shift of the plasmonic resonance band from ~650 nm to ~400 nm. In the presence of N-GOQD, an essentially smaller blue shift is noted, indicating stabilization of tAgNP/N-GOQD against NaCl-induced degradation. Varying N-GOQD concentrations demonstrated their role in maintaining tAgNP integrity under NaCl conditions, with higher concentrations preserving the characteristic UV-Vis profile of AgNPs. This suggests the potential of N-GOQDs as effective stabilizers for tAgNPs in biological and medical applications.

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Enhanced Treatment of head and neck tumor cells using polymeric nanocapsules loaded with zinc-bound phthalocyanine in Photodynamic Therapy

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Photodynamic Therapy (PDT) is a promising tool in dentistry and your application in head and neck squamous cell carcinoma (HNSCC) is still a challenge [1]. Zinc-bound phthalocyanines (ZnPcs) have desirable characteristics of a good photosensitizer (PS) [2], but its use is limited by its low solubility in organic solvents. For this reason, polymeric nanocapsules (NCs) for PS delivery are a very useful tool to improve its applications in antitumor therapy. The present study aims to investigate the cytotoxicity and cellular uptake of NC/ZnPc and antitumor efficacy through PDT in HNSCC cell lines. The NCs were prepared by the interfacial deposition method [3]. Different concentrations of NC/ZnPc were tested in HNSCC cell lines to perform cytotoxicity by the resazurin method, cellular uptake and PDT. In vitro cytotoxicity observed formulations concentrations of 0.5 to 5.4 µmol. L-1 showed no toxicity compared to the control for both cell lines tested at an exposure time of 3h. The concentration of NC/ZnPc that demonstrated the best profile in the cell uptake assay was 2,0 µmol.L-1 for all cell lines tested. The photobiological activity assay generated a significant reduction in cell viability only for the H357 cell line at doses of 30 and 50J.cm-^{2}. The results obtained so far were considered promising for the next steps in 3D biological assays.

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Green and scalable aqueous synthesis of biocompatible magnetite nanoparticles for cancer treatment by magnetohyperthermia

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Challenges for magnetic iron oxide nanoparticle (SPIONs) applications in cancer treatment via magnetohyperthermia include the costs of large-scale production and its surface functionalization for biocompatibility, increased circulation time, and tissue recognition [1]. Here, a new one-pot synthesis of functionalized SPIONs in an aqueous medium is described. The reduction-precipitation method [2,3] uses $FeCl_3$ and Na_2SO_3 to promote the in situ stoichiometric reduction of Fe^{3+} to Fe^{2+}, followed by precipitation in an alkaline medium (NaOH). This method reduces costs and does not need deaeration or an inert atmosphere, resulting in SPIONs with an average of 25±4 nm. This meets the precepts of Green Chemistry with a high yield (~2.1 g/100 mL of solution) scaled in a chemical reactor using a solution volume of up to 2000 mL. SPIONs structure by Mössbauer spectroscopy revealed a non-stoichiometric magnetite phase (oxygen vacancies, $\square$), $Fe^{3+}[Fe^{2.5+}_{1.44}Fe^{3+}_{0.47}\square_{0.09}]O_4$. The method allows the SPIONs functionalization with 3-(mercaptopropyl)trimethoxysilane (MPTMS) inside the reactor (SPIONS@MPTMS). The SPIONs@MPTM has a hydrodynamic diameter of 125 nm, zeta potential of -30 mV, saturation magnetization of 60 emu/g, and high hyperthermal efficiency (heat generation in alternating magnetic field). No cytotoxicity was observed in different tumors and healthy cell lines. The MPTMS onto the SPION surface allows simple additional functionalization via disulfide bonding with polymers, drug loading and tissue recognition molecules, e.g., folic acid. Our results show a simple, green, low-cost, and large-scale synthesis route for MPTMS-functionalized SPIONs with high potential for cancer treatment via magnetohyperthermia.

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Green synthesis of nanoparticles from almond agricultural residues with potential application in biomaterials

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A promising and sustainable approach for the synthesis of nanoparticles (NPs) in biomaterial applications involves the use of natural extracts rich in bioactive substances. These extracts can be obtained from plant residues, such as almond hulls, acting as reducing and stabilizing agents in NP synthesis. This not only reduces environmental impact but also enhances biocompatibility and allows for the customization of NPs for specific biomedical applications. Furthermore, the extraction of these compounds using green solvents such as Natural Deep Eutectic Solvents (NADES) further contributes to a sustainable process. The lactic acid:glycerol 1:1 NADES (containing 20% water) was used as the extracting solvent subjected to the miniaturized technique of microwave-assisted extraction (MAE). The extraction was optimized through a central composite design (CCD). The extract obtained was used for the synthesis of gold (Au), silver (Ag), and platinum (Pt) NPs, characterized by UV/Vis and X-ray diffraction (XRD) with s of 8 nm, 22 nm, and 8 nm respectively. These NPs will undergo evaluation for their antimicrobial potential through biological tests, aiming at the inactivation of bacterial strains for application in COREGA® adhesives against C. albicans biofilms. Using the Analytical GREEness (AGREE) metric, it was possible to quantify the environmental impact of the developed method and compare it with methods reproduced in the literature. Based on the input data entered into the software, the method developed in this study showed the greatest coverage of Green Analytical Chemistry principles and can be classified as a green method.

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Layer-by-Layer-modified lipid nanoparticles for RNAi delivery in glioblastoma treatment

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Glioblastoma multiforme (GBM) is the most common and lethal primary brain cancer. Current pharmacological interventions marginally increase the 12-month overall survival of patients with GBM. Among the novel therapeutic strategies being pursued, micro-RNAs, a class of non-coding RNAs, are receiving considerable attention for their regulation of several pathways implicated in tumorigenesis and survival. Notably, microRNA-181a-5p (miR-181a) has consistently been reported to be downregulated in GBM clinical samples, and its overexpression negatively affects tumor growth both in vitro and in vivo.

To improve the delivery of miR-181a to GBM cells, we sought to develop a modified lipid-based nanocarrier capable of encapsulating and delivering miR-181a to GBM cells in vitro and in vivo.

Optimized ionizable lipid-containing lipid nanoparticles (LNPs) were constructed by covering themiR-181a-loaded LNPs with hyaluronic acid. Hyaluronan-decorated LNPs (HA-LNP) were characterized by DLS, encapsulation efficiency, and Atomic Force Microscopy. Glioblastoma cells targeting was identified after Flow Cytometry and Confocal Microscopy. Transfection efficiency was evaluated by GFP silencing after incubation of HA-LNPs/siGFP with HeLa and U251 GFP cells. The effect of miR-181a on U87 cells was assessed in vitro (viability assay) and in vivo (tumor growth, subcutaneous model).

The resulting HA-LNPs targeted GBM cells more efficiently than non-modified LNPs and mediated siRNA and miRNA transfection in vitro. Finally, delivery of miR-181a by HA-LNPs induced significant cellular death of U87 GBM cells in vitro and delayed tumor growth in an in vivo subcutaneous tumor model..

Learning the implications of biomolecular corona formation in increasingly complex biological environments from a synchrotron perspective

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Nano-bio interactions are pivotal in nanomedicine, shaping the fate of nanoparticles (NPs) in vivo and driving novel nanomaterials' development. Biological fluids initiate intricate interactions with NPs upon administration, forming a biomolecular corona primarily composed of proteins. This corona profoundly influences NP biological responses, inducing conformational and structural changes due to heightened complexity and ionic forces [1,2]. Here, we explore NP-protein interfaces, focusing on the conformational changes of proteins in corona formation and silica NPs behavior in complex fluids (e.g. human serum and plasma). We investigate complex nano-bio interactions using synchrotron techniques such as small-angle X-ray scattering (SAXS) and circular dichroism (CD), providing perspectives into NP dynamics in diverse biological fluids. Meanwhile, we derive thermodynamic parameters characterizing the physical-chemical interactions between NP-biological components. An in-depth knowledge is made possible by the combination of SAXS and CD, which enhances data acquisition and allows for the investigation of protein conformational changes and stability upon NP interaction. Our findings in this research contribute to advancing targeted nanomedical interventions and precision medicine by bridging basic research closer to real-world applications.

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Lyophilized and Sonicated Graphene Oxide and its Nanoecotoxicity applications

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The present work aimed to perform an exhaustive structural and chemical characterization of Lyophilized-Sonicated Graphene Oxide (L-SGO) and its nanoecotoxicological applications using Chlorella vulgaris and Lactuca sativa as biological models, exposed to 0.1, 1, 10 and 100 mg L-1 of L-SGO. In addition, both exposed and unexposed organisms to L-SGO were analyzed by optical and stereoscopic microscopy, X-ray diffraction (XRD), scanning electronic microscopy (SEM), Raman spectroscopy, Fourier transform infrared spectroscopy (FTIR), and X-ray photoelectron spectroscopy (XPS) and spectrofluorimetry. The 96 h-EC50 obtained for C. vulgaris was 37.52 mg L-1, and growth inhibition at the highest concentration tested (100 mg L-1) was 62.18%. In L. sativa, germination (%) showed a significant difference between the control and the 100 mg L-1 treatment, while root elongation showed no differences between the treatments. Overall, this study demonstrated that L-SGO has slight or no toxicity on C. vulgaris and L. sativa at concentrations near and higher than 100 mg L-1, respectively, and showed that the toxicity of L-SGO is lower than that of other Graphene-related materials tested on these species. This study highlights the importance of graphene oxide like L-SGO to be used for multiple technological applications with which we can reducing pollution and having a relatively low impact on ecosystems.

Magnetic nanosystems with thermal self-regulation for magnetic hyperthermia: a new approach for lung cancer theranostics

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Introduction: Lung cancer, the second most prevalent cancer in adults, is estimated to cause 28,618 deaths in Brazil by 2025 [1]. Magnetic nanosystems with thermal self-regulation properties hold promise for cancer therapy, utilizing magnetic hyperthermia to induce cancer cell death [2]. Objective: The impact of Co/Zn/Cr doping on magnetic nanoparticles, on their magnetic properties, and evaluate cytotoxicity, internalization, and intracellular trafficking in lung cancer models (A549). Methodology: Magnetic iron oxide nanoparticles (MIONs), pure and doped with Co/Zn/Cr, were synthed and characterized by XRD, TEM, DLS, magnetic measurement, and SAR analyses. Results: The XRD diffractogram confirms the crystal structure of magnetic nanosystems. In the TEM micrograph, we observed a spherical shape in the pure sample and a cubic shape in the doped sample, with average diameter of the 10 ± 2 nm and 20 ± 2 nm, respectively. DLS analysis in water showed a bimodal hydrodynamic diameter distribution around 150 and 950 nm for both particles. The particles, presenting a SAR of 62 W/g for the pure sample, and 10 W/g for the doped sample, under conditions of 270 Oe and 224kHz. And saturation magnetization of 60 emu/g and 30 emu/g, respectively. The doped one demonstrated thermal self-regulation. Both systems did not show cytotoxicity. Although, phagocytosis and macropinocytosis were primary internalization routes for both systems, and doped nanosystems exhibited increased internalization compared to pure MIONs. Conclusion: Overall, Co/Zn/Cr-doped MIONs thermal self-regulated nanosystems show promise for lung cancer therapy, by magnetic hyperthermia. Currently, experiments are underway to apply the magnetic field to lung cancer cells that have internalized these nanosystems to validate the therapeutic application under biological conditions. References:
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Nanocomposite films based on chitosan and silver-moxifloxacin nanoparticles

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Chitosan is a natural polysaccharide greatly exploited as drug delivery systems. However, a drawback for most applications is the drug burst release. Consequently, intensive research is made to improve the control over the release from these systems. One strategy consists in the insertion of nanoparticles, containing the drugs, within the polymer matrix. This provides a second barrier to the diffusion of drugs and allows to better control the release [1]. In this work, chitosan-based films were loaded with silver nanoparticles (NPs) impregnated with moxifloxacin, a broad-spectrum antibiotic. The NPs were prepared by the dropwise addition of caffeic acid or ascorbic acid to a solution containing AgNO3 and moxifloxacin. NPs were characterized by dynamic light scattering and moxifloxacin incorporation was evaluated by HPLC-UV/VIS. Chitosan films were prepared according to Chevallier et al. (2023) [2] and loaded with the obtained NPs. Control films containing only moxifloxacin were also prepared. Films were characterized regarding moxifloxacin release kinetics and antibacterial activity against E. coli and S. aureus. The NPs showed uniform distribution, around 10-20 nm for ascorbic acid and 300-400 nm for caffeic acid, with loading capacities around 200 µg/mg. Nanocomposite films were successfully obtained, showing a significant reduction in the burst-effect, which indicated a more controlled release. Preliminary antibacterial tests by disc-diffusion assay confirmed the antimicrobial activity of the films. A more detailed characterization in terms of antibacterial activity against time is ongoing.

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Nanomaterials Comprising Unsaturated Lipid Langmuir Monolayers: A Biomimetic Exploration of Nanotoxicology of a neolignan isolated from Nectandra leucantha (Lauraceae)

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Dehydrodieugenol, a neolignan isolated from the Brazilian plant Nectandra leucantha (Lauraceae), renowned for its antiprotozoal and anticancer properties, was incorporated into Langmuir monolayers composed of selected lipids to serve as models mimicking cell membranes. The primary objective was to unravel its molecular action mechanism. Using phospholipid Langmuir films, which not only sheds light on its mode of action concerning cell membranes. Employing techniques such as tensiometry, infrared spectroscopy, and Brewster angle microscopy, we inferred the interaction of dehydrodieugenol with lipids, including 1,2-Dioleoyl-sn-glycero-3-phosphocholine (DOPC), 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine, and cholesterol. Our findings unveiled distinct effects contingent upon the chemical nature of the lipid polar head, with a notable condensation observed across all monolayers. Furthermore, the distinctive impact of dehydrodieugenol on lipids was evident, as corroborated by hysteresis assays, surface potential isotherms, and rheological measurements. Infrared spectroscopy revealed that the interaction of the drug with the monolayer not only perturbs polar groups but also influences acyl lipid chains across all lipid types. These results underscore the modulatory effect of lipid composition, particularly the polar head group, and the hydrophobicity of both lipids and the drug. The interactions observed with different lipid types suggest a correlation with the compound's antiprotozoal and anticancer properties. The implications of these findings extend to understanding the biological significance of such interactions and the impact of bioactive substances on artificial membranes. Further analysis will delve into the potential therapeutic applications of dehydrodieugenol and related compounds based on their interactions with lipid membranes. Acknowledgments: FAPESP, CNPq, INEO, and CAPES.

NOVEL BIOMIMETIC NANOSYSTEMS FOR CANCER THERAPY

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The isolation and manipulation of cell membranes (CM) to be used as efficient biomimetic nanosystems for target delivery in cancer therapy has become an important research area in nanomedicine. We report the development of cell membrane-based nanocarriers encapsulating nanoparticles and anticancer drugs for both cancer photothermal and chemotherapies, respectively. Highly stable nanoparticles containing Gemcitabine (GEM), Paclitaxel (PTX), and Temozolomide (TMZ) were obtained using the major components isolated from tumor cell membranes. The nanoparticles containing GEM or PTX (NP-GEM-PTX) induced higher cytotoxic effects on pancreatic PANC-1 cells, in comparison to the use of pure GEM+PTX, indicating that membrane-covered nanoparticle favors the targeting and interaction with tumor cells. The biomimetic NP-TMZ system was built with isolated cell membrane from a U251 glioblastoma cell line and showed a greater affinity to U251 cells compared to other glioblastoma cell lines. The internalization of MNPs-TMZ in U251 cells was almost 2 times greater compared to U87 cells, and nearly 4 times greater compared to HCB151 cells. The use of cell membrane-coated nanoparticles opens up new possibilities regarding the development of efficient biomimetic nanosystems for cancer therapy and brings benefits to the field of personalized medicines.

Polymeric unimer micelles as nanocarriers of organic fluorophores for bioimaging applications

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The fluorescence of small organic molecules is commonly exploited in many fields of biomedical sciences, including medical diagnostics and theranostics[1]. However, the use of organic fluorophores in biological environments is limited by their low water solubility, bioavailability and photostability. To address these challenges, various types of polymeric fluorescent micro and nanoparticles have been proposed. Unimer micelles are self-assembled single-chain polymer nanoparticles, typically formed by copolymers incorporating both hydrophilic and hydrophobic comonomers, representing a promising solution due to their remarkably small size.

In this work, an amphiphilic random (meth)acrylate copolymer with oligoethyleneglycol and perfluorohexylethyl side chains was chosen to encapsulate coumarin153 (C153), a water-insoluble solvatochromic fluorophore. The resulting C153-loaded unimer micelles were extensively spectroscopically characterized in aqueous suspension. Notably, C153 was solubilized in water without compromising its spectroscopic properties, yielding fluorescence quantum yield and lifetimes comparable to those observed in organic solvents. Additionally, cytotoxicity studies demonstrated the biocompatibility of the nanomaterial.

The fluorescent nanocarriers were then employed for permeation experiments in ex vivo porcine sclera, a well-recognized animal model for studying of the posterior segment of the eye. Hyperspectral two-photon microscopy revealed the distribution of the nanocarriers within the scleral tissue, with intense emission of C153 originating from the aqueous pores located between the collagen fibers[2].

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Superparamagnetic Nanoparticles as potential "drug delivery" for the treatment of Duchenne Muscular Dystrophy

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Duchenne muscular dystrophy (DMD) is a genetic neuromuscular disease primarily affecting male newborns, leading to progressive muscle loss and a reduced life expectancy. Currently, there is no cure for DMD, and its therapy relies on the use of corticosteroids. Superparamagnetic iron oxide nanoparticles (SPIONs), specifically magnetite (Fe_3O_4), are widely employed in biomedicine due to their biocompatibility and unique magnetic properties compared to other materials. Given this issue, this study aimed to synthesize, characterize, and apply superparamagnetic nanoparticles to deliver the deflazacort drug to the muscles affected by DMD through an external magnetic field. The SPIONs were synthesized using the coprecipitation method, followed by surface functionalization with cysteine (CYS). The free thiol groups (-SH) in the CYS facilitated drug anchoring to the system, which was then employed in *in vivo* studies. Characterization of SPIONs involved XRD, FTIR, DLS, and magnetic measurements. Results showed that the SPIONs:CYS system had an average crystallite size of around 10 nm in the solid state and a hydrodynamic size of approximately 120 nm, suitable for biological applications in aqueous dispersion. Regarding magnetization, the nanoparticles exhibited superparamagnetic behavior at room temperature without residual magnetism. FTIR analyses identified vibrational modes characteristic of functional groups in iron oxide, cysteine, and deflazacort. *In vivo* assays allowed the assessment of cytotoxicity and the applicability of the SPION:CYS:Deflazacort system in DMD treatment. Data from blood tests and histological analyses of mdx mouse muscle tissue after seven consecutive days of nanoparticle treatment confirmed the non-toxic nature of the system, showing normal levels of enzymes (ALTL, ASTL, CK2, creatinine, and urease) and preserved cytoplasm and shape.

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Ultradense Electrochemical Chips with Arrays of Nanostructured Microelectrodes to Enable Sensitive Diffusion-Limited Bioassays

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Nanostructured microelectrodes (NMEs) are an attractive alternative to yield sensitive bioassays in unprocessed samples. However, although valuable for different applications, nanoporous NMEs usually cannot boost the sensitivity of diffusion-limited analyses because of the enlarged Debye length within the nanopores, which reduces their accessibility. To circumvent this limitation, nanopore-free gold NMEs were electrodeposited from 45 µm SU-8 apertures, featuring nanoridged microspikes on a recessed surface of gold thin film while carrying interconnected crown-like and spiky structures along the edge of a SU-8 passivation layer. These structures were grown onto ultradense, vertical array chips that offer a promising strategy for translating reproducible, high-resolution, and cost-effective sensors into real-world applications. The NMEs yielded reproducible analyses, while machine learning allowed us to predict the analytical responses from NME electrodeposition data. By taking advantage of the high surface area and accessible structure of the NMEs, these structures provided a sensitivity for $[Fe(CN)_6]^{3-/4-}$ that was 5.5× higher than that of bare WEs while also delivering a moderate antibiofouling property in undiluted human plasma. As a proof of concept, these electrodes were applied toward the fast (22 min) and simple determination of *Staphylococcus aureus* by monitoring the oxidation of $[Fe(CN)_6]^{4-}$, which acted as a cellular respiration rate redox reporter. The sensors also showed a wide dynamic range, spanning 5 orders of magnitude, and a calculated limit of detection of 0.2 CFU mL^{-1} [1].

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Zinc Oxide Nanostructures: A Promising Approach for Bladder Cancer Treatment

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Recently, there has been increasing interest in zinc oxide nanostructures (ZnONPs) due to their biocompatibility, chemical stability, and ability to selectively target tumor cells, making them promising for biomedical applications. This study aimed to develop ZnO nanostructures and assess their anti-tumor activity using T24 cells (bladder cancer cells) to evaluate various morphologies' effectiveness.Two methods were employed to synthe ZnONPs, co-precipitation, and hydrothermal, , which were then characterized using multiple techniques including scanning electron microscopy (MEV-FEG), transmission electron microscopy (MET), X-ray diffraction (DRX), thermogravimetric analysis (TGA), and inductively coupled plasma (ICP). Zeta potential, MTT (3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide), and NMA analyses were conducted to assess the biological response and toxicity of the synthed nanostructures.The ZnONPs exhibited primarily blade, rod, and flower morphologies. Biocompatibility assessments on Vero cells (a model of normal cells) indicated the nanostructures' safety, while anticancer activity against T24 cells was observed at a concentration of 200 µg/mL, suggesting an potential application in treating human bladder cancer. Although further studies are required to elucidate cellular mechanisms related to nanostructure exposure, these experimental results support the potential use of zinc oxide nanostructures as a therapeutic tool for human bladder cancer treatment.References:[1]Wei Zhang et al.2012,[2]Muhammad Shahid et al.2018, [3] JESUS, Jeanne Louise Fernandes. Zinc oxide nanostructures: synthesis and antitumor evaluation in bladder cancer. 2021. Master's Thesis. Pontifical Catholic University of Rio Grande do Sul.

Acute and chronic cytotoxic effects of gold nanoparticles synthed via magnetron sputtering in mammalian fibroblasts.

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Gold nanoparticles (AuNPs) have been attracting interest from the scientific community in recent decades due to their optical, physical, and chemical properties, including high surface area, easy conjugation with biological material, photothermal characteristics, and different sizes and shapes. The diversity of nanoparticulate materials attribute a wide range of applications [1]. The bulk gold is considered an inert metal with potential medicinal and therapeutic properties. However, multiple variations of nanoparticles and modifications on their surface may exhibit toxic in vitro effects. Therefore, researchers have been searching for AuNPs that can exert therapeutic activities with little or no cytotoxicity, or with some favorable effect for their applications [2]. Gold nanoparticles synthed by physical method were tested on a human lung fibroblast cell line (MRC-5) at different concentrations to evaluate cytotoxicity at acute (24h) and chronic (72h) exposition, in addition to apoptosis/necrosis analysis by flow cytometry. The AuNPs generated dose-response toxicity in 24 hours, with an increase at higher concentrations after 48- and 72-hours cell exposition. AuNPs were responsible for initiating apoptosis without evidence of necrotic or late apoptotic events. These results indicate stability in the use of AuNPs at low concentrations (< 50ug/mL), which should not affect normal tissues in treatments or other applications if the tolerable limit of AuNPs is respected. [1] Masson, J.-F. (2020). The Analyst, 145(11), 3776–3800.

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Antioxidant activity of polymeric nanocapsules containing astaxanthin

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Astaxanthin (AST), a carotenoid found in vegetables, seafood, and microalgae, has a beneficial impact on organisms, highlighting antioxidant functions and photoprotective capabilities through the removal of oxygen free radicals. However, its application is constrained by challenges such as low bioavailability, poor solubility, and sensitivity to temperature. In this study, we optimized the functional properties of AST encapsulated in poly (lactic-co-glycolic acid) (PLGA) using a double emulsion technique. Subsequently, these nanocapsules were employed to hepatic cells (HTC and FC3H) to investigate their impact on oxidative stress. The optimized nanocapsules exhibited a of 112 ± 24 nm, a zeta potential of -20.9 ± 0.3 mV, an encapsulation efficiency of 54.2% by HPLC, and 78.7% by UV-Vis. The physicochemical attributes of the optimized nanoparticles were characterized using various techniques, including scanning electron microscopy, Fourier-transform infrared spectroscopy, dynamic light scattering, and nanoparticle tracking analysis. In vitro studies revealed high production of reactive species in tumor cells, as determined by oxidative stress assays, without compromising the viability of healthy cells. These results indicate that our method for synthesizing PLGA-coated astaxanthin nanoparticles is highly viable and holds promise for future oncological treatments.

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Applications of co-doping aluminum oxide with carbon and magnesium in luminescent dosimetry

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The importance of dosimetry has been steadily growing along with the industrial and medical applications of radiation sources, luminescence dosimetry is widely adopted in radiation protection personal dosimetry and area monitoring where it is used to monitor the dose from exposure of radiation workers to ionizing radiation, or to monitor the radiation levels in specific locations [1]. Currently there are only a few commercial dosimeters available, thus creating the space for new materials with different characteristics, one such material is aluminum oxide co-doped with carbon and magnesium (Al2O3:C,Mg), which has shown great potential as a fluorescent nuclear track detector in the dosimetry of neutrons as well as energetic protons [2]. This work proposes an adapted route for synthesizing the Al2O3:C,Mg powders, based on the hydrothermal synthesis method previously applied by Chobpattana et al [3], which will then be characterized by a series of techniques including: X ray diffraction (XRD), Scanning electron microscope (SEM), Thermogravimetric analysis (TGA), Differential thermal analysis (DTA) and Raman Spectroscopy; the sample applications for optically stimulated luminescence (OSL) will then be measured utilizing a Riso OSL reader, model DA-20.

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A SARS-CoV-2 impedimetric biosensor based on the immobilization of ACE-2 receptor-containing entire cell membranes as the biorecognition element

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Biomimicking nanoparticles with cell membranes are one of the most innovative approaches to enhance performance, selectivity, and functionality for biomedical applications[1,2]. The cell membrane coating provides several advantages such as enhanced biocompatibility, improved stability, and specific targeting capabilities due to inherit properties of the source cells. These advantages can be transferred to the biosensing scenario. For examples, to improve the specificity and selectivity of SARS-CoV-2 biosensors, the angiotensin-converting enzyme 2 (ACE-2) transmembrane receptor, that are overexpressed in respiratory model cells, was used as biorecognition element. In this new SARS-CoV-2 detection platform, cellular membranes from VeroCCL81 (mVero) and Calu-3 (mCalu) cells (which overexpress the ACE-2 transmembrane receptors) were extracted and immobilized as vesicles on an indium tin oxide electrode (ITO). Electrochemical impedance spectroscopy was used to optimize the performance of the developed devices for SARS-CoV-2 detection. The membrane biosensors showed limit of detection of 10.0 pg/mL and 7.25 pg/mL and limit of quantification of 30.4 pg/mL and 21.9 pg/mL were achieved with satisfactory accuracy for ITO-APTES-mVero and ITO-APTES-mCalu, respectively. Selectivity studies revealed that this platform was able to differentiate the target spike proteins from NS1 proteins from dengue and Zika viruses. The use of biorecognition between cell membranes that express the ACE-2 receptors and the virus spike protein may be a new and efficient way to diagnose SARS-CoV-2, especially in terms of the cost of production and isolation, when compared to other targets.

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Betalactamic Antibiotics Monitoring by Raman/SERS Spectroscopy using Non-conventional Nanoparticles

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Various analytical techniques, including gas chromatography, electrochemical immunosensors have been documented to identify and characterize molecules with biological significance, like antibiotics, which is crucial in biomedicine. The surveillance of drug usage in intensive care units proves pivotal in combating of infectious ailments, notably antibiotic-resistant bacteria, a significant challenge in global healthcare [1]. However, many methods demand substantial reagents, utilize costly equipment, and frequently consume considerable time. There is a need to devise inexpensive, rapid, and sensitive detection methods. Optical-based approaches like Raman spectroscopy and Surface-Enhanced Raman Scattering (SERS) present promising avenues for such diagnostic technologies [2]. Furthermore, ample opportunity exists for research into alternative materials, such as post-transition metals, to be employed in this domain (beyond Ag and Au nanoparticles (NP)) [3]. Using laser-generated NP as substrate materials, we present results on SERS for the monitoring of beta-lactam drugs (class of antibiotics that have beta-lactam ring, which imparts bactericidal activity), which are commonly prescribed in critically ill patients, being this the most important class of antibiotics. Our Raman experiments were performed by mixing aqueous solutions of antibiotics with several elements' NP (Au, Co, Cu, V). Ampicillin, Ceftazidime, and Meropenem were tested for Raman/SERS. We demonstrate the possibility of antimicrobial fingerprint identification, interesting vibrational peak changes and intense enhancement of specific Raman peaks. All tested NP are potential candidates for developing Raman/SERS biotests for molecular monitoring and characterization of antimicrobial drugs.

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Bioactive and Biodegradable Magnesium-Based Composites

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Magnesium is considered a biocompatible and biodegradable material. This material exhibits continuous corrosion in physiological environments, with the corrosion by-products being absorbed by the body and any excess being expelled. These characteristics have prompted research into its use in biodegradable implants that serve a temporary structural function and are absorbed by the body over time. However, the mechanical strength of this material is considered low, and its corrosion can be too rapid and unpredictable. This study demonstrates that processing magnesium through severe plastic deformation allows for refinement of its structure to the sub-micrometer scale, enhancing its mechanical strength and improving its corrosion behavior. These property changes could enhance the performance of this material in biological applications. Furthermore, our research group has shown pioneeringly that processing using the technique of high-pressure torsion enables the consolidation of magnesium particles with bioactive particles, producing biocompatible, biodegradable, and bioactive composites. In this study, we've delved into analyzing the corrosion behavior of an Mg–HA composite, drawing a direct comparison with pure Mg. Samples of both the Mg–HA composite and pure Mg were soaked in Hank's solution for up to 60 hours. The microstructure and corrosion products were then examined using scanning and transmission electron microscopy and X-ray diffraction. Electrochemical tests were employed to assess their corrosion behavior, alongside a hydrogen evolution test to measure the corrosion rate. Notably, our results indicate that initially, the corrosion rate of the Mg–HA composite is higher than that of pure Mg, but it diminishes significantly after about 10 hours of immersion in Hank's solution. This increased corrosion resistance in the composite is credited to the formation of a protective layer of corrosion products with an outer surface layer rich in Ca, P, and O.

Bioscaffolds based on (PMMA/gelatin)/HAp-Zn for skin regeneration

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The fragility and direct exposure of the skin to the external environment makes it highly vulnerable to the occurrence of acute and chronic wounds. Chronic wounds aggravated by diabetes, for example, is a warning sign, since the total number of adult diabetics is expected to increase to ~ 12% by 2045 worldwide, according to data from the International Diabetes Federation (IDF) [1]. On the other hand, acute wounds can occur due to surgical interventions, trauma and burns. It is estimated that burns have caused around 180,000 deaths per year worldwide and are considered the fourth most common type of trauma [2]. In some of these circumstances, traditional skin grafts are typically used to restore damaged structures and functions of biological systems. However, these approaches may present unsatisfactory clinical results due to low biocompatibility, scarcity of donors or donor areas and lack of antibacterial activity, which may lead to graft rejection. As an attractive alternative, electrospun fibrous based on polymers, due to its physical and chemical characteristics can provide better adsorption of secretions, faster regeneration and antimicrobial protection. Thus, aiming to promote urgent advances in this worrying scenario, the present study produced bioscaffolds based on PMMA/gelatin containing different HAp-Zn contents by electrospinning. These materials were labeled as (100)/0, (99)/1, (97)/3 and (95)/5 (PMMA/gelatin)/HAp-Zn (at wt%) and exhibited excellent structural, morphological, textural and optical properties, when compared to the individual components (PMMA, gelatin or HAp-Zn active [3]). In addition, it was possible to verify the influence of bioscaffold mass and HAp-Zn content on the antibacterial activity and fibroblast cell viability, being possible to inhibit Staphylococcus aureus (S. aures) bacteria with 10 mg mL-1 of (95)/5 (PMMA/gelatin)/HAp-Zn. Fibroblast cells showed a excellent viability in contact with (100)/0 or (99)/1 (PMMA/gelatin)/HAp-Zn bioscaffolds, at all concentrations tested, but for (97)/3 and (95)/5 (PMMA/gelatin)/HAp-Zn, considerable percents of cell proliferation were observed only at 2.5 mg mL-1 of respective bioscaffolds. These multifunctional characteristics overcome the limitations of traditional skin grafts, as well as the individual components used, contributing to a faster, safer and more effective recovery for the patients.

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Characterization of first- and second-generation lipid nanoparticles used as drug carriers through Dynamic Light Scattering

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Recent studies on Artepellin C, the majority compound in Brazilian Green Propolis, have shown promising antitumor effects.[1] Our study explores solid lipid nanoparticles (SLN) and nanostructured lipid carriers (NLC) to enhance therapeutic potential. We employ the solvent injection method, a rapid, straightforward, and practical approach applicable in the laboratory, that involves creating a colloid dispersion by injecting a solvent and lipids (stearic acid and oleic acid) into an aqueous solution. The nanostructures are formed through the stabilization of two phases facilitated by the interaction of a surfactant (tween 80). Herewith, we characterized the hydrodynamic diameter (DH), polydispersity index (PDI), and zeta potential (ZP) using dynamic light scattering (DLS) before encapsulation. This technique relies on the correlation of Rayleigh and Mie scattering by colloids over time to measure the DH, utilizing the translational diffusion equation of Stokes-Eisntein. Provides mean values for colloid diameter and its dispersion before encapsulation, such as DH = 71 ± 21 nm and PDI = 0.34 ± 0.04. Additionally, DLS measures the ZP by the electrophoretic movement under an applied electrical potential, yielding values like ZP = -31 ± 4 mV. However, interpreting these results requires careful consideration due to the statistical nature of the measurements. Concluding, DLS is essential for studying and developing colloidal systems for therapeutical proposes, providing essential information about their stability. However, a deep understanding of its principles and data interpretation is necessary.[2]

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Cobalt sulfide quantum dots for potential biomedical and energy applications

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Nowadays, the search to develop sustainable materials using materials from renewable sources is a great challenge. In this context, the present research evaluated producing new cobalt sulfide quantum dots for potential biomedical and energy applications, using carboxymethyl cellulose as stabilizer and eco-friendly chemical route. Spectroscopies analysis (FTIR, UV Vis), X-ray diffraction, and morphological (SEM, TEM, ZP and DLS) were used to characterize this system. The results showed that the CoS presented the of (1,72 ± 0,06) nm with a good electrical potential for application in energy areas, demonstrating a low-cost and environmentally friendly chemical route. In addition, the chemical groups stabilized the CoS QD was the carboxylates. The UV Vis showed absorption bands in the range of 250 - 325 nm and at 500 nm. Additionally, the XRD diffractogram showed characteristics peaks of $Co_{(1-x)}S$ (JCPDS 42-0826). Moreover, the nanoparticles were applied to biological analysis of cytotoxicity and antimicrobial activity, and both showed a great result. Then, these results showed the great potential of cobalt sulfide quantum dots for providing an application to renewable energy sources and biomedical areas.

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Core-satellite (magnetite-gold) functionalized with folic acid: a theranostic platform with potential application in the treatment and diagnosis of cancer

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Cancer is one of the primary diseases responsible for countless deaths worldwide. Due to its heterogeneity, no extensive and selective treatments are available, which often affect healthy cells and result in various side effects for the patient. Consequently, there is a pressing need for new studies to develop more effective treatments, such as theranostic therapy, which has been gaining attention for combining therapeutic and diagnostic agents in a single multifunctional platform. Superparamagnetic iron oxide nanoparticles (SPIONs) have been extensively studied for applications in biotechnology and the biomedical field due to their magnetic properties, particularly their superparamagnetism. Magnetites synthed in aqueous medium using the reduction-precipitation methodology[1] have shown promising results in and morphology control, as well as magnetic properties and colloidal stability. Their low production costs, simple methodology, and sustainability make them even more attractive for large-scale production, a persisting challenge. Combined with the optical properties of gold nanoparticles (AuNPs), they form core-satellite structures[2] with a high potential for diagnosing and treating cancer as theranostic agents. Core-satellites must be positioned close to or inside tumor cells for more efficient biomedical applications. Some types of cancer overexpress folate[3] receptors on their surface, so a promising alternative is the conjugation of targeting or cell recognition molecules such as folic acid. Functionalizing the surface of magnetite-gold nanostructures with folic acid via peptide bonds also directly impacts the magnetic properties and colloidal stability of these materials.

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Cytotoxic and antibacterial effects of natural rubber latex films incorporated with silver nanoparticles processed through magnetron sputtering

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Natural Rubber Latex (NRL) has a complex composition and several biomedical applications, among them are tissue engineering, pharmacological delivery systems, and tissue repair [1]. Thin layer NRL films were enriched with silver nanoparticles (AgNP) synthed by magnetron sputtering with bactericide properties. Magnetron sputtering using top-down method for producing nanoparticles is a versatility, clean and eco-friendly technology, allowing the acquisition of different types of metallic nanoparticles. To improve the properties of these materials, plasma treatment was also applied to the films [2]. Cytotoxic activity was evaluated by MTT and antimicrobial effects through agar diffusion assays. Fibroblast cell adhesion was monitored over the films by EDS and FEG-SEM. TEM revealed that AgNP presented spherical shape with approximately 20 nm of diameter. MTT assay showed non-cytotoxic effects for NRL films and samples enriched with silver nanoparticles presented antibacterial activity proportional to the increase of AgNP. Taken together, NRL enriched with promising application as films to recover wounds.

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Design a new electrochemical biossensor based in Cassava-derived carbon for S.aureus detection

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Bacterial infections have a great impact on hospitals and Intensive Care Units and can often lead to sepsis. controlling the entry of bacteria into these environments is essential [1]. In this context, this work aimed to validate the Staphylococcus aureus (S. aureus) immunosensor, which in laboratory analyses proved to be accurate, fast and safe. The sensor was developed for the detection of S. aureus during hand asepsis and artificial intelligence (AI) was employed to improve the results. Immunosensor board contains a CE, a WE, both of gold, and an Ag/AgCl reference electrode into a Printed Circuit Board base. A controlled layer of cassava derived carbon with zinc nano-hybrids was deposited on the WE, which acts to immobilize the antibodies and improve the current response. The immunosensor was constructed by cystamine-glutaraldehyde system [2] and morphologically characterized by Scanning Electron Microscopy and the electrochemical performance of the biosensors was investigated by DPV. The results, in laboratory, demonstrating good reproducibility, selectivity, and precision. The evaluation stage was carried out using 400 donor samples and comparing the results obtained from the immunosensor and with the Mannitol Salt Agar test. The results were compiled and analyzed using AI techniques, to improve the test's assertiveness. In summary, we developed a biosensor for the detection of S.aureus, which showed a similarity of over 97% to the gold standard with a high capacity to help control infections.

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Development and characterization of doxorubicin and quinizarin nanoemulsions for application in Photodynamic Therapy of oral squamous cell carcinoma using in vitro HET-CAM (Hen's Egg Chorioallantoic Membrane) assay

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The complexity of oral squamous cell carcinomas (OSCC) makes their therapy aggressive [1]. This study aims to develop a nanoemulsion (NE) system for the treatment of OSCC using Photodynamic Therapy (PDT) combined with a NE loaded with doxorubicin (DOX - chemotherapeutic) and quinizarin (QNZ - photosensitizer) to enhance the therapeutic effect. The NEs were prepared by interfacial deposition with the surfactant Pluronic F-68, soy phosphatidylcholine, 0.05 mg/mL of QNZ in the presence and absence of DOX (1% w/v). Particle , polydispersity index and zeta potential were characterized by dynamic light scattering. For the photophysical characterization and quantification of the components, absorption and fluorescence emission spectroscopy analyses were carried out in 2D/3D mode. The cytotoxicity study was carried out using the HdFn strain under dark conditions and a resazurin test and biocompatibility was defined using the HET-CAM test [2].The NE were monodispersed, between 180.8 nm and 228.1 nm and zeta potential between -22 mV and -31 mV, with a high incorporation of QNZ (86%) and DOX (95%). The NEs had no cytotoxic effects at the concentrations used in monolayer (0.2% to 6% diluted in DMEM/SFB 5%) and HET-CAM (6% and 10%). Thus, NEs were considered promising for synergistic application in anti-tumor PDT.

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Development of a Membrane Biosensor Utilizing Overexpressed SSTR2 Receptor in PANC-1 Cells for Pancreatic Cancer Diagnosis

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Pancreas cancer is an aggressive disease with an increasing number of cases due to late diagnoses. Novel methodologies, such as electrochemical biosensors, can revolutionize diagnostics by reducing costs and aiding in early-stage detection compared to traditional techniques [1]. In this context, this work aims to improve specificity in pancreatic cancer detection by utilizing the SSTR2 receptor as a biorecognition layer, given its significance in pancreatic cancer treatment methods. The biosensor will comprise an indium tin oxide (ITO) electrode modified with an amino-silane group and a vesicle membrane derived from PANC (pancreatic carcinoma of ductal cell origin) cells with high SSTR2 receptor expression, resulting in the biosensor ITO/APTES/mPANC. The (3-aminopropyl)triethoxysilane (APTES) concentration was initially optimized, and the vesicles were analyzed using various techniques such as dynamic light scattering, potential zeta, nanoparticle tracking analysis, and molecular spectroscopies. Each modification step was then confirmed using electrochemical techniques, such as electrochemical impedance spectroscopy (EIS). The optimal APTES concentration was found to be 1% v/v, and the PANC membrane vesicles exhibited absorption at 262 nm and emission at 360 nm, attributed to the presence of tryptophan protein. The vesicle after extrusion was 148 ± 18 nm, with a polydispersity index of 0.983 ± 0.030, a charge of -17.1 ± 0.9 mV, and a conductivity of 10.97 ± 0.45 mS/cm. EIS results showed an increase in charge transfer resistance after vesicle immobilization, confirming successful modifications and completing the biosensor construction with anti-SSTR2 as the analyte.

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Development of halloysite nanoclay composites based on Tetragonisca angustula (Jataí) propolis for antimicrobial applications.

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Propolis is produced by bees from a mixture of saliva, wax, and plant resins, and it has a distinct chemical composition according to the pollinated flora and the bee species. In its composition, two classes of biomolecules are of greatest interest for biomaterials development: the coumarins and flavonoids, secondary metabolites of plants to which immunomodulatory actions are related. In this work, with the aim of developing an antimicrobial system, propolis from the stingless bee *Tetragonisca angustula* (Jataí) were extracted using three different solvents: toluene, chloroform and ethanol and investigated by means of photoluminescence and antimicrobial activity against *S. aureus* and *E. coli* bacteria. Later, the extracts were mixed with halloysite nanoclays, were treated to acquire three different potentials: acid, basic, and neutral. As preliminary results, the extracts showed differences in the colour and variations in photophysical characterizations, with changes in the shape of the curves. In addition, ethanol and chloroform extracts showed positive activity against the bacteria. In the next steps, composites were prepared and they are being studied regarding photophysics and antimicrobial activity.

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Development of kaolinite nanoclay composites based on *Melipona quadrifasciata quadrifasciata* propolis extracts for antimicrobial applications.

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Antimicrobial resistance is one of the biggest challenges faced by modern medicine and has mobilized the scientific community to develop new systems capable of inhibiting bacterial growth [1]. Therefore, the development of nanocomposites, compared to traditional approaches, is more favourable to mitigating the described problem, due to their antibacterial properties and good biocompatibility. In view of this, the development of nanocomposites based on nanoclays with the addition of propolis for antimicrobial applications was proposed. In this work, the choice of materials was based on the fact that nanoclays, given their chemical inertness and large surface area, are widely used in medicine as drug carriers [2], while the antioxidant and anti-inflammatory characteristics of propolis, further optimized by the association with nanoclay, can result in new means for microbial inactivation [3]. To this end, composites were prepared from acidic, basic, and neutral kaolinite nanoclays (KAO), which were mixed with propolis extracts (in three different organic solvents - ethanol, chloroform, and toluene) from *Melipona quadrifasciata quadrifasciata* (Mqq). Subsequently, composites were characterized by absorption, photoluminescence (PL) and excitation photoluminescence (PLE), in order to determine their physicochemical characteristics.

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Development of polyfullerene-based photoinactivation systems for antimicrobial applications.

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Antimicrobial resistance poses one of the foremost threats to global health, with significant implications for modern medicine and public health. Since Alexander Fleming's discovery of penicillin, the rapid evolution of antibiotic resistance in many human pathogens has led to a global crisis in microbial resistance (AMR), impacting treatment effectiveness and escalating healthcare costs [1]. Photodynamic Inactivation (PDI) emerges as a promising approach to combat microbial resistance, utilizing light-activated photosensitizing substances to generate reactive oxygen species (ROS) and irreversibly damage microorganisms. In this context, the unique structure of fullerenes, coupled with their ability to produce ROS in response to light irradiation, offers a promising alternative to conventional antibiotic treatments. Due to the dependence of pro-oxidant activity and formation of triplet species, the understanding the photophysics of fullerenes into different physical chemical conditions is essential for the development of efficient photosynthers. In this work, C_{60}-based polymers [2] have been characterized by means of photoluminescence and photoluminescence excitation in two different temperatures (293 and 303 K), showing a decrease of PL emission of C_{60} into the block, in comparison to the poly-C_{60}. The decrease in the PL intensity can be an indication of higher triplet species formation and this result is currently being investigated by PLE and antimicrobial tests, to further development of photoinactivation systems with high triplet species formation with a lifetime as long as possible.

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Development of polymeric nanocarriers for lung cancer therapy

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Nanotechnology presents a promising alternative for developing more effective methods compared to conventional treatments for cancer therapy. Poly(lactic-co-glycolic acid) (PLGA) stands out as a biodegradable polymer with high biocompatibility, FDA approval for drug delivery systems, and versatility in accommodating various types of drugs—ranging from hydrophilic to hydrophobic, small molecules to macromolecules. In this study, we synthesized PLGA nanoparticles with a diameter of 130 nm, exhibiting a surface charge of -35 mV and a polydispersity index (PDI) of 0.2. The encapsulation of carboplatin reached an efficiency of 41.5%, ensuring the stability of the nanoparticles for up to nine days. This stability contrasts with free carboplatin, which hydrolyzes within three days of dilution in water. Consequently, the encapsulation of the drug allows prolonged usage, making this system a promising candidate for further studies on prolonged release and in vitro cell viability assays.

Development of scintillating nanodevices for application in X-Ray PDT (X-PDT)

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A significant number of cancer cases are expected in the next triennium, underscoring the urgent need for effective technologies. Radiotherapy remains the primary treatment modality, with Photodynamic Therapy (PDT) emerging as a promising adjunct. Combining PDT with radiotherapy, particularly through X-ray activation, enhances treatment efficacy. However, most photosensitizers rely on visible light, limiting their penetration depth. To address this, a nanodevice emitting visible light upon exposure to ionizing radiation was proposed. These nanodevices, composed of lanthanide-doped inorganic matrices, facilitate deep tissue penetration and generate reactive oxygen species upon activation. Synthed nanoparticles, primarily Ca□2:Tb3+, demonstrated high purity, (~ 20 nm), high radioluminescent emission within the therapeutic window, and singlet oxygen production (measured by ESR technique) especially when conjugated with the photosensitizer Rose Bengal. This innovative approach integrates radiotherapy with PDT, promising improved cancer treatment outcomes. So far, this study has unveiled a potential active agent for treating deep tumors through the production of ROS. This is because it has generated a nanoparticle with defined structure, high purity, appropriate , high emission, synergy with the photosensitizer employed and ESR relevant gain (2,78 ± 0,56), which is directly linked with the reactive oxygen species generation. Further studies are still needed to determine the optimal distance between RB and the nanoparticle in order to maximize the ROS generation.

Development of theranostic nanoplatforms based on colloidal silver and paramagnetic chelates

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There is a growing interest in the development of theranostic tools that facilitate the high-precision detection and efficient treatment of cancer cells with lower invasion and adversary effect. In this way, magnetic resonance imaging (MRI) is one of the most non-invasive and efficient diagnostic tools of cancer. Moreover, as antitumoral drugs can often cause collateral damage to non-cancer cells, a promising alternative to these treatments is plasmonic photothermal therapy (PTT) [1]. In this context, silver nanoparticles (NPs) have been arise as promising tools for PTT. These NPs combine good plasmonic properties, simple synthetic procedures with high control over and morphology, and cost-effectiveness. Besides, AgNPs still have the versatility to attach molecules to their surface, such as providing more specificity and/or signal for another technique, such as paramagnetic chelates that are contrast agents (CAs) for MRI. Thus, in this work AgNPs were conjugated with Gd3+ chelates to obtain theranostic nanoplatforms for MRI and PTT. For this, AgNPs stabilized with glucose were prepared in water and thiolated DOTA-Gd complexes were conjugated to their surface. Our results showed that these theranostic tools exhibited good colloidal stability, similar plasmonic bands to the bare AgNPs, and longitudinal relativities per Gd3+ analogous to the CAs used clinically (at 20 MHz and 37 °C) [2]. Thus, the results indicate that combining the plasmonic property of AgNPs with the relaxometric efficiency or Gd3+ chelates are promising for the preparation of theranostic systems for MRI and PTT.

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Effect of the pesticide glyphosate on mimetic system of the plasma membrane

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The current demand for food results in the increase of using pesticides in Brazilian crops, with glyphosate being one of the most widely used pesticides, particularly in soybean cultivation [1]. Once glyphosate was found to, potentially affect sperm development in rats [2], studies of its effects on human health are necessary. However, since in vitro and in vivo studies require more complex experimental procedures, model systems are a useful alternative to provide some insights. Thus, in this study, mimetic systems of the lipid structure of the cell membrane based on giant unilamellar vesicles (GUVs) were used to investigate the interaction between glyphosate and such structures. The GUVs were composed of a ternary lipid mixture of POPC (1-palmitoyl-2-oleoyl-sn-glycero-3-phosphatidylcholine), POPE (1-palmitoyl-2-oleoyl-sn-glycero-3-phosphoethanolamine), and SM (sphingomyelin), in a molar ratio of 2/2/1 mol %, approaching both the fluid phase of the plasma membrane of mammalian cells and the composition of the sperm membranes [3]. The GUVs were also formed with the fluorescent probes DiIC18 and Alexa Fluor and were analyzed by phase contrast and confocal microscopies for 60 minutes, in an aqueous solution of glucose and glucose with glyphosate (10-4 mol/L). The results demonstrate that in the presence of glyphosate, there was a greater loss of phase contrast and spherical shape of the GUVs, indicating that the pesticide may negatively alter the membrane of sperm cells.

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Effects of ultrasmall Gold Nanoparticles on Local Dose Enhancement and Toxicity in *Drosophila melanogaster* Model

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The study of gold nanoparticles (AuNPs) in radiotherapy highlights their potential to improve treatment efficacy by increasing the radiation dose delivered specifically to tumor cells while minimizing the impact on surrounding healthy tissue. The of these nanoparticles is a critical factor affecting their efficacy. In this study, we evaluated the toxicity and radiation-enhancing effects of AuNPs as local dose enhancers in radiotherapy, using *Drosophila melanogaster* as an in vivo model organism. AuNPs were synthed by the chemical reduction method. Their and morphologies were characterized by transmission electron microscopy (TEM) and dynamic light scattering and presented an ultrasmall of approximately 4 nm. The UV-visible spectroscopy showed a characteristic peak plasmonic band of AuNP around 534 nm.

Flies were exposed to a diet containing 100 pmol/L AuNps followed by 30 Gy of X ray irradiation. We assessed measures such as embryonic development, pupation, lifespan, and DNA damage. The results indicate that exposure to ultrasmall AuNPs delays embryonic development but does not significantly affect hatching rates or lifespan. An interesting observation is the protective effect observed in irradiated adult flies, where AuNPs contributed to increased lifespan. This study demonstrates that ultrasmall AuNPs enhance the efficacy of radiotherapy and reduce its side effects, possibly due to their bactericidal activity.

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Elaboration of a novel magnetic nanohybrid composite (Fe_3O_4@Zr-MOF) to extract metabolites from serum samples in biomarker detection studies

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Blood is a biological sample widely used in the diagnosis of human diseases. However, its complex composition presents analytical challenges, especially in detecting human disease biomarkers [1,2]. In this context, this study proposes a new adsorbent material to extract metabolites (potential biomarkers) from blood, simplifying it and increasing sensitivity in the detection of metabolites in blood serum. The material was developed based on a metal-organic framework based on zirconium (Zr-MOF) and magnetic nanoparticles (Fe_3O_4), named as Fe_3O_4@Zr-MOF. Fe_3O_4 and Zr-MOF were synthed employing solvothermal method. 1,4-Benzenedicarboxylic acid as ligand and Zr salt were used for MOF synthesis. The nanohybrid composite was prepared using the MOF post-synthesis approach. After synthesis, the material was characterized using FT-IR, SEM, BET, DLS and Zeta potential. As a result, material with a particle of 143.16 nm and a polydispersity index (PDI) of 0.03 was successfully obtained, suggesting high homogeneity. The composite Zeta potential was -21 mV. Furthermore, Fe_3O_4@Zr-MOF showed significant surface area (186.35 m^2/g) and pore s of 1.7 nm. Then, using the obtained composite, metabolite extraction studies were initiated. For this, the amino acid L-tryptophan was used as a standard analyte. Multivariate analysis using full factorial (2^3) was used. Three independent parameters (pH, material mass and incubation time) were tested to evaluate the adsorption capacity of the composite. The ideal condition was achieved using pH (5.5), material mass (21 g) and incubation time of 123 minutes, achieving recoveries greater than 80%. Adsorption isotherm and adsorption kinetics experiments, as well as application are in progress, and the results will be presented at the event.

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Electrochemical activation of carbon electrodes functionalized with graphene/conducting polymer nanocomposite for application in colorectal cancer biosensing

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The development of nanomedicine is constantly searching for solutions for the early diagnosis of cancer. An interesting approach is the detection of tumor biomarkers in the early stages of the disease. The high sensitivity of these devices is directly linked to the materials used to transduce the generated signal. Graphenes and conductive polymers have stood out for this purpose. In addition to the nanomaterial, another important aspect is the stability of the surfaces on which the detection platforms are built. Electrochemical activation can promote a significant improvement in sensor sensitivity [1]. This work aims to evaluate the stability and electrochemical response of commercial electrodes, through electrochemical activations promoted for different amounts of voltammetric cycles in KOH (0.5M), -1.5 to 1.0 V. The results obtained showed that the number of cycles directly affects the electrochemical behavior of the electrodes. Applying just two cycles, it is possible to observe a significant difference between the initial surface and the treated surface in terms of electrochemical reversibility, which corroborates the lower values of resistance to charge transfer obtained by electrochemical impedance spectroscopy, ensuring greater stability and reproducibility of the analyses. After this treatment, the electrodes were functionalized with a nanocomposite based on chemically exfoliated graphene, conductive polymer and specific biomolecule for detecting colorectal cancer biomarkers. The results showed that, for activated electrodes, modification with the nanocomposite allows a better detection response compared to isolated materials, presenting great potential to be explored in the diagnosis of colorectal cancer as electrochemical biosensors.

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Enhanced Uptake of Cisplatin-Loaded Biomimetic Nanoparticles for Lung Cancer Therapy

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Nanotechnology has enhanced therapeutic outcomes through nanoparticle-mediated drug delivery, mitigating drug toxicity [1]. Cisplatin, a commonly used chemotherapeutic, often induces dose-dependent toxic effects [2]. In this study, we propose the synthesis and physicochemical characterization of poly(lactic-co-glycolic acid) (PLGA) nanoparticles coated with hybrid membranes derived from lung adenocarcinoma cells (A549) and T lymphocytes (Jurkat) for the encapsulation of cisplatin, a standard chemotherapy agent in lung cancer treatment. We evaluated nanoparticle uptake with and without coating on *in vitro* A549 and MRC-5 (lung fibroblast) cell cultures using flow cytometry and confocal fluorescence microscopy. Initially, membrane-free nanoparticles showed a diameter of 98 ±1 nm and a surface charge of -17 ±4 mV. After functionalization with the membranes, nanoparticles had a of 104 ±1 nm and a surface charge of -18 ±5 mV. The coating of nanoparticles was suggested by infrared spectroscopy, showing characteristic protein bands. Drug-containing and functionalized nanoparticles showed increased internalization in tumor cells compared to fibroblast cells, suggesting homotypic recognition of the system. This study represents an advancement in the development of nanoparticles for lung cancer treatment, with the prospect of improving treatment efficacy and minimizing its adverse effects.

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Enhancement of encapsulation efficiency of Artepillin C in solid lipid nanoparticles via solvent injection method

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Solid lipid nanoparticles (SLNs) have emerged as a promising option in biomedical applications, demonstrating stability and the ability to encapsulate, along with controlled and targeted release. The study to be presented focuses on encapsulating artepillin C, a lipophilic compound derived from green propolis, utilizing the solvent injection method [1], alongside additional modifications aimed at enhancing efficiency. The compound is incorporated into the organic phase before being injected as part of the SLN formulation. The primary modification involves pH adjustment to 2.0, as the drug exhibits low solubility at acidic pH levels, enhancing encapsulation efficiency. Furthermore, the temperature of the aqueous phase was set to 35 °C, resulting in smaller particle and polydispersity, yielding more favorable results compared to lower temperatures, leading to rapid lipid precipitation at the interface between droplets and the aqueous medium, thus preventing drug leakage [2]. Additionally, sonication was introduced to reduce particles and mitigate aggregation. These methodologies were evaluated through characterization techniques encompassing polydispersity (PDI), z-average measurement via Dynamic Light Scattering (DLS), and Transmission Electron Microscopy (TEM), demonstrating the production of smaller, more stable particles with enhanced encapsulation efficiency.

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Enhancing Photodynamic Therapy with Green-Synthed Zinc Oxide Nanoparticles

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Photodynamic therapy (PDT) is an emerging form of treatment in cancer research that uses a combination of light, oxygen and a photosensitizer (PS) to target disease. PSs are carefully selected for their non-toxicity in the dark and their ability to cause damage when exposed to light. Recent research has highlighted the role of nanoparticles, particularly zinc oxide nanoparticles (ZnO-NPs), in enhancing the efficacy of PSs in PDT [1]. This study investigates the environmentally friendly preparation of PS from ZnO-NPs via a microwave-assisted hydrothermal method using Glycine max (soybean) extract as a reducing agent. We investigated the green synthesis with different zinc salts (acetate, chloride, nitrate) at three microwave temperatures (100°C, 150°C, 180°C). Analytical methods included X-ray diffraction, Fourier transform infrared spectroscopy, scanning electron microscopy and UV-Vis spectroscopy. Samples were analyzed before and after calcination at 400°C. The characterisation confirmed the crystalline structure of ZnO, the chemical absorption bands and the morphology of the nanoparticles. Photodegradation tests were carried out with methylene blue dye under black light, and the three materials most effective in generating reactive oxygen species (ROS) were further functionalised with methylene blue and the photodegradation was compared. The photodegradation tests showed the relationship between the morphology and the bandgap value of the materials. The three best syntheses were found to have degradation rates close to 100%. These results suggest promising possibilities for the use of green-synthed ZnO-NPs as photosensitizers in PDT, potentially leading to more effective and environmentally friendly cancer treatments.

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Exploring Myrsinoic Acid Toxicity in Cell Membranes Using Langmuir Monolayers as Bioinspired Nanomaterials

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Natural plant-derived compounds show promise as foundational structures in drug development. Among these, Myrsinoic acid stands out for its antitumor and anti-inflammatory properties. These compounds often interact with lipid surfaces, including cell membranes, which can be effectively modeled using Langmuir films. This study aims to investigate Myrsinoic acid's interaction with two simple membrane models composed of phospholipids: dipalmitoyl phosphatidylcholine (DPPC) and dipalmitoyl phosphatidylserine (DPPS), serving as erythrocyte and tumorigenic cell models, respectively. We analyze the drug's effects on each lipid, employing techniques such as tensiometry, Brewster Angle Microscopy, and Infrared Spectroscopy. Surface pressure-area isotherms reveal that the acid expands both DPPC and DPPS monolayers, inducing visible morphological changes and forming interfacial aggregates. Moreover, the compound stabilizes previously compressed monolayers up to 30 mN/m, accompanied by a decrease in surface potential. Compression-decompression curves exhibit hysteresis in the presence of the compound, and rheological measurements indicate a reduction in the monolayers' viscoelastic modulus, altering film fluidity. Infrared spectroscopy highlights alterations in bands related to both hydrophobic and hydrophilic chains, elucidating specific interactions across all membrane regions. These results offer insights into the potential biological implications of the drug in cell membrane models, providing valuable information about molecular-level interaction mechanisms dependent on lipid composition. This research was supported by FAPESP (2023/07185-8, 2022/03736-7) and CNPq.

Exploring the Nanotoxicity of Senecioyloxy Kaurenoic Acid Utilizing Langmuir Monolayers as Nanomaterials Mimicking Cell Membranes

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Naturally occurring phytochemicals can manifest diverse biological effects, including antimicrobial and tumorigenic. These activities often entail interactions with lipid surfaces, such as those constituting cellular membranes. Langmuir films are a valuable tool for modeling these membranes, comprising an unimolecular assembly of amphiphilic molecules at the air-water interface. In this study, we isolated 15-senecioyloxy kaurenoic acid methyl ester, a compound with potential antiprotozoal properties, and incorporated it into Langmuir monolayers of 1,2-dihexadecanoyl-sn-glycero-3-phosphoethanolamine (DPPE), known to mimic protozoan membranes. We then characterized the monolayer through tensiometric measurements, Brewster Angle Microscopy, and rheological analyses using oscillating barriers. The pressure-surface area isotherms revealed that the antiprotozoal compound expanded the DPPE monolayer. Surface compressional data indicated that the compound hindered the lipid monolayer from attaining the solid state, rendering the film more fluid. Moreover, it destabilized previously compressed monolayers up to 30 mN/m and altered the morphological characteristics of the films. Compression-expansion curves exhibited hysteresis for the mixed monolayer, distinguishing it from the pure lipid. Rheology demonstrated that the compound reduced the viscoelastic modulus of the DPPE monolayer, rendering the film more fluid, a phenomenon correlated with hysteresis and surface compressibility. Notably, the monolayer containing the compound remained in the condensed liquid state even at low surface areas. Conversely, the pure and mixed lipid monolayers exhibited insignificant viscous contributions, primarily displaying elasticity. These findings underscore the interaction of this antiparasitic compound with cell membrane models, providing critical insights into its mechanism of action at the molecular level. This work was supported by FAPESP (2022/03736-7) and CNPq

Exploring the properties and applications of biogenic silver nanoparticles synthesized using Gomphrena vaga root extract

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In recent years, nanotechnology has been extensively utilized in research and development of materials with varied applications across multiple fields. Metallic nanoparticles, particularly silver nanoparticles (AgNPs), are notable in medicine for their biological, antimicrobial, and antiviral properties. Biogenic methods for obtaining AgNPs, using extracts and natural products, are preferred for their sustainable, easy, and biocompatible production. In this study, we synthesized AgNPs using the extract from Gomphrena vaga (G. vaga) root, an endemic Brazilian species used in traditional medicine, known for its analgesic, anti-inflammatory, and bronchodilator properties. The nanoparticles were characterized using UV-Vis spectroscopy, infrared spectroscopy, dynamic light scattering (DLS), transmission electron microscopy (TEM), and atomic force microscopy (AFM). Results showed the production of spherical and electrostatically stable AgNPs with an average yield of 68 ± 1%, diameter of 33.29 nm, zeta potential of -35.9 mV, and a polydispersity index (PdI) of 0.170. Antimicrobial tests determined the minimum inhibitory and bactericidal concentrations of AgNPs against Gram-positive and Gram-negative bacteria (P. aeruginosa, S. aureus, E. faecalis, E. coli), revealing significant bacteriostatic and bactericidal effectiveness starting from 13.18 µg/mL. Ongoing tests aim to investigate the main biomolecules involved in AgNP synthesis and stabilization via liquid chromatography-mass spectrometry (LC-MS), the impact on microbial metabolism through nuclear magnetic resonance spectroscopy, and the potential incorporation into bioactive material formulations, such as cosmetics.

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Fabrication of nanostructured devices inspired by the SARS-Cov 2 viral envelope: applications for sensing and understanding molecular interaction mechanisms

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Since the declaration of the global pandemic by the World Health Organization (WHO) due to the novel coronavirus SARS-CoV-2 and the ensuing COVID-19 outbreak, the urgency of long-term research aimed at developing antiviral medications, robust vaccines, and diagnostic sensors for detecting viral infections has become increasingly apparent. Understanding the chemical and morphological composition of viruses, as well as the biological processes involved in their infection, replication, and interaction with host cells, is crucial in this endeavor. The present study focuses on investigating the interaction between the SARS-CoV-2 Spike protein receptor (RBD) and heparins with Langmuir films composed of phospholipids, serving as models of cell membranes. Specifically, dipalmitodilphosphatidylserine (DPPS) and cholesterol were selected to mimic the viral envelope and the human cell membrane, respectively. The interaction between these compounds and lipid monolayers was evaluated through various measurements, including surface potential and pressure-surface area isotherms, compression-decompression cycles, surface pressure-time stability, surface rheology using oscillating barriers, and Brewster Angle Microscopy (BAM). By incorporating RBD and heparin into the monolayers, we observed changes in thermodynamic parameters, thereby shifting the isotherms. Rheological measurements were conducted to analyze the viscoelastic modulus of the monolayers, assessing whether the behavior of the films would become more fluid. Additionally, BAM was utilized to examine the morphological patterns of each monolayer. The results were evaluated to infer potential biological implications based on the effects induced by the bioactive compounds on artificial membranes. Through experimental analyses, could elucidate part of the mechanisms underlying the interaction between these compounds and phospholipids. This research received support from FAPESP (2022/03736-7) and CNPq.

Functionalization of Graphene oxide-based photosensitizers for application in photodynamic therapy

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Photodynamic therapy (PDT) is a therapeutic treatment for tumors, less invasive and with fewer side effects compared to chemotherapy and radiotherapy. The technique uses photosensitizers (PS) that, when activated by electromagnetic radiation, produce reactive oxygen species (ROS) with cytotoxic potential, resulting in the destruction of tumor cells. In this context, graphene oxide (GO) emerges as a promising PS, due to its biocompatibility, photothermal properties, high absorption in the near-infrared energy range (NIR), and capacity for fluorescence resonance energy transfer by (FRET) to adjacent chromophore molecules, aiming for increased therapeutic efficacy. In this study, our objective was to obtain GO with improved characteristics of hydrophilicity, dispersion, and biocompatibility. GO was synthed, characterized, and functionalized with methylene blue and the polysaccharide chitosan. Characterization of GO identified its structure and functional groups via X-ray diffraction (XRD) and Fourier-transform infrared spectroscopy (FTIR), while electron microscopy analyses (SEM and TEM) revealed the morphology and dimensions of the nanoparticles. Characterization by UV-Vis absorption revealed significant peaks corresponding to the specific absorption band of graphene oxide, confirming the efficiency in NIR light absorption, essential for the activation of photosensitizers in PDT. Functionalization with methylene blue enabled ROS production capacity, and conjugation with chitosan improved the hydrophilicity and dispersion properties of GO, which may be crucial for increasing its biocompatibility and distribution in the organism. These results suggest that the obtained PS presents significant potential for applications in PDT.

Gold-Decorated Graphene Oxide for Enhanced Biophotovoltaic Cells and Electrochemical Sensing Applications

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Carbon-based electrochemical sensors, such as graphene, stand out in electroanalysis due to their unique properties including chemical stability, mechanical strength, and superior thermal and electrical conductivities; coupled with low preparation costs and long-term stability. Graphene oxide, an oxidized form of graphene, is primarily prepared via the Hummers method and can be reduced to produce surfaces with oxygenated functional groups at the edges. This reduction results in reduced graphene oxide (rGO), which is significant in electrochemical sensors due to the enhanced conductivity from the restoration of conjugated carbon atoms. The use of rGO as a chemical modifier on various surfaces increases electron transfer kinetics, generating an electrocatalytic effect that enhances electroanalytical performance. The large-scale production of graphene nanomaterials faces challenges such as complex and costly traditional methods. Seeking alternative synthesis routes is essential to unlocking graphene's transformative potential. A promising strategy involves combining graphene with metal nanoparticles to form nanocomposites with enhanced synergistic properties. Metal nanoparticles, like gold, can modulate graphene's properties to meet specific application demands. Over the past two decades, there have been significant advances in developing various gold material morphologies, such as nanolayers and nanorods, driven by the phenomenon of localized surface plasmon resonance (LSPR). This optical phenomenon, involving the interaction between conduction band surface electrons and incident light, results in light scattering and absorption; influenced by the physical dimensions of the nanomaterials and their dispersion medium. This work explores the synergistic properties arising from the combination of reduced graphene oxide with gold nanoparticles in specific morphologies for biosensor applications. Understanding this combination is essential for developing new materials.

Hybrid Nanovesicles for Tumor-Specific Delivery of Bevacizumab in Lung Cancer

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Solid tumors, such as lung cancer, heavily rely on adequate blood supply for their growth, which is enhanced by angiogenesis. Bevacizumab (BVZ) is an antiangiogenic drug widely used in solid tumor chemotherapy, showing significant therapeutic efficacy by inhibiting angiogenesis and consequently, blood supply and tumor growth1. However, adverse effects related to intravenous administration of BVZ should not be ignored2. The development of nanocarriers capable of directing the drug to the site of action emerges as a promising alternative to optimize therapeutic efficacy and reduce side effects. Hybrid nanovesicles (NV), composed of tumor cell membranes (A549) and T lymphocytes (Jurkat), offer important advantages, such as specific delivery of the drug to the tumor microenvironment and the ability to evade the immune system. In this study, hybrid NV were synthed and characterized for tumor-specific delivery of BVZ. The NVs showed nanometric diameters, with drug-free samples (NV_Br) with a mean diameter of 243.1±30 nm and PDI of 0.45±0.05, while NV loaded with BVZ (NV_BVZ) exhibited a mean of 622.4±21 nm and PDI of 0.54±0.06. The zeta potential was -31.69±1.74 mV and -11.64±0.76 mV for NV_Br and NV_BVZ, respectively, indicating the physical stability of the systems. AFM demonstrated the spherical shape of the NVs. Total protein quantification revealed concentrations of 0.411 µg/mL, 0.441 µg/mL, and 0.189 µg/mL for A549, Jurkat, and hybrid membranes, respectively. The results indicate significant potential for the development of more effective and targeted therapies in lung cancer treatment.

Hypericum perforatum MEDIATING THE GREEN SYNTHESIS OF AuPt NANOPARTICLES FOR ANTIMICROBIAL APPLICATION

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The advancement of nanotechnology has enabled the development of nanoparticle (NP) based drugs applied in the treatment of microbial infections. Studies show that the simultaneous use of two metals in the preparation of NPs, results in nanomaterials with new properties due to the synergistic effect between them1. The use of natural processes to synthe NPs offers benefits such as resource availability and simplicity in the process. The green synthesis of bimetallic NPs mediated by natural extracts occurs through the reduction of metal ions to metallic NPs, due to the presence of reducing biomolecules contained in these extracts2. Thus, the present study aimed to obtain and characterize gold-platinum bimetallic NPs (AuPt-NP) from extracts of the plant Hypericum perforatum3 for antimicrobial application. AuPt-NP were obtained by mixing aqueous solutions of HAuCl4.3H2O and K2PtCl4 in a molar ratio of 4:1 for 1h. After this, the plant extract was added to the reaction medium under magnetic stirring for 24h. The obtained suspension of AuPt-NPs was characterized by UV-vis, XDR, and TEM. The UV-vis spectra showed a large band at 613 nm (AuPt-HYP), indicating a shift of the plasmonic band to longer wavelengths compared to the standard absorption peak at 520 nm of Au, suggesting a coating of the Au seed with Pt. The TEM images revealed NPs of 60 nm in and spherical structures of Au coated with a dendritic shell of Pt, as indicated by the arrows. The X-ray diffraction pattern showed characteristic peaks of Au and Pt. Thus, it is concluded that AuPt-NPs were successfully obtained through green synthesis using Hypericum perfuratum extract, and the evaluation of antimicrobial activity is planned for the next stage.

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Impact of Allura Red AC on mimetic gastrointestinal lipid membranes

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Consumption of Allura Red AC (AR), a synthetic dye commonly used in processed foods for enhancing color and texture, has been linked to an increased risk of developing inflammatory bowel diseases (IBD), characterized by chronic gastrointestinal inflammation1. Despite advancements in understanding and treating IBD, it remains incurable for many patients. Recent research has highlighted alterations in specific phospholipid ratios in intestinal cells of IBD patients, including phosphatidylcholine, phosphatidylethanolamine, and sphingomyelins (SM)2. This study aimed to explore the effects of AR on lipid mimetic structures resembling the plasma membrane of gastrointestinal cells. Lipids such as 1 palmitoyl-2-oleoyl-sn-glycero-3-phosphatidylcholine (POPC), 1-palmitoyl-2-oleoyl-sn-glycero-3 phosphoethanolamine (POPE), and SM were utilized to form lipid monolayers and giant unilamellar vesicles (GUVs), reflecting lipid bilayer structures in the gastrointestinal tract with a molar proportion of POPC/POPE/SM 3/1/1. Langmuir techniques, including π-A isotherms and Brewster Angle Microscopy (BAM), were employed to study monolayers, while GUVs were generated using the electroformation method and analyzed through fluorescent and phase contrast confocal microscopies. Interaction between AR (10-4 mol L-1) and ternary monolayers, observed throughout all compressed stages in π-A isotherms, displayed distinct lipid domain behaviors under specific surface pressures. In bilayers, AR incorporation induced various morphological changes on the GUVs, such as non-spherical shapes, budding transition, and lipid protrusions, illustrating the possible impact of AR on gastrointestinal cell membrane lipids and its role in potential damage to cellular integrity.

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Influence of synthesis parameters on magnetic nanoemulsion formulations loaded with xanthene photosensitizer

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According to the World Health Organization, prostate cancer ranks second in incidence and fourth in mortality among male oncological disease. In this scenario, photodynamic therapy and magnetic hyperthermia are promising treatment tools [1]. However, these techniques have limitations related to the bioavailability, toxicity in the body and non-selective accumulation in tissues, which can be reduced using nanotechnology by encapsulating the photosensitizer and magnetic nanoparticles in nanostructures. Thus, synthesis parameters of these nanostructures play a key role in achieving the appropriate , charge and stability for the formulation, especially the method of synthesis, homogenization and the interactions between the nanostructure components and the photosensitizer/magnetic nanoparticles. The aim of this study was to evaluate time and solvent extraction speed in ultra-homogenization, intrinsic to the method of synthesis by spontaneous emulsification in the nanoformulations. The effects of the concentration of Erythrosine, a xanthene-derivate photosensitizer, and maghemite magnetic particles on the particle , Zeta Potential and Polydispersity Index parameters were evaluated. Concentration values of 0.1 mg/mL and 1.0 mg/mL for the magnetic particle and concentrations of Erythrosine 0.5 mg/mL were tested with different Ultraturrax times (515 min.). Dynamic Light Scattering technique (DLS) was used for the analysis. In essence, was possible to elucidate the influence of concentration and intensity of homogenization on the stability profile of the MNE.

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Innovation in Physical Barriers: Development with Chitosan and Molle Essential Oil via Airbrushing

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In response to the growing demand for natural and sustainable products, this study explores the production of innovative physical barriers using chitosan and Molle essential oil through the airbrushing technique. Chitosan, a biopolymer of natural origin, is known for its antibacterial properties, biodegradability, low toxicity, and biological compatibility. Molle oil, originating from the Amazon region, has anti-inflammatory, antibacterial, healing, antiseptic, antifungal, and antioxidant properties, which can intensify the activity of the physical barrier to be produced. Preliminary results indicate that the distance between the tip of the airbrush and the collecting surface interferes with the formation of the films. The best distance found was 20 cm, as the resulting films were more uniform and flexible, while for the application at a distance of 30 cm there was a significant expenditure of material that was mostly projected by the airbrush outside the application surfaces due to the distance, in addition to less flexible and rougher films. Furthermore, the concentration of the polymer also proved to be an important factor, with the ideal concentration being 1.0% m/m. The films produced under these conditions showed greater flexibility, uniformity, and more suitable thickness. After standardizing the film production steps, the developed material, initially composed only of chitosan, was evaluated under different operating conditions. The best control membranes were selected for the subsequent addition of Molle oil. The resulting films will be characterized in relation to mechanical properties, cytotoxicity, controlled release, antioxidant capacity, thickness, water absorption capacity, water vapor permeability, infrared spectroscopy, and scanning electron microscopy. This study represents a significant advance in the production of biopolymeric physical barriers, with potential for applications in various industries.

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Integrating Folic Acid Targeting, PET Imaging, and Novel Chemotherapy into a Mesoporous Silica Nanoparticle Platform for Breast Cancer Treatment

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Breast cancer, a significant global challenge, necessitates substantial advances in diagnostics and therapy. This study addressed theranostics of breast cancer as a promising approach by combining 64Cu-based positron emission tomography (PET) diagnostic imaging with a novel mesoionic chemotherapy agent, MIH 2.4Bl therapy, into a single platform. By incorporating MIH 2.4Bl into mesoporous silica nanoparticles, this study also overcame an insolubility challenge of the drug. In addition, conjugation of the nanoparticles with folic acid (FA) allowed for the specific targeting of cancer cells that overexpress the receptor. The synthesis of the nanomaterial was achieved through functionalization with APTES, surface modification with FA, conjugation with DTPA, and adsorption of MIH 2.4Bl, which culminated in an integrated system. The resultant nanomaterial underwent comprehensive physical and chemical characterization. Testing confirmed the efficacy of drug adsorption, controlled release, and selective antitumor activity against the 4T1 and MCF-7 breast cancer cell lines over normal mammary epithelial cells. After complexation with 64Cu [1], PET phantom and in vivo imaging in BALB/c mice demonstrated the potential of the radiolabeled nanomaterial as a diagnostic agent. This study embodied an innovative nanotechnology approach by integrating FA targeting, PET diagnostics and therapeutic modalities for breast cancer treatment.

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Integrating Magnetic Resonance Imaging and Novel Chemotherapy for Breast Cancer Treatment: The Potential of Mesoporous Silica Nanoparticles

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Breast cancer poses significant global challenges, necessitating advancements in diagnostic and therapeutic techniques. This study explores an innovative theranostic approach using the nanomaterial called MCM-41-NH_2-DTPA-Gd^{3+}-MIH 2.4Bl, which combines mesoporous silica MCM-41 with the mesoionic drug MIH 2.4Bl and gadolinium, providing both drug delivery and Magnetic Resonance Imaging (MRI) capabilities. The extensive surface area and porosity characteristics make MCM-41 ideal for drug loading, and its conjugation with the ligand diethylenetriaminepentaacetic acid (DTPA) and complexation with Gd^{3+} further facilitates MRI applications. The synthed nanomaterial was characterized using SEM, FTIR, XRD, ICP-OES, porosimetry, and TEM techniques. Adsorption studies indicated that 15% of MIH 2.4Bl was effectively adsorbed onto the material, demonstrating its capacity for drug loading. The drug release assay revealed that approximately 50% of MIH 2.4Bl was released by 12 hours in a PBS/Methanol medium, confirming controlled release capabilities. In MRI phantom studies, the material demonstrated a significant longitudinal relaxivity (r_1) of 8.997 $s^{-1}\cdot mM^{-1}$, compared to 4.3 $s^{-1}\cdot mM^{-1}$ for the commercially available Magnevist, indicating superior imaging potential. Furthermore, in vitro cytotoxicity assays showed that the material effectively killed MDA-MB-231 breast cancer cells at an ED50 concentration of 12.6 mg/mL. The dual functionality of MCM-41-NH_2-DTPA-Gd^{3+}-MIH as a diagnostic agent was tested in vivo in a mouse model of breast cancer. These results demonstrated enhanced MRI signal after intratumoral administration of the nanomaterial. This work underscores the potential of MCM-41-NH_2-DTPA-Gd^{3+}-MIH 2.4Bl to enhance breast cancer diagnosis and treatment, combining high-sensitivity MRI imaging with effective drug delivery.

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INVESTIGATION OF BIOLOGICAL AND IMMUNOMODULATORY PROPERTIES OF BIOMIMETIC DELIVERY SYSTEMS

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The development of biomimetic nanosystems applying isolated cell membranes has enabled the creation of homologous structures that enhance nanoparticles' ability to interact with biological systems.1 Among their well-recognized advantages, the capacity to activate specific cellular components of the immune system towards processes of phenotypic reestablishment and functions initially impaired, provides to this structures, immunomodulatory properties.2–5 Here, we investigated the therapeutic / immunomodulation potential of a biomimetic nanostructured delivery system based on polylactic/glycolic acid (PLGA) carrying temozolomide drug decorated with cell membrane isolated from U251 glioma cell and T lymphocyte. Our results from the cell viability assay have shown a tumor cell viability decrease, especially compared with non-tumoral cells as a result of biomimetic nanosystems treatment. Further, the isolated membranes also have the potential to reduce cell viability, especially against its source cell. Therefore, further assays are undergoing to better understand the biological and immunomodulatory potential of those systems.

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LiCaAlF6:Eu nanoparticles for application in ionizing radiation dosimetry

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Ionizing radiation is widely used in medicine and industry, but its use must be controlled as it can cause serious harm to exposed people. Studies on LiCaAlF6:Eu single crystals showed that it has dosimetric properties such as radioluminescence/scintillation (RL), thermoluminescence (TL) and optically stimulated luminescence (OSL). Therefore, in this work we studied the synthesis and characterization of LiCaAlF6:Eu nanoparticles (NPs), as well as investigating and testing whether their excellent dosimetric properties observed in bulk are maintained when produced at the nanoscale. NPs are synthed by the hydrothermal method and the amount of solvents and dopants is varied. Structural and morphological analyzes were carried out, in which we observed that we obtained spherical particles with an average of approximately 170nm. These present good RL and OSL intensity, with the sample doped with 1% Eu being the best. These results demonstrate that LiCaAlF6:Eu NPs can be used as OSL dosimeters, providing a high degree of sensitivity. Furthermore, due to the fact that LiCaAlF6:Eu presents good RL intensity, its applicability in X-ray activated photodynamic therapy (X-PDT) is suggested for future studies.

Magnetic Fluid Hyperthermia (Fe_3O_4@SiO_2) Integrated with Thermally Induced Polymer UCST for Controlled Drug Release.

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Iron oxide magnetic nanoparticles, such as magnetite (Fe_3O_4), have been widely studied due to their potential in biomedical applications [1]. Their superparamagnetic property makes them excellent agents for magnetic hyperthermia (MH), a promising route in cancer treatment. However, the colloidal instability of Fe_3O_4 nanoparticles has been a challenge for their clinical application. In this study, we propose the synthesis of core-shell Fe_3O_4 nanoparticles coated with mesoporous silica (MS) and the copolymer poly(allylamine)-*co*-poly(allylurea) (AMPU), which has a Upper Critical Solution Temperature (UCST). The pores of MS will serve as reservoirs for the chemotherapeutic agent 5-fluorouracil (5-FU), while the thermally induced phase transition of AMPU will control the drug release [2, 3]. We anticipate that the heat generated by MH will elevate the local temperature, triggering the conformational transition of AMPU chains, resulting in the opening of silica pores and the controlled release of 5-FU.

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Mesoporous silica nanocarriers carboplatin encapsulated for lung cancer therapy

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Lung cancer was the most commonly diagnosed cancer in 2022, with approximately 2.5 million new cases reported. The standard treatment is platinum-based drugs, widely used for chemotherapeutic eradication of lung cancer. However, the side effects of these drugs, such as lack of selectivity, high systemic toxicity, and drug resistance, limit their clinical application. Nanotechnology is an alternative to resolving the gaps in conventional treatments through designing drug delivery systems. The mesoporous silica nanoparticles (MSN) are proposed as a potential drug delivery for targeted non-small cell lung cancer therapy. These nanoparticles were synthed by a co-condensation method and can act as nanocarriers of the chemotherapeutics drug carboplatin. Calcined MSN nanoparticles showed a diameter of ca. 90 nm, as observed by TEM microscopy, and a surface charge of -15.4 mV. MSNs functionalized with (3-aminopropyl)triethoxysilane (APTES) were treated with reflux registered a diameter of 120 nm with a surface charge of 35,2 mV. The conversion surface between siloxanes and hydrogen-bonded silanols along APTES functionalized led to MSNs with a hydrophilic surface, which is more advantageous for drug delivery systems, which was reviewed by Raman and FTIR spectroscopy. This condition increased the drug load by 10%, producing an encapsulation efficiency of around 50%. Cell viability analysis and cell uptake results showed that the nanocarrier was more effective than the isolated drug. Moreover, MSNs present low toxicity in non-cancer cells for up to 48 hours of treatment.

Mg-doped hydroxyapatite: synthesis, characterization and bioactivity evaluation for use in bone tissue regeneration

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In recent decades, the incidence of chronic degenerative diseases, cancer, injuries, and, osteoporosis, has increased due to the accelerated growth of the older population. Since autologous bone grafting is hampered by a rejection rate of more than 50%, this scenario has driven the search for alternative and innovative treatments. In this sense, materials as metals, polymers, ceramics, and composites have been extensively studied in order to improve their physicochemical and biological properties aiming its use in substitution to the natural bone transplantation [1]. Among innumerous materials, calcium phosphates, especially nano-hydroxyapatite (Ca10(PO4)6(OH)2), have been highlighted for their similarity in composition and physicochemical properties to the inorganic phase of bone tissue, as well as for their biocompatibility, bioactivity, and osteoconductivity [2]. Besides, hydroxyapatite (HA) similarities to the bone are enhanced when mimicking its porosity, particle, and the presence of essential ions such as magnesium (0.72 wt%), known to play a key role in mineralizing, growing, and forming hydroxyapatite by directly influencing in osteoblast proliferation. Furthermore, antimicrobial studies of hydroxyapatite doped with Mg2+ (HAMg) have demonstrated efficacy against gram-positive and gram-negative bacteria, reducing the risk of implant failure due to bacterial infection [3]. Aiming to contribute and promote advances in bone regeneration researchs, in this study we synthesized bioactives based on HAMg NPs with different Mg2+ contents (0; 2.5; 5, and 10 mol%) which were named HA, HAMg2.5, HAMg5, and HAMg10. The structural, textural and morphological properties of these bioactives were evaluated by FTIR, XRD, TEM, SEM and EDS, evidencing the production of nanomaterials similar to the bone, with adequate crystallinity, constituted by a main phase of porous HA and HAMg with flake-like morphology, and rod-like particles with size ranging between 20-180 nm.

Multiplex electrochemical biosensor for simultaneous detection of cutaneous leishmania and paracoccidioidomycosis

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Vulnerable populations frequently have little access to primary healthcare conditions. Neglected tropical diseases (NTDs) are ancient diseases that mainly affect these people. Some NTDs present similar symptoms, complicating diagnosis. Point-of-care (POC) devices based on biosensors that use nanotechnology bring the prospect of rapid and accurate diagnosis, avoiding the need for clinical laboratories. In this context, electrochemical biosensors offer the potential to employ an inexpensive tool with immediate results. This work aimed to develop a multiplex electrochemical immunosensor for differential diagnosis of cutaneous leishmania and paracoccidioidomycosis. The immunosensor board contains a gold counter electrode (CE), two gold working electrodes (WE) with a unique design interconnected by tracks, and an Ag/AgCl reference electrode (RE). The idea is to obtain distinct current ranges in the WEs and reduce production costs using one potentiostat. The antigen-antibody interaction was performed for L. *amazonensis* and P. *brasiliensis* antigens using the dot blot technique and electrochemical measurements. The immunosensor was constructed using the cystamine-glutaraldehyde system to immobilize the antigen in the WEs. The L. *amazonensis* and P. *brasiliensis* antigens were immobilized on different WEs and characterized by Fourier Transform Infrared Spectroscopy (FTIR), demonstrating the immobilization of the antigen to the sensor. Confocal microscopy analyses corroborate the efficiency of antigen immobilization. Electrochemical measurements DPV and CV demonstrate good reproducibility and stability of the biosensor. Initial evaluations of the developed multiplex electrochemical sensor showed promise for a new diagnostic multiplex test for cutaneous leishmania and paracoccidioidomycosis. Acknowledgments: CTI's Open Labs, Finep, CNPq (Nº 308649/2020-6 and 445443/2023-5) and CEPID/FAPESP-CDMF 2013/07296-2.

Nanoparticle Development for Chemotherapeutic Delivery in Lung Carcinoma Therapy

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Lung cancer ranks as the second most prevalent cancer in Brazil. While Paclitaxel (PTX) serves as a common chemotherapeutic agent for this disease its said effective are concerning. Among the new therapeutic strategies are delivery systems like solid lipid nanoparticles (SLN), combined with photodynamic therapy (PDT), recognized as a treatment modality for various neoplasms. This study endeavors to develop SLN for encapsulating PTX with the 5-aminolevulinic acid (5-ALA), aiming coning both therapies as strategy for lung cancer treatment. SLN were crafted utilizing the high-energy method. A high-shear homogenizer was used to the production of four systems: NLS, NLS-PTX, NLS-5-ALA, and NLS-PTX-5ALA. The resulting nanoparticles exhibited an average ranging between 170 and 222 nm, with a polydispersity index (PDI) around 0.2 and zeta potential ranging from -20 to -3mV. Stability assessments conducted over 35 days at 4°C revealed that the formulations remained stable over time. The encapsulation efficiency of PTX has reached an 99%, while that of 5-ALA 80%. The release profile demonstrated the nanoparticles' capability to control PTX release rates. Scanning electron microscopy (SEM) revealed nanoparticles with a spherical geometry and uniform distribution. The in vitro cellular viability assessment of NLS-PTX-5ALA revealed significant cytotoxicity of irradiated nanoparticles, underscoring their promising therapeutic potential in inhibiting cell proliferation.

Nanoproduct Contamination in Aquatic Ecosystems: Implications for Coastal Phytoplankton

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The daily use of nanoproducts has been exponentially increasing in recent decades. Cosmetic industries have been investing in the use of nano sunscreens in pursuit of stable and safe formulations, with high UV protection capacity and reduced opacity. However, there is still a scarcity of research on contamination caused by nanoproducts in aquatic ecosystems. In order to assess the nanoecotoxicological effects of nano products on representative phytoplankton communities of the Brazilian coast, this study conducted morphometric analysis of microalgae Tetraselmis sp. and *Chattonella subsalsa* exposed to increasing concentrations of a raw material for the production of nano-TiO_2-based sunscreens. Microalgae agglomeration were evaluated by morphological analyses by SEM micrograph and measurements using ImageJ software. The response to oxidative stress was verified by catalase and superoxide dismutase (SOD) assays. The results showed that *Tetraselmis sp.* microalgae formed cellular aggregates that increased in area in a dose-dependent manner, starting from 25 mg/L. *Chattonella subsalsa* algae did not show aggregate formation and exhibited a significant increase in catalase production after 96 hours. The increase in antioxidant enzymes, cellular growth, and absence of aggregate formation in *Chattonella subsalsa* cells suggest potential impacts on organism selection, favoring certain species over others in the marine environment.

Nanostructured layer-by-layer immunosensors for detection of the cancer biomarker p53

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The molecular control imparted by methods such as the layer-by-layer (LbL) film assembly allows for fabricating tailored devices, including high-performance biosensors. In this work, we developed nanostructured architectures using the LbL technique to produce a biosensor for detecting the cancer biomarker p53 antigen. LbL films with 1, 3, and 5 bilayers of chitosan/chondroitin sulfate were deposited on interdigitated gold electrodes, with the carboxylic acid molecules in the LbL film being activated using a combination of EDC/NHS. The active layer of the immunosensor contained anti-p53 antibodies. Detection of the p53 antigen was made by measuring the capacitance spectra in the frequency range from 1 Hz to 10^6 Hz. Upon interaction with the antigen, changes in capacitance occur at medium and low-frequency regions owing to electrical double layer effects [1]. An increase in capacitance due to the antigen-antibody complex formation [2] may be interpreted as the accumulation of charges on the sensors. The detection limit was calculated using the IUPAC method described by $\text{LoD} = S_0 + 3 \times \text{SD}$. The highest sensitivity was obtained with a single bilayer of chitosan/chondroitin sulfate, probably because of the small film thickness which had a large influence on the charge accumulation in film [3]. Taken together, these results indicate that optimized biosensing of cancer biomarkers can be obtained with tailored molecular architectures.

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NdNiO3 NANOWIRES APPLIED TO BIOSENSOR DEVICES

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Nowadays flexible and wearable electrochemical devices have been extensively studied as no-invasive tools to monitor biological substances, for example, dopamine, ascorbic acid, and glucose.[1-2] These biosensors are important in the prevention and the control of several diseases. This work focuses on the production of Fe-doped NdNiO3 nanowires with electrospinning procedures, which are characterized and applied in electrochemical devices. Preliminary results of X-ray diffraction revealed the presence of Bragg reflections belonging to the orthorhombically-distorted perovskite structure (Pbnm) of the NdNiO3 phase, without any additional phase.[1] Scanning electron microscopy revealed nanowires microstructure with diameters of 100 to 200nm and lengths of several micrometers. These samples will be decorated with gold nanoparticles, which will be linked to cysteamine and the necessary enzyme to detect biological substances. Then this material will be used in flexible electrochemical electrodes to evaluate their biosensor responses.[2]

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Nonwoven membranes of poly (L-lactic Acid) with Basil Essential Oil for Skin Wound Healing

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Advanced wound dressings have properties of biocompatibility, physical-mechanical adaptability, and hygroscopic control [1, 3]. However, the potential risk of bacterial resistance due to the inappropriate use of antibiotics and the considerable volume of infectious waste discarded during the wound care period entails a negative impact on the ecological balance, an increase in the prevalence of diseases, and the generation of important economic expenses at a global level [1-3]. In this work, were developed electrospun fibers of poly (L-lactic acid) (PLLA) with basil essential oil (BEO) at concentrations of 1%, 5%, 10%, and 20% to obtain non-woven membranes with improved biological and mechanical properties for potential use as wound dressings with minimal ecological impact post-use. Were identified the active components Estragole and Linalool in BEO, which contribute to its antibacterial, anti-inflammatory, and analgesic properties. PLLA fibers with encapsulated BEO were successfully produced, free of defects, with an average distribution ranging from 620-787 nm and improved mechanical characteristics. The PLLA/BEO non-woven membranes exhibited initial degradation effects during soil burial after 60 days of exposure, with a subsequent loss of mass after 210 days. In in vitro degradation assays, they showed the onset of degradation, indicated by mass loss after 120 days of exposure in simulated physiological medium (PBS) at a temperature of 39 ± 1 °C.

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Novel biopolymeric nanocapsule for controlled release of lithium in the treatment of neuropsychiatric disorders

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Neuropsychiatric disorders (ND) are currently among the leading causes of global disability [1,2]. Lithium carbonate (Li2CO3) is one of the main drugs used for treating such disorders, but it is often associated with side effects. This study describes the synthesis and application of a novel biopolymeric nanocarrier to encapsulate Li, with the aim of mitigating side effects while increasing therapeutic efficacy. To achieve this objective, the preformed polymer interfacial deposition method for Li encapsulation was employed, using poly-ε-caprolactone (PCL), Span and Tween 80. The prepared nanocarrier was characterized using TEM, FT-IR, XRD, DLS, and Zeta . The results revealed a spherical morphology with an average of 219 nm, and a particle dispersion measurement of 0.97, indicating a homogeneous distribution of the nanocapsules. Furthermore, the Zeta potential was measured at -32 mV. In vitro studies to evaluate (i) drug loading capacity, (ii) controlled drug release, (iii) permeation and penetration of biological barriers, and (iv) toxicity are in progress and will be presented at the event.

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Novel Synthesis of Cerium Oxide Nanorods via Hydrothermal Method for Enhanced Biosensor Applications

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Nanotechnology and the use of nanoparticles (NPs) are fundamental for advancements in biomedicine, especially in biosensor technologies. In this context, cerium oxide nanoparticles (CeO2NPs) stand out due to their unique mode of interacting with biological systems and their applicability in detecting and monitoring biomedical conditions with high precision. The choice of the synthetic route is crucial for defining the morphology of NPs, especially in obtaining cerium oxide nanorods (CeO2NRDs), due to their capacity to directly influence the shape, surface, and crystalline structure of the particles. Hydrothermal methods, such as conventional and microwave-assisted hydrothermal (MAH), are fundamental for controlling the characteristics of NPs. Thus, the motivation of this project is to understand the effect of synthesis time on the formation of CeO2NRDs obtained by conventional and MAH hydrothermal methods. For the MAH synthesis, the procedure will be carried out using cerium(III) chloride heptahydrate [CeCl3 . 7H2O, 0.05 M] and potassium hydroxide [KOH, 6M] as precursor and mineralizing solution, respectively, under different radiation times (1, 2, 4, and 8 min) at 180°C. The XRD results showed a cubic fluorite-type structure. FESEM images revealed that different times form nanorods, but at shorter times, other morphologies are formed. The optical bandgap of the samples is around 3.2 eV. Raman data revealed specific characteristics of CeO2, such as vibrational modes related to the fluorite structure, including the F2g band at approximately 465 cm^{-1}, with a linewidth of 12 cm^{-1}, indicating the cubic symmetry of the material. Additionally, the Raman spectrum showed the presence of a secondary band at 600 cm^{-1}, associated with oxygen defects. . Understanding the effects of synthetic processes will enable the development of innovative new materials for biomedicine.

Paclitaxel encapsulation in cell membranes-coated PLGA nanoparticles for Neuroblastoma therapy

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Neuroblastoma (NB) is an extracranial malignant tumor that mainly affects newborns, infants, and children. Despite advances in conventional treatments, few successes have been achieved in terms of patient survival rates, which are still considered very low. This scenario underscores the severity of the situation and the urgent need to seek more effective therapeutic alternatives. Nanotechnology represents a promising strategy, offering numerous possibilities for directing drugs to specific tumor targets, thereby improving their pharmacokinetic and pharmacodynamic properties while reducing toxicity [1]. In this study we used a high-performance liquid chromatography (HPLC) method to quantify the amount of paclitaxel (PTX) encapsulated in poly(lactic-co-glycolic acid) nanoparticles (PLGA NPs). The nanoparticles were synthed using the nanoprecipitation method and a high Encapsulation Efficiency (EE) (99.3%) was achieved. For PTX quantification, an analytical C18 column was used with a mobile phase of water and acetonitrile (55:45, v/v), at 40 °C and flow rate of 1.1 mL/min. The method exhibited selectivity, accuracy (100.3%) and reproducibility, indicating its suitability. With a limit of detection of 0.607 µg/mL of PTX and rapid analysis (~6.5 min of retention time), it allowed the effective quantification of PTX in PLGA NPs. The utilization of nanotechnology for PTX delivery may enhance therapeutic efficacy, overcome the limitations of conventional treatments, and advance targeted NB therapy [2].

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PASSIVE DIFUSIVITY IN STRATUM CORNEUM MEMBRANE OF NANOEMULSION BASED ON *CARAPA GUIANENSIS Aubl.* and Fe_3O_4 NANOPARTICLES

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The present work aimed to evaluate the passive diffusivity of a nanostructured complex based on nanoemulsions (CGNE), derived from the vegetable oil of *Carapa Guianensis Aubl.* and doped with Fe_3O_4 nanoparticles, through the *Stratum Corneum* (SC) membrane. Fe_3O_4 was synthed by the coprecipitation method and CGNE by ultrasonic homogenization [1]. To evaluate passive diffusivity, in vitro permeation studies were carried out using an adapted Franz-type diffusion cell [2]. Nanoemulsions were prepared in four different proportions and characterized by TEM, OM, XRF and UV-vis. To measure diffusivity, 3 ml of CGNE were added to the donor compartment and 50 ml of a receptor solution to the lower phase. Using UV-Vis and XRF measurements, it was possible to estimate the molecular flow and permeability coefficient of the samples. TEM Micrographs showed the spherical shape of CGNE. The XRF data indicates traces of Cu and Fe. For passive diffusivity calculations, the CGNE sample showed the highest molecular flux and permeability coefficient, followed by CGNE 1 and CGNE 2. For the CGNE 3 sample, the data were inconclusive. OM micrographs of the SC membrane showed high concentrations of the samples in the SC capillaries. The data indicate that the developed nanoemulsions permeated the SC membrane. The efficiency in the diffusion process may be related to the concentration of Fe_3O_4 in relation to *C. Guianensis oil*. The data indicated that the diffusion process occurred intercellularly. The material showed good diffusivity and could be useful for encapsulating drugs.

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Pectin-based hemostatic biofilms doped with Bi-NP for medical and dental use.

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Despite the existence of a diversity of hemostatic agents, whether organic or inorganic, there is still a need for new and more effective materials in surgical centers and emergencies. This work was dedicated to studying the anti-hemorrhagic effect of biofilms based on Pectin (Citrus), which were incorporated into calcium by the Cross-Linking method[1], and also the synergistic and antimicrobial effect of metallic Bismuth[2] nanoparticles, which were synthed, characterized and incorporated into these biofilms using the nanodispersion technique and the casting method[3]. This new investigation into Bi-pectin nanocomposites presents a hybrid material with excellent potential due to the synergy between the hemostatic effect and antimicrobial action, preventing bacterial infections, thus improving wound treatments and surgeries and controlling bleeding in general.

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Pectin nanoparticles for encapsulation of antidiabetic agents

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Type 2 diabetes mellitus (DM2) is an exponentially growing condition of dysfunctional glucose regulation in the body[1]. Sotaglioflozin has emerged for innovative treatment which acts as an inhibitor of sodium-glucose co-transporters 1 and 2 but has shown side effects such as chronic diarrhea[2]. Encapsulation of the drug in pectin nanoparticles is expected to provide controlled and targeted release into the kidney to reduce adverse effects and to improve efficacy. Herein, pectin nanoparticles were synthed using an aqueous solution at 1.5% in mass and dripping of chloroform under magnetic stirring. The particles were characterized regarding size and morphology by dynamic light scattering and transmission electron microscopy. The release kinetics were studied by synthesizing pectin nanoparticles with rodhamine B. Then, aliquots of the stock suspension were incubated at 37 °C for different times. UV-Vis spectroscopy was carried out in the 260-800 nm range (FS5 Edinburgh S.A.) to quantify released rhodamine B. Cytotoxicity was evaluated by the MTT method with mesangial kidney cells (CMHI) for 24 h. Hydrodynamic diameter distribution of pectin nanoparticles in aqueous suspension was wide with a predominance of nanoparticles in the 70 nm range, although other particles were present between 260-3000 nm. TEM micrographs showed irregularly-shaped quasi-spherical nanoparticles with 62 nm average diameter. The release kinetics of rhodamine B followed the model of Korsmeyer-Peppas with a diffusional coefficient of 0.388 that is attributed to a pseudo-fickian mechanism. Therefore, the release was driven by the diffusion of rodhamine B throught the polymer. The CMHI cells showed viability of 73% when incubated with pectin nanoparticles at 3.75 mg/mL. In conclusion, pectin nanoparticles showed suitable properties for the encapsulation of sotaglioflozin and the future in vivo assays as antidiabetic agents.

Photoactivated sensor based on plasmonic nanoparticles for thyroid hormone detection.

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Plasmonic nanoparticles have an important intrinsic characteristic after photoactivation. The localized surface plasmonic resonance is capable of being activated by irradiating light at the same wavelength as the plasmonic band found in nanoparticles, increasing the number of “hot electrons”. The photoactivation of sensors containing gold nanorods (AuNRs) is advantageous, as it increases these electrons generated by irradiation on the surface of the sensor, which can make it more catalytic, and, therefore, increasing the sensitivity and detection limit of the analyte of interest. The objective of this study was to synthe and build a photoactivated sensor based on gold nanorods for the detection of the thyroid hormone Thyroxine (T4). For this, gold nanorods (AuNRs) were synthed, modified with PAMAM-G2 dendrimers, whose longitudinal is 59.24 ± 4.16 nm and transversal of 3.19 ± 0.04 nm, with PdI of 0.702 ± 0.026, Zeta potential of +15.2 ± 1.18 mV and conductivity of 0.015 ± 0.007 mS/cm. The sensors were built using indium tin oxide electrodes modified with PEDOT: PSS and AuNR using the layer-by-layer technique for the construction of sensors with 5, 10 and 15 bilayers, with the aim of seeing the response in function of the greater production of hot electrons. Chronoamperometic measurements were performed in phosphate buffer 0.1 mol/L pH 7.0 in the presence and absence of the hormone T4, and in the presence or absence of laser at 808 nm, close to the maximum value of the AuNR plasmon resonance length 820nm. The results indicated a considerable increase of 100.17 % in current due to photoactivation, indicating that the method used is suitable for analyzing this analyte.

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Photoactivity of iron-phenanthroline complexes conjugated to nanoparticles

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Iron-phenanthroline complexes are under investigation as alternatives to photosensitizers to be applied in photodynamic therapy. These complexes act under UV light irradiation and some studies have reported on their high photoactivity even in the absence of oxygen. In this work, the photoactivity of organocalcogen derivatives1 of iron-phenanthroline complex, Fe(PhenSe)3 and Fe(TDZP)3 was characterized at different concentrations and irradiation conditions in metastatic melanoma B16-F10Nex2 tumor cells. The cytotoxicity and photoactivity of the complexes were evaluated using the MTT assay in B16-F10Nex2 cells at different concentrations and irradiation conditions. It was observed that the Fe(TDZP)3 was more photoactive and showed greater cytotoxic effect when irradiated under 252 nm (0.053 W/cm2) for 10 min and at 17.5 µM. Under these conditions, the cell viability was about 35% but the photoactivity did not increase with the complexes concentration. Therefore, Fe(TDZP)3 and Fe(PhenSe)3 were encapsulated into PLGA nanoparticles and also conjugated to gold nanoparticles in order to enhance the complexes cell internalization and their in vitro photoactivity. PLGA nanoparticles presented hydrodynamic diameter of 139 ±30 nm and gold NPs 36± 1 nm. The highest photoactivity was observed in the PLGA nanoparticles encapsulating Fe(TDZP)3 at 3.2 and 0.64 µM. At these conditions, cell viability decreased 20% and 40% after irradiation (252 nm; 0.053 W/cm2; 10 min) compared with the control group (irradiated cells in the absence of complexes). Notably, the NPs were photoactive at a concentration 100 times lower than the reported concentration of iron-phenanthroline complexes that induced DNA degradation2. <div>Aknowledge: PIBIC CNPq; FAPESP 2022/00662-2</div> <div>References: 1Braga, H.C., Salla, C. A.M., Bechtold, I.H., Bortoluzzi, A.J., Souza, B, Gallardo, H. The effect of spin–orbit coupling on selenadiazolo- and thiadiazolo- fused 1,10-phenanthrolines. Dyes and Pigments. V.

Physical-chemical characterization of biomimetic nanovesicles loaded with doxorubicin and erlotinib

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The use of biomimetic nanovesicles as drug delivery carriers has gained attention as a promising strategy for cancer treatment. This strategy relies on homotypic recognition of nanovesicles (NVs) to their parental cell, promoting improved bioavailability and specific targeting. In the present study, NVs were synthed from A549 lung cancer cell lineage and loaded with doxorubicin (DOX) and erlotinib (ERL). Their physical-chemical parameters such as , zeta potential, morphology and chemical composition were assessed. Dynamic Light Scattering (DLS) data showed, for blank and loaded NVs, an average of 187±43 nm and 257±23 nm, and zeta potential of -10±3 mV and -18±5 mV, respectively. Nanoparticle Tracking Analysis (NTA) revealed s of 163±9 nm and 187±17 nm for blank and loaded NVs. Images of the NVs were obtained using Atomic Force Microscopy (AFM) and Transmission Electron Microscopy (TEM), allowing for a better visualization of NVs surface and morphology. In addition, Raman and Fourier Transformed Infrared (FTIR) Spectroscopy studies were conducted to characterize samples according to their chemical composition. These results of the NVs physical-chemical characterization demonstrate the potential of this novel nanosystem for targeted lung cancer treatment.

Polyelectrolyte nanocomplexes: a strategy to overcome bevacizumab resistance in glioblastoma cancer therapy

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Monoclonal antibody therapy with Bevacizumab (BVZ) have been a promising treatment option. However different mechanisms of resistance alter significantly the extracellular matrix (ECM), leading to cancer recurrence. Nanoparticles were synthed by combining oligomeric chitosan and dextran sulfate to form polyelectrolytic complexes (nanoPECs), which were used to encapsulate BVZ. Both compounds exhibit ECM activity water solubility, biocompatibility, and biodegradability. NanoPECs were planned using Minitab software by desirability function, which led to a formulation with a maximum encapsulation efficiency of 86% (213 µg/mL) and presented a of 244.2 ± 10.3 nm and Pζ of -34 mV. NTA analysis showed a concentration of 2,04 x 10 09 ± 0,36x 109 particles/mL. NanoPECs showed high colloidal stability for 11 weeks in coherent values for , zeta potential, and PDI. Cell viability in human adenocarcinoma (A549) was analyzed using MTT assay. After 48 hours, up to 30% mortality rate was observed. In conclusion, the NanoPECs are promising BVZ delivery system with anti-angiogenic application in glioblastoma cancer therapy.

Polymeric Nanoparticles Functionalized with RGD Tripeptide for Targeted Delivery of 5-Fluorouracil in the Treatment of Colorectal Cancer.

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Cancer ranks among the leading causes of mortality globally, with colorectal cancer standing as the second most lethal [1]. 5-fluorouracil (5-FU) is a chemotherapy drug commonly used in its treatment. However, in advanced cases, its efficacy is limited, with response rates below 15%, and it often induces hematological, neural, cardiac, and dermatological side effects [2]. Hence, exploring alternatives to enhance cancer chemotherapy is imperative. In this study, we fabricated nanoparticles composed of poly(lactic-co-glycolic acid) (PLGA) for delivering 5-FU (NP-5-FU) via the double emulsion method [3]. These nanoparticles exhibited a medium of 233.2 nm, a low polydispersity index (PDI) of 0.1, and a zeta potential of -30.62 mV, with a concentration of approximately 1012 nanoparticles/mL. Additionally, the encapsulation efficiency reached 71.4%. These findings highlight promising attributes such as favorable and stability. Functionalizing the nanoparticles with RGD holds the potential to enhance chemotherapy by enabling targeted and more effective treatment. Moreover, toxicity assessments and studies on internalization kinetics will complement our understanding of the nanoparticles' behavior.

Polyurethane-based flexible nanocomposites for tactile sensing applications

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Wearable devices are great allies in the healthcare field, as they offer the possibility of real-time monitoring in a much more accessible way to the population and in their daily activities. The main characteristic that these sensors must present is to be flexible and soft so that a good mechanical contact is achieved between device and biological tissues such as human skin [1]. Following this idea, the focus of our project is the fabrication of flexible composites to be incorporated in wearable devices for potencial neuroplastic training of patients with motor deficits. Aligned with this goal, we studied the synthesis of polyurethane foam/nanomaterial composites. The polyurethane used in our work was treated with additives to delay their degradation, and PEDOT:PSS [3] or reduced graphene oxide (rGO) were used as nanomaterials. The composites were characterized structurally and electromechanically in order to determine if these low-cost materials provide suitable conversion coefficients, strength, and resilience for use as pressure sensors, targeting ranges of interest for tactile transduction (for humans: 100Pa a 100kPa)[2]. Using Raman Spectroscopy, scanning electron microscopy and resilience test with a step motor-based setup, we were able to determine that the nanomaterial incorporation into the foam volume is uniform and that the time and electrical response of the synthed composite are suitable for the intended applications.

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PPy/SiO_2 film for electrochemical adsorption of organic micropollutants

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In recent years, conductive polymers, particularly PPy and PANI, have been highlighted in their use as adsorbent materials, due to their properties, such as hydrophobicity, acid-base character, π-π interactions, functional groups, ion exchange properties, and electroactivity. The combination of conductive polymers with inorganic particles is currently common in literature, numerous works report this combination to apply in the most different areas, in particular, silica-based materials are very attractive for adsorption purposes. The association of silica with conductive polymers provides unique characteristics and properties, with great potential in the application for adsorption of micropollutants in environmental matrices with electrochemical control. The present work proposes the electrochemical synthesis of hybrid materials (PPy and SiO2), to be used as adsorbing materials for micropollutants. The silica was obtained by the Stober method and was used in the SDBS solution and the pyrrole monomer was used to form the PPy/SiO2 film. By using SEM it was possible to observe the formation of a polypyrrole globular, the energy dispersive spectroscopy technique confirmed the presence of silica on the polymeric matrix. FTIR spectra confirmed that no structural changes occurred in the PPy film during silica formation. Adsorptive experiments with electrochemical control were carried out indicating that the material is promising as an adsorbent substrate for organic micropollutants with electrochemical control.

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Production and main properties of green hybrid reinforcement containing montmorillonite and nanobioglass from agroindustrial waste for bone regeneration

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Currently, bone systems denote a series of consequences mainly in the reduction of properties compromising the quality of life [1]. The (agro)industrial waste constitutes a major socio-environmental problem when incorrectly managed [2]. The combination of nanomontmorillonite (MMT-NPs) in a glassy system as nanobioglass (MgNPs-BV) facilitates the adsorption of biomolecules enabling the entry of ions with a focus on increasing the rate of bone formation [3]. The work aims to produce/characterize a hybrid reinforcement (MMT-NPs@MgNPs-BV) for application in bone regeneration, where the ideal synthesis condition was determined by CCRD. The samples were characterized by XRD, SEM-FEG, ZP, and contact angle measurement. *In vitro* safety profile was carried out in 293T and OFCOL II cell lines to verify the bioactivity; and biodegradation for verifying the release of ions (P^{3-}, Mg^{2+}, and Ca^{2+}). The ideal condition was [MMT-NPs]=30 wt.%, [MgNPs-BV]=6 wt.%, and calcination temperature of 1273 K with cell viability around 66% (293T), average crystallite diameter around 12 nm, and contact angle of 17°. The characterization confirmed the impregnation method with the following characteristic phases Muscovite 2M1, Neighborite, Quartz Low, Kaolinite 2M, and Phosphorus pentoxide, and ZP=-12.05 mV. MMT-NPs@MgNPs-BV showed cell proliferation of around 96% (OFCOL II) compared to the NC with biodegradability of 82% (56 days) and release of ions with a Ca/P ratio of 1.42. Therefore, the MMT-NPs@MgNPs-BV may offer a promising alternative to replace or increase bone tissue regeneration.

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Reduced Graphene Oxide Quantum Dots for bioimage applications systems

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Quantum dots are semiconductors that do not exceed a few nanometers of dimension. Their optical, electronic and chemical properties, which may be adjusted by changing composition, , and synthesis parameters. This tunability pushes these nanocrystals into different types of applications such as biomedical and environmental ones [1]. Thusly, material presents different properties than usual due to quantum confinement, making it a promising choice for applications in analytical chemistry, cell biology and medicine [2]. Therefore, these nanomaterials provoke some concerns about their use regards the inherent toxicity related to the most efficient emission QD based on heavy metals [1]. In this sense, the reduced graphene oxide quantum dots (rGOQDs), due to their excellent photoluminescence properties, biocompatibility and good water solubility, they have become excellent alternatives in the development of materials [3]. Then, this research produced rGOQDs by converting graphite into graphene oxide using the modified Hummers method. The material was characterized by FTIR, UV-Vis, XRD and TEM. In FTIR, bands related to the graphite oxidation process were observed, with bands at 3123, 2364, 2107, 1559, 1339 and 1038 cm-1. In the UV-Vis spectrum, bands at 233 and 300 nm referring to the π→π* transition were visualized. In the XRD spectrum, the presence of peaks at 25.05°, referring to graphite oxidation. Additionaly, in the TEM images, rGOQDs quantum dots with a distribution of 1.1 ± 0.23 nm were observed. These results demonstrated that the QDs obtained are of excellent quality, very promising for applications in bioimaging systems.

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SANS data analysis of poloxamer-based drug delivery systems

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Poloxamer-based drug delivery systems are widely used in the pharmaceutical industry. The structural characterization of these systems is crucial for the development of new drug delivery systems and for the optimization of their properties. In this study, we used small-angle neutron scattering (SANS) to investigate the structure of poloxamer-based drug delivery systems. The samples were measured using the VSANS-V16 instrument at the Helmholtz-Zentrum-Berlin (HZB), Germany. The samples contained 20% poloxomer (PL407) and between 0.1% and 1% of the drug (Nystatin, Prednosolone, Resveratrol, Doxycycline, Rambutan, Mangustan, Diclofenac, Ketoprofen, Ibuprofen, Paracetamol, Ethanol), in deuterated water (D2O). The samples varied in terms of drug quantity and temperature (25ºC, common storage temperature; 37º C, human body temperature; 40ºC, the temperature of an individual with fever). The analysis of the systems consists of modeling the data using a model assuming an interacting isotropic solution of polydisperse spherical micelles with interparticle structure factor described within the local monodisperse approximation regime. This allows us to obtain important information about the system, such as the radius of gyration, average radius, aggregation number, and total excess scattering density of a chain in the core and corona [1,2]. The results will contribute to the development and optimization of new drug delivery systems that are more effective and safer for medical applications.

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Silica nanoparticles as a dopamine inducer vehicle to increase fish fertility

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Environmental techniques related to nanotechnology have shown great potential for overcoming environmental challenges, such as the extinction of species crucial to their ecological niches. Inducing fertility through controlled release of inducers has proven effective for both commercial reproduction and river repopulation. Among the materials studied in the literature, silica (SiO_2) presents a unique combination of desirable properties, such as low toxicity, high biocompatibility, and biodegradability, having been investigated for its applications in different fields, such as potential applications in the medical area for drug delivery, tissue engineering, and imaging diagnostics, and in the environmental area for water treatment, air purification, and soil remediation. In the current context, the insertion of dopamine inducers into mesoporous SiO_2 nanoparticles is being explored as an alternative method for repopulating rivers and producing these fish in captivity on a commercial scale, which would reduce production costs, preserve rivers, and ensure the effectiveness of the method. This study focuses on the effects of different nanoparticle s and hormonal inducers on the reproduction of rheophilic fish of the Brycon genus, threatened by sports fishing and meat trade. In this work, the synthesis, characterization, and optimization of the parameters of adsorption and release of dopamine-inducing drugs, such as the drug domperidone, were studied. Silica nanoparticles were synthed by the modified Stober method with different s and subjected to optical, spectroscopic, and structural characterizations, as well as release and incorporation assays with dyes.

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Spectroscopic pH responsive analysis of the coumarin derivate 4-Methylesculetin

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Coumarins have been highlighted in biotechnology because of their therapeutic effects such as anti-inflammatory, antioxidant, and antimicrobial. A derivative compound of coumarin, 4-Methylesculetin (4-Me), showcases distinctive optical qualities, positioning it as a promising theranostic agent possessing both therapeutic and diagnostic capabilities. The chemical structure of 4-Me depends on the medium pH, influencing its biological activity and optical properties in living organisms. This study aimed to analyze the molecule 4-Me using UV-Vis absorption and fluorescence emission spectroscopies. Data were collected at different pH levels (2-12). Additionally, time-resolved fluorescence experiments were employed to investigate the pH-dependent interactions of 4-Me. Coumarin 4-Me exhibited variations in spectral behavior depending on the pH of the aqueous solutions. The positioning of the bands in both UV-Vis and fluorescence spectra was influenced by increasing pH, shifting towards longer wavelengths. There was also a significant alteration in emission intensity which can be correlated with the quantum yield and time-resolved analyses: longer average lifetime calculated for deprotonated 4-Me at pH 12 goes to shorter values at pH 2,0, suggesting faster fluorescence decay for neutral 4-Me species. Such understanding supports the rational design and optimization of 4-Me as a potential therapeutic agent for inflammatory diseases.

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Stability and in vitro release assessment of quercetin nanoemulsion

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Quercetin is a flavonoid belonging to the sub-class of flavanol with recognized biological activities. However, these activities are limited due to its poor aqueous solubility. Therefore, this study aimed to develop and characterize nanoemulsion (NE) containing quercetin. NE formulations were prepared using phase inversion temperature method [1] and characterized in relation to size, polydispersity index (PdI), physical stability, and in vitro release. For unloaded NE formulations, droplet size ranged from 65 to 470 nm and PdI values between 0.09 and 0.63. Quercetin-containing NE (Qct-NE) showed average diameter of 60.6 nm (±4.08) and PdI 0.085 (±0.005) demonstrating that nanosized oil droplets were formed with narrow distribution. Stability study was performed using the analytical centrifugation method with photometric detection. According to stability testing, F1, F2, F3, F4, and Qct-NE formulations were considered stable with lower droplet migration velocities and instability index below 0.076. In addition, there was no statistically significant difference ($p > 0.05$) of droplet and PdI from NE before and after analytical centrifugation assay. In vitro release experiments were carried out using the dialysis technique and under sink conditions. Following 154 h of experiment, 71.4 % (±8.12) and 8.9 % (±1.25) of nanoemulsified and free quercetin, respectively, were released. Hence, in vitro release study confirmed that NE could modify the quercetin release profile improving its dissolution rate when compared to coarse dispersion (free quercetin). In summary, we have successfully developed a stable NE containing quercetin using a low-energy emulsification approach.

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Strategies for improving radiotherapy effectiveness of bismuth sulfide nanoparticles

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Radiotherapy is a fundamental tool for treating over 50% of cancer patients. However, its impact can affect healthy tissue, leading to adverse effects on patients. One potential solution lies in the use of radiosensitizers, which enhance the effectiveness of radiation on tumor cells, thereby reducing the necessary radiation dosage.

In this study, we investigated bismuth sulfide (Bi2S3) nanoparticles as promising radiosensitizers. These were synthed via the hot injection technique, followed by ligand exchange with Polyvinylpyrrolidone (PVP) to enhance their suspension in biological media and biocompatibility [1].

Nanoparticles can be captured in tissues passively or actively. Active capture, which can be achieved through ligand addition, can enhance nanoparticle arrival and/or retention in tumor cells, improving therapeutic efficacy [2]. Therefore, to enhance the selectivity of Bi2S3 nanoparticles, we proposed functionalizing them with Flavin Mononucleotide (FMN). FMN is a derivative of riboflavin, which has several elements implicated in its internalization, including its carrier protein and three transporters found to be overexpressed in various cancers [3].

To achieve this functionalization, we explored different methods including sonication with a point sonicator and heating with reflux. Subsequently, the obtained nanoparticles were analyzed using infrared spectroscopy, photoluminescence, and epifluorescence microscopy.

It was possible to discern distinctive peaks within the infrared spectrum, along with the fluorescence exhibited by the nanoparticles functionalized with FMN, indicating the successful functionalization process.

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Studying the interaction between a uridine derivative and Langmuir monolayers as membrane models

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Understanding the interaction between a compound with potential biological activity and the cell membrane is pivotal for predicting its efficacy as a pharmacological agent. In this sense, Langmuir films, ultra-thin layers with the thickness of a single molecule formed at the air-water interface, serve as an invaluable tool to mimic cell membranes and their interaction with bioactive compounds. Thus, the focus of this study is to explore the interaction between 3,4-acetonide-uridine-succinate-cholesterol (PNM3), a uridine derivative with potential anticancer properties, and Langmuir films comprising dioleoylphosphatidylcholine (DOPC), a primary lipid constituent of erythrocyte cells, and dioleoylphosphatidylserine (DOPS), a prevalent lipid in mammalian cells, notably overexpressed during early apoptosis. Various techniques, including surface-pressure isotherms, surface potential isotherms, tensiometric stability tests, and Brewster angle microscopy (BAM), were employed to evaluate the effects of PNM3 on the lipid monolayers. Observations revealed alterations in the isotherms post-PNM3 introduction, indicating an interaction between the compound and the monolayer, shedding light on whether the compound was incorporated or expelled from the air-water interface. Noteworthy changes in film stability were observed after PNM3 addition. Furthermore, shifts in surface potential isotherms depicted distinct orthogonal ordering, suggesting altered molecular arrangement upon PNM3 integration. Additionally, BAM images illustrated morphological changes in the film after the drug introduction. In summary, PNM3 induced significant changes in the lipid monolayers' thermodynamic and morphological characteristics. This study unveils critical insights into the molecular-level interaction between PNM3 and the cell membrane, providing valuable knowledge for understanding its pharmacological action.
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Study of the filler-matrix interaction of natural rubber/SBR composites with PU waste

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In the present study, composites of natural rubber (NR) and synthetic styrene-butadiene rubber (SBR) were manufactured in a 50/50 ratio using micronized polyurethane (PU) waste from the refrigeration industry as filler. The vulcanization system used was semi-efficient (SEV). The interaction of the filler with the polymer matrix, the rheometric and mechanical properties of the composites were investigated. The composites were produced by varying the filler content between 0-40 phr in an open mixer, and the test specimens were manufactured using thermopressing at a temperature of 160°C (ASTM D 3182), with dimensions of 15 x 15 cm and a thickness of 2 mm. The characterization of the composites was carried out using the techniques of rheometry (ASTM D 5289), density (ASTM D 297), hardness (ASTM D 2240), tensile strength (ASTM D 412), density of crosslinks by swelling in organic solvents using the Flory-Rehner equation. Furthermore, the composites were subjected to Lorentz-Park analysis to study the interaction effect between the filler and the polymer matrix. The results showed a strong interaction between the filler and the matrix. The crosslink density values increased with increasing filler. Mechanical properties have improved. The hardness went from 50 (pure gum) to 75 Shore A (composite with 40 phr of PU), and the tensile strength value went from 4.2 MPa (pure gum) to 7.3 MPa (composite with 40 phr of PU), demonstrating excellent dispersion and matrix-filler interaction. However, the deformation at break was reduced from 800% (pure gum) to 300% (composite with 40 phr PU). Composites have mechanical properties for industrial applications, such as casual shoe soles.

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Sustainable Development of PLLA Polymeric Films and Muña Oil for Medical Applications Through the Airbrushing Technique

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The growing demand for natural products has driven the exploration of synthetic polymers, such as poly lactic acid (PLLA), and natural products, such as Muña oil, in the manufacture of films for medical applications. PLLA is recognized for its biodegradable properties, low toxicity, and biological compatibility. When combined with Muña oil, which has notable properties, it can result in films with enhanced characteristics. These films have the potential to be used in a variety of medical applications, opening new horizons for the treatment and prevention of skin diseases. To overcome the challenges in the production of these films, the airbrushing technique has been explored, which stands out for its sustainability and respect for the environment, as it consumes less energy compared to other techniques, such as electrospinning. Airbrushing involves spraying polymeric solutions into fine streams, forming fibers as the solvent evaporates. This provides precise control over the thickness and uniformity of the films, resulting in significant improvements in properties such as breathability and moisture absorption. In this project, the aim is to develop PLLA polymeric films enriched with Muña oil, using the airbrushing technique. The optimization of operating conditions will take into account the PLLA-solvent solution, the air pressure in the airbrush, and the distance between the airbrush and the collection surface. Preliminary results indicate that the solubilization time of PLA in the solvent (acetone) influences the type of fibers formed. The longer the solubilization time, the fibers obtained present more uniform characteristics, but result in physical equipment problems such as clogging. Lower solubilization times favor the operation of the equipment and the films obtained present PLA beads. The best distance found was 20 cm and at a concentration of 6 m/v. Studies are being carried out to better map opperating conditions and addition of the bioactive.

Synthesis and Characterization of Bacterial Cellulose and Silver Nanoparticles Composite

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Cellulose is an abundant biopolymer, with various means of obtaining it, including the use of bacteria to produce bacterial cellulose (BC), which possesses unique mechanical and structural properties, and high biocompatibility, enabling applications in various areas, such as medicine for wound healing dressings [1]. Similarly, metallic nanoparticles have been gaining prominence for their multiple applications, including silver nanoparticles (AgNps), which are effective antibacterial agents [2]. This study aims to evaluate the synthesis and characterization of the composite of bacterial cellulose and silver nanoparticles, in order to access such benefits targeted towards the medical field and their applications. Firstly, the best culture medium for the bacteria was determined, followed by two routes of silver nanoparticles insertion: (I) ex-situ method, incorporating pre-synthed AgNps into the polymeric matrix, and (II) in-situ method, synthesizing AgNps directly in the matrix through photochemical reduction of silver nitrate (AgNO3) in the presence of UV light. Finally, analyses were performed using techniques such as Fourier Transform Infrared Spectroscopy (FTIR), X-ray Diffraction (XRD), and Scanning Electron Microscopy (SEM) with Energy Dispersive X-ray Spectroscopy (EDS). Additionally, in vitro tests were conducted to evaluate bioactivity and antibacterial efficacy against Gram-negative and Gram-positive bacteria, as well as antibiofilm action. The results obtained confirm the silver incorporation by the methods, as well as its antibacterial, antibiofilm, and cytocompatibility activity, with the best response coming from method (II).

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Synthesis and characterization of biomaterials for medical use using cellulose nanofibers from orange peels with embedded silver nanoparticles

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Due to the growing demand in the tissue engineering market to replace synthetic polymers with natural materials that simulate skin functions such as thermoregulation, protection, and healing, cellulose@AgNPBio was strategically designed to combine cellulose properties with the antibacterial activity of the biogenic nanoparticles, thus creating a sustainable and biocompatible gel that would meet therapeutic demands.[1] Cellulose was isolated from orange biomass, such as orange peel (OP), rich in this biopolymer. In the process, OP went through acid, and then, a base treatment and was transformed into nanocellulose fibers (CNF), a material with a high surface area, excellent mechanical and elastic strengths, and an ability to form composites. Cellulose was obtained from OP with a high yield (~15% w/w) by applying the methodology described by Marino et al.[2] with some modifications. Then, the cellulose fibers were nanonized to CNF in acid conditions by varying H2SO4 concentration (5, 10, and 20%). The cellulose and CNF were characterized with ATR-FTIR, and ^{13}C NMR ssNMR (CP/MAS). In the final step of the project, we produced a biomaterial using CNF from the OP in combination with proteins and polysaccharides such as collagen and carrageenan, with the incorporation of biogenic silver nanoparticles. Finally, biomaterial gel interactions with the biogenic silver nanoparticles synthesized by other research group members[3] were investigated. A gel was fabricated, whose healing, cicatrizing, and antioxidant properties are going to be observed in the skin.

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Synthesis and characterization of Biomimetic nanoparticles for the delivery of paclitaxel in lung cancer therapy

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Paclitaxel (PTX) is among the first-line chemotherapeutic agents in the treatment of non-small cell lung cancer (NSCLC). However, its use is associated with the emergence of adverse effects and resistance [1]. Nanomedicine has offered a diverse range of alternatives aiming to improve parameters such as biocompatibility, bioavailability, circulation time and, recently, homotypic targeting through the use of biomimetic nanoparticles with tumor cell membrane coatings [2]. This study presents the synthesis of PLGA nanoparticles loaded with PTX, the extraction of lung tumor cell membranes (A549) for coating, and their respective characterizations, with the goal of using them as an innovative and targeted strategy for NSCLC treatment. PLGA nanoparticles loaded with PTX were synthesized using the nanoprecipitation/solvent evaporation method. Extraction and isolation of A549 cell membranes were performed through trypsinization, centrifugation and ultracentrifugation. The physical-chemical characterization of NPs was evaluated in Dynamic Light Scattering (DLS) and Nanoparticle Tracking Analysis (NTA). The NPs show a diameter of approximately 211 nm; PDI was 0.191 and ZP -21.4mV ± 7.47 mV, indicating the NPs electrical stability. NTA revealed s corroborating DLS results. The scanning electron microscope (SEM) revealed particles with nanometric diameters and spherical geometry. A549 membranes exhibited a diameter of approximately 289.9nm; PDI was 0.339 and ZP -29.5mV ± 10.1 mV. NTA results also corroborated DLS values. SEM images were in accordance. The afore mentioned results suggest both NP_PTX and A549 extracted membranes are viable for nanosystem construction.

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Synthesis and characterization of niobium-based nanoparticles functionalized with natural antioxidants

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Ascorbic acid (AA), tannic acid (TA), and quercetin (QUE) are natural antioxidants with potential in the treatment and prevention of various diseases. However, their efficacy is limited by poor absorption and degradation in physiological conditions. Niobium (Nb) is a metal that possesses favorable physical and chemical attributes, low cytotoxicity, and significant biomedical applications. In this study, niobium-based nanoparticles (Nb-NPs) were synthed and functionalized with AA, TA, and QUE to obtain nanoantioxidants. The synthesis involved dissolving the metallic precursor ($NbCl_5$) in deionized water [1], and functionalization occurred either during the Nb-NPs synthesis or by immersing Nb-NPs in an antioxidant solution [2]. The charge, , morphology, and crystallinity properties of the obtained samples were determined respectively by Zeta Potential, DLS, AFM, and XRD. UV-Vis and FTIR spectra confirmed the formation of hydrated niobium oxide (Nb_2O_5 nH_2O). The FTIR spectra of functionalized Nb-NPs indicated the presence of organic traces in each sample. The UV-Vis spectra of functionalized Nb-NPs show a shift in maximum absorbance to shorter wavelengths, suggesting a smaller compared to non-functionalized ones. Additionally, the spectra also indicate the presence of bioactives in each sample as well as a successful functionalization. Preliminary results from biological assays with cell cultures showed that even non-functionalized Nb-NPs exhibit properties against the formation of bacterial biofilm.

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Synthesis and Characterization of Plasmonic Gold-based Nanoparticles for Melanoma Photothermal Therapy

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Plasmonic nanoparticles based on gold exhibit a diverse physical-chemical feature, high dependent on their and morphology. Among these, the localized surface plasmon resonance (LSPR) stands out, enabling these nanoparticles to efficiently absorb light in the near-infrared (NIR) region. This effect can be modulated to enhance the therapeutic potential of nanomaterials, especially in photothermal therapy, where the interaction between light and nanomaterials induces localized heating, that can be valuable for cancer treatment. Thus, gold nanorods (AuNRs) and gold nanobipyramids (AuBPs) were synthed and characterized by spectroscopies, dynamic light scattering, nanoparticle tracking analysis, and transmission electron microscopy. The synthesis was optimized to obtain the LSPR effect on the NIR range. The AuNRs synthed exhibit an LSPR effect at 874 nm, with dimensions of length 62±2 nm, width 4±2 nm, zeta potential of +39.7 ± 0.45, and a polydispersity index (PdI) of 0.460±0.006. The AuBPs demonstrated an LSPR effect at 898 nm, with dimensions of length 77±1 nm, width 10±1 nm, zeta potential of +38.4±0.52, and (PdI) of 0.301 ± 0.005. Additionally, a crucial step was incorporated into the synthesis to enhance the purity of the AuBPs, utilizing depletion flocculation with a specific surfactant (BDAC). This study lays the groundwork for a comparative analysis of the morphological characteristics of AuNRs and AuBPs in the context of their potential applications in melanoma photothermal therapy.

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Synthesis and characterization of porous β-cyclodextrin/manganese ferrite nanoparticles and their application as an electrochemical sensor of dopamine

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Superparamagnetic manganese ferrite nanoparticles stabilized with β-cyclodextrin (βCD-MFO) were prepared by co-precipitation at room temperature and hydrothermal methods, using temperatures of 120 and 140°C. Similar samples, without βCD, were prepared for comparison (MFO). Samples called βCD-MFO140 and MFO140 showed the best characteristics when heated at 140°C during the synthesis in autoclave. The βCD-MFO140 is formed by nanoparticles of 5 nm and presented the highest surface area, the highest porosity, and a hydrophilic surface. Alternatively, the MFO140 presented crystallite near 25 nm and a hydrophobic surface.

Both nanocomposites were applied to modify carbon paste electrodes and evaluated using differential pulse voltammetry for determination of dopamine. They showed promising responses such as sensitivities of 0.09 and 0.23 µA µmol^{-1} L, and low detection limit of 2.28 and 0.39 µmol L^{-1} for MFO140 and βCD-MFO140, respectively, which are good answers in a linear range between 11.97 and 39.68 µmol L^{-1} for MFO140 and between 3.99 and 15.95 µmol L^{-1} for βCD-MFO140. Both sensors demonstrated good reproducibility with relative standard deviation of 12.7 %. The CPE βCD-MFO140 exhibits better selectivity for dopamine. The sensors were tested using commercial urine presenting a recovery of 109 and 103 % for MFO140 and βCD-MFO140, respectively. According to these results, the βCD-MFO140 electrode demonstrated better electrochemical performance with potential for application in real samples. The superior response of the βCD- MFO140 electrode can be ascribed to its higher surface area and porosity, as well as, its hydroxylated surface that makes this electrode more hydrophilic.

Synthesis of Carbon Dots Using Orange Juice for Next-Generation Nanotechnology Applications

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Since the discovery of Carbon Dots (CDs) [1], a wide range of scientific areas have experienced notable progress due to the incorporation of these promising materials, noted for their stability, solubility, unique optical properties, and low toxicity, making them useful in semiconductors, theranostic agent, photodynamic therapy, drug delivery, among other applications. This research delves into the sustainable synthesis of CDs via a microwave-assisted hydrothermal method, employing orange juice, attributed to the predominance of ascorbic acid as the carbon source. We aim at green methods by adjusting temperature, time and microwave power, replacing less efficient equipment and toxic solvents. The synthesis protocol was optimized through the original article [2] and added other techniques by current literature. Analytical methods included UV-Vis spectroscopy, TEM, DLS, static and time-resolved photoluminescence spectroscopy. Characterization confirmed the CDs optical properties, , structure, and absorption bands. These findings offer a straightforward path for CDs synthesis, enhancing their applicability in various fields and promoting the adoption of advanced nanomaterials.

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SYNTHESIS OF PHOTOSENSITIZING NANOSYSTEMS FROM NANODIAMOND – HYPERICIN/FAGOPIRIN FOR APPLICATION IN PHOTODYNAMIC THERAPY

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Nanotechnology is a useful tool[1] in the development of nanosystems with photosensitizers (PS), obtaining NPs as a strategy to reduce PS deactivation in biological media, increasing photoactivity for application in PhotoDynamic Therapy. Among the promising NPs, nanodiamonds (ND) are biocompatible and present a versatility of chemical groups suitable for reactions with PS[2]. In nature, a variety of PS can be found, with emphasis to, Hypericin and Fagopirin, present in the plant Hypericum perforatum and Fagopyrum esculentum, respectively, being candidate for obtaining photosensitizing NPs[3]. This work was based on the extraction, purification and chemical conjugation of PSs to NDs to obtaining nanosystems for PDT application. The methanolic extraction of the plant's flowers were conducted under microwave (20min/80°C) and purified by thin-layer chromatography with eluents of suitable polarity. The nanosystems were synthed by esterification between the PSs and ND under microwave, using EDC/NHS (1h/75°C). In the UV-vis spectra of the extracts, banda at 591nm corresponding absorption to the anthraquinone structures (FSs), which was also observed in the phases recovered after the purification processes. By fluorescence, a band at 644nm was observed after excitation at 500nm. The efficiencies of conjugation were investigated by UV-vis with limitations due to scattering caused by the NDs; however, band near 591nm was observed with low intensity. IR spectra showed the carbonyl (carboxylic) band shifting to a lower wavenumber characteristic of the ester carbonyl. This, it is concluded that the novel nanosystems, ND-HYP and ND-FAG, were successfully obtained, and ROS generation and antimicrobial assays are planned for a next step for PDT application.

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Synthesis, physicochemical characterization and cytotoxicity assay of nanoemulsion containing chloroaluminum phthalocyanine colorant for photodynamic treatment of cervical cancer

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Cervical cancer is one of the main causes of cancer mortality in women [1]. Approaches to transport photosensitizers have been widely explored due to their low solubility in water [2]. This study aims at the synthesis and characterization of nanoemulsions (NE) containing the chloro-aluminum phthalocyanine (ClAlPc) for photodynamic treatment (PDT) of cervical cancer in vitro. The NE preparation process was based on the mixture of oil and aqueous phases. The quantification of the incorporation content of ClAlPc in NEs was obtained through the spectrofluorimetric method developed. The particle (PS), Zeta Potential (ZP) and Polydispersity Index (PDI) of NE were evaluated using the Zetar equipment. The physicochemical stability of NE/ClAlPc was monitored for 12 weeks. Cytotoxicity study was conducted using NIH-3T3 cell line under dark conditions by the resazurin method and PDT using NE/ClAlPc was performed using HeLa cell line. The results indicated the stability of the formulation during the analyzed period. NE showed homogeneous distribution, between 172.91nm and 252.83 (TP), and ZP between -22mV and -11.21mV, with a ClAlPc incorporation rate of 51.9%. In the cytotoxicity assay using the NIH-3T3 cell line, viability exceeded 75% across all tested concentrations (0.5-20 µmol.L^{-1}). The PDT assay resulted in a 69.38% reduction in viability of the HeLa cells, showing promise for cervical cancer photodynamic treatment.

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Tailoring Swelling Properties of Alginate Films through Beta-Caryophyllene Nanoemulsion and Hyaluronic Acid: A Comprehensive Study

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Hyaluronic acid (HA) and beta-caryophyllene (bC) have gained attention for their therapeutic properties. Their incorporation into sodium alginate (SA) films can significantly affect the swelling behavior of the resulting material [1]. Understanding the release mechanisms of polymeric films are linked to parameters governing their swelling kinetics. The aim of this work was to understand the effect of HA and bC-based nanoemulsion (NE-bCP) on the properties of SA films. For this purpose, a 2^2 full factorial design was applied to investigate the effect HA and NE-bCP concentration. The films were obtained by casting method. Control films consisted of an aqueous SA-HA solution, while NE-bCP were prepared by mixing the nanoemulsion with the SA-HA solution. The formulations were characterized by macroscopic appearance, thickness, FTIR, and swelling behavior (SB). The transparent SA films were obtained, whereas incorporating NE-bCP gave opaque films. The film thickness was 0.15 ± 0.37mm (n = 24). FTIR analysis revealed that the presence of SA indicates a potential interaction, where the COOH group of HA reacts with the OH group of SA, contributing to cross-link formation [2]. The analysis of SB using the Peppas equation [3], indicated that HA displayed a dominant influence on the diffusional mechanism (n) in SA films containing NE-bCP. This influence was attributed to the presence of hydroxyl groups in HA, facilitating solvent retention and enhancing film hydrophilicity. These findings, elucidated by factorial analysis, provide valuable insights for design films using SA, NE-bCP, and HA by highlighting the critical role of HA-NE-bCP interaction in governing SB of SA films.

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The impact of phytosterol on ethosome formulation

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Ethosomes are a promising tool in cosmetic science, offering enhanced skin penetration and delivery of active ingredients [1]. Incorporating cholesterol in ethosomes is a topic of interest as it may influence their characteristics and performance [2]. Raw material from animal sources is undesirable for the cosmetics industry, so this work studied the possibility of using phytosterols instead of cholesterol in that formulation. Ethosomes were prepared using phosphatidylcholine (ET) or phosphatidylcholine and phytosterol (ETP); for comparison purposes, a model ingredient, ascorbyl glucoside, was encapsulated in both system types. The two formulations were characterized by particle size by laser diffraction, encapsulation efficiency by high-performance liquid chromatography, and instability index using the Lumisizer equipment. The average particle size , D[4,3], of ET, was 3.2 ±0.4µm and of ETP was 3.4±0.6µm. The encapsulation efficiency was 21±1% for ET and 20±4% for ETP; The instability index was 0.58±0.01 and 0.58±0.02 for ET and ETP respectively. The ET and ETP formulations across the tested parameters did not differ statistically significantly. This lack of difference could be attributed to the low phytosterol concentration. Therefore, additional studies will be required to assess the impact of phytosterol on ethosome formulations.

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Thiolated SPIONs for biological applications - Synthesis and characterization

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In this research we developed methodologies for synthesizing superparamagnetic iron oxide nanoparticles (SPIONs) specifically approach for biomedical purposes, motivated by the diversity that nanostructured systems offer in applications spanning technological, industrial and biomedical domains [1]. Thus, we conducted the synthesis, characterization and evaluation of the cytotoxicity and genotoxicity of this nanomaterial, aiming to enhance its biocompatibility and suitability for applications in nanomedicine. Among the variety of available methods, we chose coprecipitation due to its simplicity and the best cost-benefit, resulting in nanomaterials suitable for biomedical applications [2]. The SPIONs were synthed by combining ferric and ferrous chlorides in acidic aqueous solution, followed by precipitation with ammonium hydroxide. To improve the biocompatibility of the SPIONs and enable precise targeting at specific sites through an external magnetic field, we functionalized the surface of the SPIONs with organic ligands (Cysteine or Glutathione - mass ratio, SPIONs:ligand = 1:5), incorporating a functional group (-SH). Nanoparticles characterization was carried out using Fourier Transform Infrared Spectroscopy (FTIR), UV-Vis spectroscopy, RAMAN microscopy, X-Ray Powder Diffraction (XRPD), Dynamic Light Scattering (DLS), Transmission Electron Microscopy (TEM) and SQUID magnetic measurements. Finally, following physicochemical analysis, we conducted biological analysis of the nanomaterial through in vitro assessments of cytotoxicity using healthy and tumor cell cultures, as well as genotoxicity analysis.

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Understanding the Impact of Ethephon on Sperm Plasma Membrane: Insights from Mimetic Systems

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Among a wide list of pollutants permitted for using in Brazil, ethephon (2-chloroethylphosphonic acid) stands out, which is a growth regulator that functions by releasing ethylene. Recently, a study [1] indicated that the exposure of male rats to ethephon significantly affected the reproductive system of these animals, decreasing the sperm count and increasing the number of abnormalities and damages in the testicular tissue. Although in vivo studies show the effects resulting from animal exposure to ethephon, the mechanism of action of this agrochemical on the body is poorly understood. In this context, aiming to avoid the complexity of in vivo systems, an investigation of the effects of ethephon on mimetic systems of the sperm plasma membrane is proposed, using giant unilamellar vesicles (GUVs) for lipid bilayer formation. Such systems are formed by a ternary mixture of: 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphatidylcholine (POPC), 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphoethanolamine (POPE), and sphingomyelin (SM), in a 2/2/1 molar ratio, which were chosen to ensure the fluid phase, like the plasma membrane of mammalian cells, and to be close to the mass proportion found in sperm membranes [2]. The method used for GUVs formation was gel-assisted, being the GUVs observed under an inverted confocal microscope (Nikon C2/C2si Eclipse Ti-E, Kyoto, Japan). It was observed that ethephon causes various effects on GUVs: formation of buds, formation of lipid collars, deformation of the spherical shape, loss of contrast, and rupture of the vesicles. The evident interaction of ethephon with structured lipids in bilayers found in sperm and testicular tissue confirms the harmful biological effects of the agrochemical.
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Unraveling the ACE2 and TMPRSS2 arrangements in nanostructured platforms: Insights into the SARS-CoV-2 interaction with host cell membrane

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SARS-CoV-2 enters the host cell through two main events: (i) binding of the Spike protein (S) to a cellular receptor, angiotensin-converting enzyme 2 (ACE2), and (ii) fusion of the virus envelope with the host cell membrane mediated by cell proteases, such as the transmembrane serine protease 2 (TMPRSS2) [1]. Hence, understanding the arrangements of ACE2 and TMPRSS2 on the cell membrane and their interactions with the S protein is crucial for comprehending SARS-CoV-2 infection and developing strategies against COVID-19. Given the complexity and dynamic nature of biomembranes, one approach to studying the incorporation of these proteins involves using platforms that partially replicate these structures, enabling the extraction of intricate molecular information [2]. In this work, we employed Langmuir films to replicate the host cell membrane and investigate the molecular arrangement of ACE2 and TMPRSS2 proteins. We used a mixture of cholesterol (CHOL), 1,2-dioleoyl-sn-glycero-3-phosphocholine (DOPC), and 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (DOPE) as a model of the human plasma membrane. Additionally, we investigated the contribution of lipid rafts formed by CHOL, DOPC, and sphingomyelin (SM) to protein incorporation. Langmuir monolayers were evaluated through tensiometric, microscopic, and spectroscopic measurements. Our findings confirmed the incorporation of ACE2 and TMPRSS2 on the mixed lipid monolayers, and we observed an influence of the lipid matrix on the arrangement of ACE2 and TMPRSS2, which potentially may affect their interaction with the spike protein of SARS-CoV-2.

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Zinc Oxide Nanoparticles: antimicrobial and photocatalic activity

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Zinc oxide nanoparticles are known for their photocatalytic ability, which induces antimicrobial activity. Advanced oxidative processes are triggered when irradiated, producing reactive oxygen species (ROS) and promoting antimicrobial action [1]. In this work zinc oxide nanoparticles were produced by precipitation, using the process adapted from Sharma et al [2] with thermal treatment at 150 ^{0}C for 2 hours. SEM images show the formation of nanoparticles with diameter between 20 and 30 nm, organized in sheets. The antimicrobial activity was tested using the broth microdilution process, resulting in a minimum inhibitory concentration of 0.78 µg/mL against *Stapylococcus aureus* (ATCC-33591). The band gap of the nanoparticles was determined by U-Vis spectroscopy, resulting in 2.6 eV. Preliminary results of phototacalilytic activity mediated by UV light indicate a reduction in the absorbance of methylene blue dye (2 mg/L) and ZnO (50 mg/L) from 0.65 to 0.4 at $\lambda = 662$nm when exposed to 30 min of UV-C radiation (18 W). Therefore, these preliminary results demonstrate the potential of this nanomaterial to combat microorganisms and can direct future work to create antimicrobial surfaces, extremely useful in hospital environments, the food industry, among others. References [1] de Maria, V. P. K., de Paiva, F. F. G., Tamashiro, J. R., Silva, L. H. P., da Silva Pinho, G., Rubio-Marcos, F., & Kinoshita, A. (2024). Advances in ZnO nanoparticles in building material: Antimicrobial and photocatalytic applications–Systematic literature review. Construction and Building Materials, 417, 135337. [2] Sharma, D., Rajput, J., Kaith, B. S., Kaur, M., & Sharma, S. (2010). Synthesis of ZnO nanoparticles and study of their antibacterial and antifungal properties. Thin solid films, 519(3), 1224-1229. Acknowledgments: JGKUZ thanks FAPESP (2024/00424-0), JRT and FFGP thanks CAPES (88887.691142/2022-00) and AK CNPq (306096/2023-4)

EP01-Semiconductor Nanocrystals: A Noble Prize Winner Class of Material

Advanced Structural Characterization of Defects in Luminescent Wide Band Gap Halide Perovskite Nanostructures

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Semiconductor materials play a pivotal role within contemporary society due to their substantial economic, technological, and social implications. These materials are indispensable components in optoelectronic devices, including televisions, cell phones, computers, and various other appliances. Perovskite nanostructures, also known as perovskite quantum dots, hold significant potential for advancing optoelectronic technologies. Achieving high quantum fluorescence yields and control over optical properties are fundamental for optimizing semiconductor usage in such devices. To obtain perovskites with good optical properties, especially in the blue spectrum, precise control over the morphology, chemistry, and structural attributes of nanoparticles becomes imperative. This requires the application of statistically accurate structural characterization methodologies capable of identifying atomic-level defects in the fabricated systems. Transmission Electron Microscopy provides valuable insights into the morphology and structural correlations of nanomaterials. However, challenges arise due to the interaction of perovskite constituents with the electron beam, resulting in structural degradation. Consequently, there is a scarcity of advanced TEM investigations on perovskites in the literature, predominantly due to the inherent difficulties in mitigating electron beam-induced damage. In this study, innovative approaches to sample preparation and data acquisition will be explored, including low-dose imaging and serial image capture techniques reminiscent of Cryo-EM procedures. These methodologies aim to provide crucial insights into identifying structural imperfections that hinder the efficiency of the final devices, which can be corrected through inventive synthesis methodologies. Such advancements hold promising prospects for future applications in perovskite light-emitting diodes (PeLEDs), thereby facilitating the production of more efficient optoelectronic devices.

Exploring the Potential of Bismuth Chalcohalide Semiconductors: Synthesis, Properties, and Applications

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Bismuth chalcohalide semiconductors have gained significant attention in recent years due to their unique properties and potential applications. The combination of bismuth with chalcogens and halogens leads to a wide range of semiconductor materials with tunable bandgaps, making them promising candidates for photodetection, ionizing radiation detection, photocatalysis and solar cells [1]. However, their ternary nature makes synthesis complicated and requires precise control to obtain the desired composition. In this work, we explored the synthesis methods, structural properties, and potential applications of $Bi_{19}S_{27}I_3$ and BiSI [2]. We have developed different synthesis methods, such as hot injection and solvothermal, which have allowed us precise control over the composition and morphology of nanostructures of both compounds. We have studied the applications of these nanostructures obtaining a promising photocatalytic activity for the reduction of Cr(VI) for the case of $Bi_{19}S_{27}I_3$, and we constructed pellet detectors with BiSI, obtaining a high sensitivity and a low detection limit for X-rays. In summary, our ability to control the nanostructures of these materials not only promises enhanced performance but also facilitates their integration into emerging technologies. Thus, our findings represent a significant step toward unlocking the full potential of bismuth chalcohalide semiconductors across various technological domains.

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Development of nanoprobe based on positively charged quantum dots for detection of HSO_4^- and SO_4^{2-} ions

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Quantum dots (QDs) are fluorescent semiconductor nanocrystals ranging from 2 to 10 nm with unique optical and electronic properties, and for this reason they have gained prominence in sensor development [1]. Detecting anions such as HSO_4^- and SO_4^{2-} is essential, given their broad implications in both industrial and environmental contexts. HSO_4^- is present in nuclear fuel, industrial waste, and agricultural fertilizers, with severe environmental impacts. In this sense, the present work aims to evaluate the application of positively charged quantum dots (CdTe-CYA) as nanoprobes for HSO_4^- and SO_4^{2-} ions detection in water [2]. The QDs' optical features were evaluated by UV-Vis absorption spectroscopy and emission spectroscopy titrations, and the calibration curves were obtained from the titration-acquired data and statistically validated by ANOVA. The QDs exhibited favorable optical properties and high photostability. The results revealed a gradual increase in the QDs' emission intensity with successive anion additions, indicating the sensitivity of CdTe-CYA to the anions and exhibited good linearity, likely due to interactions between the positively charged amino groups of the CdTe-CYA and the anions, indicating that the probable detection mechanism is by electrostatic attraction. Regarding the SO_4^{2-} ion, the analytical parameters exhibited good linearity ($R^2 = 0.995$) with a limit of detection (LOD) of 10.51 µM. Similarly, the HSO4- also demonstrated a good linearity ($R^2 = 0.995$) with a LOD of 1.95 µM. Thus, CdTe-CYA QDs shows potential as fluorescent sensors for monitoring HSO_4^- and SO_4^{2-} ions in water sources.

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Effect of the crystallographic orientation of the surface of Si wafers on the morphology of $NiSi_2$ nanoplates endotaxially grown in Si

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Nanocomposites formed by crystalline $NiSi_2$ nanoplates embedded in silicon wafers have attracted the attention of many researchers due to the potential applications of this material in nanotechnology [1]. In this study, we describe a process for growing crystalline nickel disilicide nanoplates in a thin layer close to the surface of silicon wafers with different crystallographic orientations, namely Si[001], Si[011], and Si[111]. The synthesis of the disilicide nanocrystals involved depositing a Ni salt solution onto bare surfaces of each Si wafer, followed by thermal treatments of the samples under 5%H_2+95%He flow. The shape, orientation, average thickness and diameter of silicide nanoplates formed in Si were determined through scanning electron microscopy (SEM) and grazing-incidence small-angle X-ray scattering (GISAXS) techniques. It was observed that irrespective of the crystallographic orientation of the surface of the wafer this preparation method results in the formation of $NiSi_2$ nanoplates with the shape of nearly regular hexagons having their larger surfaces parallel to one of the planes of Si{111} crystallographic form. Samples were annealed at different temperatures ranging from 500 °C to 700 °C during 2 h. Our analysis of the GISAXS patterns enabled us to determine how the crystallographic orientation of the surface of the Si wafers and the temperature of thermal annealing affect the average and number density of the nanoplates.

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Enhanced Photodegradation of Bisphenol F Using g-C3N4:Nb2O5 Heterostructure: Synthesis, Characterization, and Potential Application

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The study investigated the photodegradation of Bisphenol F using a heterostructure of g-C3N4:Nb2O5. X-ray diffraction analysis revealed the crystallographic structure, showing the presence of pseudohexagonal phases of Nb2O5 and g-C3N4, indicating a successful synthesis of the heterostructure. BET analysis revealed an intermediate surface area for the heterostructure (44.64 m2/g), suggesting effective integration between the constituent materials and how their mass proportion impacts BET surface area values. Thermogravimetric analysis showed a gradual mass loss for the heterostructure, indicating enhanced thermal stability compared to pure g-C3N4. Morphological characterization by electron microscopy confirmed the formation of the heterostructure and revealed a uniform distribution of Nb2O5 nanoparticles on g-C3N4 sheets. This direct interaction between Nb2O5 nanoparticles and g-C3N4 sheets may promote effective transfer of photo-generated electrons, potentially enhancing the photocatalytic activity of the heterostructure [1]. These results highlight the potential of the g-C3N4:Nb2O5 heterostructure as an efficient photocatalyst for Bisphenol F degradation under UV light, achieving a C/C0 ratio of 0.98 after 60 minutes of photolysis, and a degradation rate of 0.85.

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Enhancing the yield of ZnO synthesized via solution combustion by adding Zinc Acetate as fuel

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Solution combustion (SCS) is an effective technique to synthe pure metal-oxide nanostructured powders and simultaneously provide an in situ doping [1]. The fuel-type used in SCS influences the control of the materials' characteristics [2]. This study aims to produce zinc oxide (ZnO) nanoparticles by SCS using zinc acetate as a fuel and a $Zn2+$ source to improve the synthesis yield. Zinc nitrate hexahydrate was used as the oxidizing agent and, for the fuel, two mixtures of reducing agents were applied: sucrose/urea (NSU) and sucrose/urea/zinc acetate (NASU). The fuel-to-oxidizer ratio was fixed at 1.4 and the amount of zinc nitrate was kept at 12,288 mMol for both formulations. The syntheses were performed at a muffle furnace at 500 °C, followed by calcination at the same temperature for 20 minutes. SEM, XRD, and DLS techniques were used to characterize the materials. The use of zinc acetate as one of the fuels increased the yield to 23.2%, which is a considerable amount compared to the yield of 20.7% observed for the synthesis without this zinc source. On the other hand, the NASU sample exhibited larger particle and crystallite s than the NSU sample, as well as a larger hydrodynamic diameter of the agglomerated particles going from 298 nm for NSU to 436 nm for NASU. The results of this investigation show that the addition of zinc acetate can successfully improve the yield of the SCS synthesis without significantly altering the ZnO morphology, however it should be noted that this higher yield synthesis also results in a slight increase in particle and a reduction in surface area.

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Fine-Tuning Zinc Oxide Nanoparticles: Insights into Organic Ligand Mediated Synthesis

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Tailoring nanoparticles (NPs) with precise control over dispersity, , and shape is crucial for various applications, whose features are fashioned by the synthesis process. Therefore, controlling the main mechanisms in synthesis process is fundamental to achieve the desired structure [1]. The first mechanism, nucleation, provides the nuclei that will ultimately form, by acting as a template, the nanoparticle itself. By using fast nucleation based synthesis protocols, such as hot injection method, homogeneous nucleation and then monodispersity can be favored. The subsequent synthesis step is responsible for the NP growth, due to the complex influence of the synthesis media and the NPs characteristics. Despite its complexity, this later synthesis is the most suitable for NP shape control, particularly by the influence of organic ligands [2].

In this context, this study provides fundamental insights into the influence of two organic ligands, oleic acid (OAc) and oleylamine (OAm), on the synthesis of zinc oxide (ZnO) NPs by using the hot injection approach. ZnO is a wide band gap semiconductor, valued for its affordability and eco-friendly properties, finding applications in electro optical devices, transducers, UV absorbers, gas sensors and solar cells [3]. Those characteristics are fundamentally linked to the exposed crystallographic facets, NP and shape. Our findings demonstrate the role of the OAc/OAm in these characteristics in the ZnO NPs synthesis, open a new venue for improved catalysts.

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Hydrothermal synthesis and optical characterization of graphene-CdTe QDs hybrid nanocomposite

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The development of graphene/semiconductor quantum dots hybrid nanocomposite remains a frontier area of research to design optoelectronic, photovoltaic, and light harvesting devices based on an electron transfer process. In this study graphene-CdTe QDs hybrid nanocomposite was prepared by direct mixing of graphene and CdTe QDs submitted to hydrothermal treatment [1,2] at 150oC@90min and was characterized with UV-Vis absorption. PL, PLE, and PL-RT techniques. To compare the effects on the optical properties CdTe QDs and graphene-CdTe nanocomposite have been obtained by same the experimental conditions. We have obtained high quality nearly monodisperse CdTe nanocrystals have been supported on graphene with no evidence of aggregation. Direct evidence is presented for the efficient quenching of photoluminescence from the CdTe nanocrystals by graphene. It is observed that the quenching of photoluminescence peak of QDs due to GO shell produced an applicable strategy and could be conveniently extended for other applications, such as, sensors, catalyst and so on. With the help of absorption (440nm) and emission spectra (750nm), it was found that the of the QDs obtained, was 3,67nm and hence induce a red shift of fluorescence emission. In conclusion, the change in fluorescent intensity through fluorescence resonance energy transfer from quantum dots to GO demonstrates the potential optoelectronic and various application of this new type of graphene-based semiconductor hybrid system.

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Optimization of synthesis processes for obtaining nanoparticulated KNbO3 semiconductors with good performance for photocatalysis

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In this article, potassium niobate (KNbO3) was obtained by hydrothermal synthesis utilizing an autoclave heated by a resistive blanket. The concentration of the reactants in synthesis vessel were 12mol/L of KOH and 1mol/L of ammonium niobate oxalate hydrate, the temperature used on each synthesis was 160°C the time used in one was 1h and another was 6h, and the synthesis was based on Kumada, N. [1]. The structure of the samples was characterized by XRD, and the microstructure was characterized by SEM. Photocatalytic activities of the materials were tested on the degradation of indigo carmine (IC), and the kinetics of this photoreaction was studied. The tests were done on a reactor created by the researchers. The system consists of an ultraviolet lamp and a thermal system that controls the temperature in the reaction vessel at 25°C. XRD analysis revealed an orthorhombic phase for the synthed materials, while SEM imaging indicated that in one of the samples, the particle s were approximately 2 µm, exhibiting a parallelepiped-like morphology, with agglomerates reaching s of approximately 10 µm. In contrast, the other sample, subjected to different synthesis conditions regarding time and concentration, exhibited larger particles with cubic morphology and smaller particles with a needle-like appearance. This observation underscores the influence of synthesis parameters such as time and reactant concentration on the morphology and structure of KNbO3. The photocatalytic activity for the degradation of organic pollutants was correlated with the properties of the materials.

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Optimization of the optical properties of hydrophilic $AgInSe_2$ quantum dots through a chemometric approach

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Recently, environmental concerns have risen regarding the use of quantum dots (QDs) due to toxic components like Cd and Pb in their synthesis [1]. Consequently, there has been a push for heavy metal-free alternatives such as $AgInSe_2$ to mitigate environmental impact. This study aimed to optimize a one-pot procedure for producing hydrophilic $AgInSe_2$ QDs, maximizing their emission intensity through multivariate optimization. Therefore, a full factorial experimental design 2^4 was carried out, with a central composite design, varying the synthetic parameters: MSA:(Ag:In) and (Ag:In):Se molar ratios, temperature, and reaction time. The optical characterization of the QDs was performed by UV-Vis absorption spectroscopy and emission spectroscopy, and structural characterization was determined by XRD and FTIR. Statistical validation of the model was performed through Analysis of Variance (ANOVA) and lack of fit F-test, at a confidence level of 95%. Under the ideal conditions determined by response surface analyses and desirability function, the experimentally obtained response for emission intensity value was 159.9±11.1, consistent with the predicted value (147.7±27.5), corroborating the predictability of the mathematical model. The XRD pattern revealed the presence of overlapping peaks that may be related to the orthorhombic crystal structure of $AgInSe_2$, and FTIR confirmed the surface passivation of the nanocrystal by the stabilizer. Therefore, it is believed that it was possible to synthe hydrophilic $AgInSe_2$ QDs with optimized emission intensity through a chemometric approach.

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Photoelectrochemical Biosensing Platform Based on Quantum Dots and Cramoll Lectin to Detect Glycoproteins

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Photoelectrochemical biosensing platforms (PECs) use photocurrents generated by photoactive species immobilized on a conductive surface, under optical illumination, as a signal to detect analytes of interest. PECs combine characteristics of purely optical and electrochemical biosensing platforms and can promote greater sensitivity of detection. Quantum dots (QDs) exhibit advantageous characteristics as photoactive species in PECs due to their: (i) intense tunable fluorescence determined by the vs. bandgap energy relationship, (ii) photostability, and (iii) chemically active surface for immobilization on electrode surfaces. The main objective of this study was to develop a PEC based on an Indium Tin Oxide (ITO) electrode modified by carboxyl-coated CdTe QDs and Cramoll lectin (specific for glucose and mannose). The potential of the platform was evaluated by detecting fetuin (glycoprotein used as a model) since it is a biomarker of heart disease and cancer. QDs of 3.4 nm presenting red emission were synthed and physicochemically characterized. Sodium ascorbate was employed as the redox probe for the photocurrent generation by chronoamperometry, upon LED illumination at 420 nm. As a result, the ITO electrode modified by QDs exhibited photostability and generated a detectable photocurrent (> 200 nA), remaining intensely fluorescent for at least 6 months. Additionally, Cramoll lectin (200 µg/mL) was effectively immobilized, as evidenced by the photocurrent decrease, compared to the signal for the platform containing only QDs. The platform recognized fetuin at a concentration 10× lower than the one used for Cramoll lectin. Thus, the developed steps favor the assembling of a PEC based on QDs that holds potential for biosensing applications.
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SELF-DOPING OF TiO_2 NANOTUBES: variables effects and experimental optimization

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Nanomaterials, particularly TiO_2 nanotubes (TNT), are widely used in electrochemical systems due to their unique properties such as high surface area, chemical and mechanical stability, and low toxicity. The band-gap value, found in the anatase phase (3.2 eV), requires an external radiation source in the UV spectra region to transfer electrons from valence to conduction band. To decrease this band-gap value, several strategies are employed, such as combination of different crystalline phases (e.g., anatase and rutile), decoration and/or doping with nanoparticles (e.g., Pt, Ag, Au) and self-doping (e.g., cathodic polarization). The effect of variables such as temperature treatment, applied potential, and self-doping time in the properties of self-doped TNT (SD-TNT) were investigated simultaneously and optimized by response surface methodology (RSM). Cyclic voltammetry (CV) showed that self-doping increases the current density ascribed to reduction of Ti^{4+} to Ti^{3+} in lattice structure and shift this peak to lower cathodic overpotential. Electrochemical impedance spectroscopy (EIS) shows that charge transfer resistance (R_{ct}) process is favored for longer times of cathodic polarization, promoting reduction of the capacitance, then favoring the charge transference. Finally, diffuse reflectance spectroscopy (DRS) analysis of TNT calcined at 550 °C give a band-gap of 3.09 eV. Rietveld refinement applied in the X-ray diffractograms provided a proportion of 76 and 24% of anatase and rutile phases, respectively.

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Studies of Graphene Quantum Dots for testing efficiency of natural and synthetic antioxidants

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Problem: Reactive oxygen species (ROS) are naturally produced in the human body. However, when in excess, they can cause pathologies, as they may react with macromolecules such as proteins, sugars and DNA. This is the case of the close relationship between the exacerbated production of ROS and diseases such as cancer and diabetes. **Solution:** One way to inhibit or delay the effects of ROS is by supplementing food with antioxidants capable of neutralizing them. That said, there is a need to understand the efficiency of antioxidants. And for this reason, graphene quantum dots (GQDs) prove to be potentially useful molecules in evaluating antioxidant potential, as they are fluorescent and oxidizable. **Objective:** Apply the intrinsic fluorescence of GQDs to evaluate antioxidant activity subjected to oxidation by hypochlorous acid (HOCl) and hypobromous acid (HOBr). **Methodology:** A study was carried out on the absorption and fluorescence properties of GQDs at different pHs (4.0-9.0), followed by kinetic tests with HOBr and HOCl. The antioxidant melatonin was used to evaluate the efficiency of inhibiting the oxidation of GQDS. **Results and Discussion:** The maximum absorption was 366 nm and the fluorescence was 450 nm in the entire pH range studied. The addition of HOCl or HOBr decreased the fluorescence signal, indicating the oxidation of GQDs. Kinetic studies showed that the reaction was more efficient with HOBr. The addition of melatonin caused concentration-dependent inhibition of GQDs, being even more efficient for HOCl. **Conclusion:** HOCl and HOBr are oxidants of GQDs and cause loss of fluorescence. The process can be inhibited by melatonin, suggesting that we can develop an assay for antioxidant efficiency based on monitoring the oxidation of GQDs through their fluorescence.

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Synthesis and Characterization of Colloidal Cadmium Selenide Quantum Dots

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This study explores the optical properties of Cadmium Selenide Quantum Dots (CdSe QDs) for potential applications in advanced optical devices. CdSe QDs, semiconductor nanocrystals known for size-dependent optical properties, are valuable in diverse technological applications. The research aims to understand the light emission characteristics of CdSe QDs and how various factors influence these properties. Specific objectives include the controlled synthesis of QDs in various sizes, crystal structure characterization, and evaluation of optical behavior in relation to particle size. CdSe QDs were synthesized using kinetic control, and UV-VIS spectrometry was used to analyze 10 samples. The results revealed a clear correlation between QD size and absorption peak shift, showcasing the precise tunability of their optical properties.

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Synthesis of nanostructured films of TiO_2 decorated with silver nanoparticles for the determination of anthocyanins in grape extracts by SERRS technique.

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Natural colorants are widely used in the food industry, especially anthocyanins found in different natural sources, such as grape skins, which are responsible for the reddish color of grape cultivars [1]. The factor that is closely related to color is that the pigment coexists, in equilibrium, in four different species, depending on the pH of the medium [2]. In this way, this work proposes to develop a SERRS (Surface Amplified Resonant Raman Scattering) sensor using titanium dioxide nanotubes (TiO_2NTs), obtained by electrochemical anodization, together with a colloidal solution of silver nanoparticles (AgNPs) for the determination of anthocyanins present in extracts obtained from grape skins. The characterization results of the TiO_2NTs films showed the presence of the anatase phase. UV-Vis spectroscopy identified the anthocyanin species in equilibrium as the pH of the medium changed. In the analysis of Raman spectra, it was possible to identify the SERRS effect only in the presence of silver nanoparticles, showing that this intensification of the anthocyanins' vibrational modes occurred both in the extracts diluted in AgNPs and on the TiO_2NTs films. The deconvolution of the SERRS spectra of the different extract dilutions showed that the signal from the flavylium cation (the cationic structure of the anthocyanin) was intensified as the amount of extract was reduced and the ratio of AgNPs/amount of anthocyanins increased. Compared to the standard methodology (UV-Vis), the SERRS sensor proved to be more sensitive, which shows the potential of TiO_2NT films coated with AgNPs as a SERRS sensor capable of assessing the anthocyanin content in grape skin extracts.

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Synthesis of WO_3/Nb_2O_5 heterostructures applied in organic compounds removal from aqueous solution

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Water pollution is a global issue. Among the methods used for removing organic compounds such as dyes and pharmaceuticals from water, the two most studied are adsorption and heterogeneous photocatalysis. As the Nb_2O_5 exhibits both adsorptive and photocatalytic properties, heterostructures between Nb_2O_5 and WO_3 were synthesized to enhance these features—the synthesis aimed to create a novel nanoscale material. The synthesis of isolated materials was based on previous reports. To synthesize the WO_3/Nb_2O_5 heterojunction, acid tungstic was dissolved in hydrogen peroxide (H_2O_2). Ammonium niobium oxalate was dissolved in distilled water, and H_2O_2 was added to this solution. The volume was completed with distilled water, and the solution was treated at 200 ºC for 24 h. Isolated materials were prepared for comparison in the same conditions. The samples were characterized, and the results showed the presence of WO_3 and Nb_2O_5, indicating heterojunction formation. The adsorptive properties of the samples were analyzed through kinetic and isotherm adsorption tests using dyes methylene blue (MB) and rhodamine B (RhB). Regarding kinetics, it was observed that the heterostructure adsorbed both dyes faster than the pure oxides. Particularly for the RhB dye, the isolated oxides exhibited minimal adsorption, in contrast to the heterostructure. The photocatalytic properties of the samples were analyzed using the dyes MB and RhB under UV light. The results showed that the heterojunction was more effective than the pure materials. Therefore, WO_3/Nb_2O_5 heterojunctions have the potential to be applied in photocatalytic processes for the degradation of organic compounds.

Synthesis optimization of nanoparticulate materials of $NaNbO_3$ via the hydrothermal route for use in photocatalytic processes

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The present study addresses the synthesis of sodium niobate through the hydrothermal route, a high-pressure procedure carried out in a steel autoclave, which enables the acceleration of material production, allowing good control over material properties through crystal growth and formation. The employed system ensures a reduced heating time up to the synthesis temperature, through personalized heating monitoring, which allows controlling time and temperature variables. The concentrations of the reagents in the synthesis were 12 mol/L of NaOH and 0.077 mol/L of niobium ammonium oxalate. One synthesis was conducted at 160°C for 2 hours and another at 160°C for 6 hours, as described by Shu, Y. W. Subsequently to the synthesis, the materials were subjected to analysis by X-ray Diffraction (XRD) which allowed the identification of sodium niobate phases and Scanning Electron Microscopy (SEM) for microstructure evaluation. Through SEM, it was possible to identify particles with distinct morphologies and dimensions. The niobates produced at 160°C for a period of 2 hours exhibited a cubic conformation, with s ranging from 0.9 to 3 µm. In contrast, those generated under the same thermal conditions, but for a six-hour interval, showed a one-dimensional morphology, with a minimum width of 0.19 and maximum of 0.3 µm, and lengths ranging from 6 to 27 µm.

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Synthetic approach to obtain hydrophilic silver indium telluride quantum dots

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Quantum Dots (QDs) are semiconductor nanocrystals that vary in from 2 to 10 nm. Due to the quantum confinement effect, these nanocrystals present unique optical properties, high photostability, resistance to photodegradation, and a chemically active surface, enabling a variety of applications such as sensors, solar cells, cellular probes, and drug delivery systems [1, 2]. The QDs most studied in the literature have high toxicity due to the presence of heavy metals such as cadmium and lead, in addition to being prepared with harsh synthetic conditions and in organic medium. To achieve more environmentally friendly QDs, the development of silver-based QDs has been growing. Ternary QDs containing silver have excellent optical properties, low toxicity, and emission from the visible to the near infrared region [2]. Among these QDs, silver indium tellurides (AgInTe2) appear as promising nanocrystals for biomedical and sensing applications. Thus, the present work aimed to obtain AgInTe2 QDs in aqueous media with optimized optical properties. A chemometric study was carried out to evaluate several synthetic parameters, such as reaction time, reagents molar ratio, nature of the stabilizer, and reducing agent, to optimize the AgInTe2 QDs fluorescence intensity. The optical results were promising, presenting a narrow and intense fluorescence spectrum, which remained stable for at least two months after synthesis. Our results indicate the formation of the desired AgInTe2 QDs with good fluorescence features, which are promising for being applied as optical sensors.

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The influence of synthesis on obtaining carbon quantum dots obtained from pumpkin seeds and their luminescent properties.

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Carbon quantum dots (CQDs) are a class of 0D nanomaterials with excellent luminescent properties, presenting superior performances than organic molecules and semiconductors [1]. They are quasi-spherical particles with a smaller than 10 nm, composed of sp2 and sp3 carbon, and depending on their synthetic route, they can have several functional groups, such as heteroatoms inserted in their structure [2]. The synthetic route and the raw material chosen to produce these nanomaterials will directly influence their chemical composition and, consequently, their properties. In this work, pumpkin seeds were selected as raw material to produce carbon quantum dots using three different methodologies. The synthed nanoparticles were characterized by XPS, FTIR, DLS, and Fluorescence Spectroscopy. The results showed that the endogenous self-doping CQDs were successfully obtained; however, even using the same raw material, the quantum dots obtained had a different chemical composition. The influence of compositional difference can be observed in the emission spectra of nanomaterials. The CQDs obtained by synthesis 1 had their maximum emission at excitation wavelengths of 330 nm, while synthesis 2 and 3 had maximum emission at 320 and 370 nm, respectively. Regarding quantum yield, the CQDs obtained by synthesis 2 were much superior to the other materials, the worst of which was obtained by synthesis 3. These results show that the synthesis was decisive in the formation of CQDs and directly influenced the properties of the materials, in addition to showing an excellent alternative for using agro-waste in the production of CQDs, which, from an environmental and economic point of view, is extremely advantageous.

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Titanium Dioxide Quantum Dots: Synthesis and Investigation of Application in VOC Detection

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The production of oxide-based chemical sensors has been extensively researched, but the majority are only effective above 100 ºC working temperatures [1]. This research proposes an VOC sensor that operates at room temperature, utilizing titanium oxide quantum dots (TiO_2 QD). The TiO_2 QD were synthed via the Sol-Gel method, where the precursor solution was a mixture of titanium isopropoxide with isopropyl alcohol. After stirring, the precursor solution was slowly mixed with a previously prepared and heated solution of hydrochloric acid diluted in ultrapure deionized water. After cooling, the liquid was centrifuged to separate the QD that were later dispersed in isopropyl alcohol, as reported in [2]. The material characterization was done through X-ray Diffraction (XRD), Transmission and Scanning Electron Microscopies (TEM and SEM), which revealed average crystal s of 5 nm. The material was used as an active layer in a chemical sensor for the detection of several VOC by casting the TiO_2 QD dispersion on electroless nickel immersion gold (ENIG) interdigitated electrodes on FR-4 substrates. The sensor characterization was conducted through impedance spectroscopy measurements at different analyte concentrations, within a measurement range of 20 Hz to 1 MHz, in a sealed static chamber filled with filtered nitrogen at room temperature. For isopropyl alcohol, the optimal frequency of 1 kHz showed a limit of detection of 103 ppm, with response and recovery times of 106 s and 34 s, respectively, indicating a potential application of titanium oxide quantum dots as an active material in the detection of VOCs as chemical gas sensors operating at room temperature.

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Tuning the color of CdTe nanoparticle emission through synthesis methods. Electronic states and coupling between states.

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The ability to control the color of light emitted by semiconductors makes them essential components in many modern electronic devices such as LEDs, electronic device screens, fiber optic communication, lasers, etc. Controlling the parameters in synthesis methods is crucial for obtaining high-quality structures. In the preparation of semiconductor nanostructures, the first step is the formation of stable solid cores in solution, followed by the growth of solid particles conditioned on the complete consumption of the reactants. One of the most important parameters in growth kinetics, and therefore the size of nanoparticles, is temperature. In this work, aqueous colloidal synthesis methods were used to control the size and tune the light emission color in CdTe nanoparticles, with reflux and hydrothermal techniques. Highly luminescent nanoparticles were obtained with emission ranging from green (500nm) to near-infrared (750nm). Different electronic transitions were analyzed through absorption, PL, PLE, and PL-RT measurements. Through the results obtained in optical characterizations, we observed coupling between different electronic states, which is essential for evaluating efficient energy transfer between different parts of the materials, enhancing the nanostructures for applications in solar cells, sensors, and optoelectronic devices.

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EP02-Memristor devices from theory to system level integration for next generation of computation and communication

Advancements in Memristor Device Development: From Material Stack Optimization to Physical Modelling

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)Analog and parallel processing architectures are promising computing paradigms to implement energy-efficient artificial intelligence (AI) hardware systems that resemble biological brains. As result, the development of novel materials/devices and integrating them to neural and synaptic functionalities have been successfully demonstrated by showing analog signal processing of neuron and synapse devices (e.g., oscillatory neurons and analog in-memory computing of synapse arrays) [1]. This presentation delves into the pivotal role of material science in shaping various devices based on Phase Change Materials and Oxide Resistive Random-Access Memories (RRAMs), fundamental components for emulating artificial neural and synaptic functions in neuromorphic computing [2,3]. These devices, grounded in diverse physical mechanisms and materials, necessitate comprehensive understanding through experimental and theoretical approaches for optimization and integration into higher layers of computer architecture. Their rich spectrum of switching and oscillating behaviors, governed by a myriad of factors such as material compositions, fabrication techniques, and device morphologies, offers substantial design flexibility to tailor devices to specific application requirements. We will see examples of how material and device engineering can lead to breakthroughs in device performance. Nonetheless, device variability among other non-idealities still hinders the hardware scaling to large networks required to solve more complex AI tasks. Challenges at the device and hardware level may also be overcome through a complementary research effort to develop more robust, hardware-friendly algorithms and computational models that could compensate for the variability issues of devices.
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Electronic Switching and anti-doping in heavily defected resistive memory devices

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Resistive memories have huge potential for electronic devices, but poor reproducibility and control of device properties remain a major drawback. The basic design is as simple as a metal-insulator-metal sandwich structure. The insulator layer of some tens of nanometers is the active medium, whose resistivity can be switched by applying bias to the metal electrodes. An obvious cause of inconsistencies and poor reproducibility of device functionality arises from the fact that the active medium typically is a highly defective oxide (e.g. titania, zinc oxide, or nickel oxide), and new defects are formed and migrate during device operation, manifested by structural changes observed in TEM observation of resistive memory operation. We first show how local phase transformations manifested by filament like structures exhibit electronic defect like behavior via the so called anti-doping mechanism, and then present a purely electronic mechanism for resistive memory switching, which occurs in highly defective insulators sandwiched between metal electrodes. Here, the switching occurs via charging and de-charging the defects in the active medium, controlled by external bias. This type of concerted charging of defects is due to multiple solutions of Poisson's equation for the device, which exist only for highly defective systems of no larger than some tens of nanometers. Thus, defects play a crucial role in this electronic switching mechanism, and switching properties can be controlled by modulating the defect species and their abundance. We show how filament like structures can act similarly to multivalent defects, and can yield multiple intermediate resistive states in addition to the conventional binary ON/OFF operation, and even may offer a control of sample magnetization in case of spin-polarized defects. This work is done in collaboration with G. M. Dalpian, A. R. Rocha, and A. C. M. Padilha.

Oxide Thin-Film Integrated Circuits with Memristors

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Analog systems are inherently very power-efficient parallel computers. However, the lack of long-term analog memory is arguably the greatest challenge facing analog computing systems. Spike-timing-dependent plasticity, spike-rate-dependent plasticity, and short- and long-term memory properties have been reported for the memristor, providing the necessary opportunity for efficient analog and spike-based neuromorphic computing implementations to become a reality. Systems using memristors are typically based on hybrid approaches (e.g., CMOS - memristor), which pose integration difficulties and raise costs. However, costs can be greatly reduced if memristive masks are part of the supporting electronic circuitry and are processed with similar steps, thus favoring integration density. With this premise in mind, our work has been aimed at innovating the status quo by developing computational memristor networks based on thin-film technologies, integrated together with thin-film transistors (TFT) for the necessary electronic control [1]. The opportunities for memristor technologies are not limited to this scope, RF switching can also benefit from this technology and is currently being explored for Reconfigurable Intelligent Interfaces (RIA) with applications on incoming 6G communications. However, electronics with TFTs have its own set of challenges that need to be carefully addressed, such as the lack of complementary devices and low speed. In addition, the modeling of memristor devices [2] is also a challenge that needs to be tackled to enable the design of complex systems. We will present some advances on these different aspects.

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Thermal aspects of filamentary switching VCM devices

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Recently, redox-based resistive switching devices based on the valence change mechanism (VCM) entered the market as non-volatile memories for smart card applications and in microcontrollers for automotive applications. As a two-terminal device the devices suffer from the so-called voltage time dilemma: While the data should be stable for years at low read voltages, a programming pulse of less than 3 V should be sufficient to switch the device on the nanosecond timescale. It has been demonstrated that local Joule heating is the dominating process in resolving the voltage-time dilemma [1]. Thus, temperature can be considered as a crucial factor for determining the device's operation.

In this talk, the influence of the local Joule heating on the switching dynamics of VCM cells is discussed. It will be shown that the appearance of digital and analog switching in a single device can be attributed to the thermal feedback of the system [2-4]. This opens design strategies for improving the device stacks towards the targeted application. The intrinsic Joule heating leads to thermal crosstalk effects in memory arrays. It will be discussed how this crosstalk effect can be exploited for security talks, but also how crosstalk can be mitigated. On the other hand, thermal crosstalk can be exploited to implement basic learning rules [5]. It will be shown that for small distances, short pulse lengths and delays associated learning rules, spatio-temporal correlations in VCM arrays occur. In the end, a perspective of exploiting thermal effects for different applications will be given.

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Unveiling the Complexities and Opportunities of Memory Responses in Electrochemical Processes and Electronic Devices

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Our studies explore the nonlinear responses of conductive materials and electronic devices, investigating phenomena like redox reactions on the surface of metamaterials, photodiode currents, memristive effects in semiconductor oxides, and other electrochemical processes. Our primary aim is to elucidate the physical origins of these effects, offering a unified theoretical interpretation for diverse experimental outcomes. To attain a comprehensive understanding, our research encompasses the classification of memory devices based on geometric principles, facilitating the identification of universal subgroups. Additionally, we provide insights into optimally manipulating memory responses to external stimuli, delineating constraints for controlling on-off strength rates, content area, and retention times. Our efforts extend to developing design guidelines for fabricating memory devices with tailored figures of merit, ensuring optimal performance across various applications. Furthermore, we unravel intricate interactions among different memory functionalities, proposing protocols for individual improvement. We aim to broaden traditional equivalent circuit representations offering a microscopic view for accurate interpretation. Addressing complexities in spectral impedance analyses within systems exhibiting intrinsic memory, our study advocates for a nuanced approach to refine analytical methodologies. Particularly challenging is the separation of dynamic contributions from non-equilibrium components and underlying steady-state characteristics. Inherent systematic errors pose an accuracy floor, limiting measurement precision. Effectively addressing these errors is crucial to surpassing this limitation. We aim to provide valuable insights into understanding and manipulating nonlinear responses in electronic materials and devices, emphasizing the challenges and opportunities presented by memory responses in electrochemical processes.
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Emulation of Neuronal Action Potential Using Graphene-Based Memristors

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In this work, the goal is to emulate the behavior of the neuronal membrane using graphene-based memristors. The memristor was a device theorized by Chua back in the 70s [1]. In this research, memristors were manufactured based on a graphene layer with bottom contact made of indium tin oxynitride (ITON) and top contact made of aluminium. ITON is a transparent material with a wide band gap. This oxynitride was obtained by evaporation and annealing in a conventional oven with nitrogen flow and four different temperatures (300 °C, 400 °C, 500 °C and 600 °C). The devices were electrically characterized to obtain important parameters such as SET and RESET. Memristors can be characterized as unipolar, and the phenomenon possibly responsible for threshold switching is the formation of oxygen vacancies. Considering that the contacts are not active, but the bottom contact is a thick oxide, and the fact that the intermediate layer is tens of nanometers thick, the justification for the formation of the resistive filament would lie in the defects present in the graphene layer, especially oxygen-related vacancies. Additionally, the ITON as a contact could also be influencing due to its oxide nature. In the Raman spectrum of graphene, the presence of defects that have the potential to act as oxygen vacancies was noted. The devices were tested in association with a circuit that emulates the behavior of the neuronal membrane. It was noted that the behavior became non-linear and could emulate the interference of an external element in the behavior of the action potential.

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ITO/polymer/Al device: from diode-like to memory behavior

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The pristine diode-like device ITO/ MEH-PPV/Al, needs an electroforming process to turn it into a resistive switching memory device. During electroforming, I-V sweeps are described using Schottky Emission (SE) and Fowler-Nordheim (FN) models, resulting in an injection barrier around ~ 0.8 to 0.9 eV that may be associated with injection through polymer/Al interface [1]. At a high resistance state (HRS), the linear coefficient of the logIxlogV curve is n □ 1 at low voltages and presents a transition to n □ 2 when the device is close to switching voltage. At low resistance state (LRS), we observe n□1 up to the negative differential resistance (NDR). Exploring the reverse bias NDR at different levels, it is possible to observe multilevel conducting states in direct bias sweeps (opposite polarizations), unlike unipolar memories, which show multilevel states when exploring NDR at different levels in the same polarization direction. I-V multilevel sweeps are following the Quantum Point Contact Model (QPC). The resulting fitting parameters show that the number of filaments increases from one (at HRS) to 70 as the multilevel states approach LRS. Also, the t_{gap} decreases from (0.59 ± 0.02)nm to (0.44 ± 0.01)nm. The conductance found in terms of G $(=2e^2/h = 7.75\text{x}10^{-5}\text{S})$ was $1G_0$ up to $11.5G_0$, compatible with values found from QPC model on I-V multilevels.

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Memristors in SURMOFs: Unlocking Novel Functionalities for Electronic Devices

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Memristors (MRs) hold promise for surpassing the limitations of complementary metal-oxide-semiconductor (CMOS) technology, nearing its scale limit. Metal-organic frameworks (MOFs), particularly surface-supported metal-organic frameworks (SURMOFs), offer high mechanical flexibility and low cost, making them suitable for MR-based hybrid materials. This presentation integrates highly porous sub-15 nm thick HKUST-1 films into functional devices, utilizing a rolled-up nanomembrane approach, demonstrating room-temperature negative differential resistance (NDR) in SURMOF vertical heterojunctions. Precise control of relative humidity (RH) and electric fields tailors NDR, with a peak-to-valley current ratio (PVCR) of about two at low voltages (<2 V). Band diagram analysis, density functional theory (DFT) calculations, and molecular dynamics simulations elucidate the underlying mechanisms. Furthermore, integrating SURMOF films in scalable-functional devices overcomes challenges, offering versatile, low-power ambipolar resistive switching. This research presents a pathway toward leveraging MR-SURMOF hybrid structures for future scalable functional devices in various strategic fields, from electronics and computing to energy, healthcare, and beyond.

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ZTO-based memristors for novel computational architectures

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Although the processing performance of computing systems has been increasing over the last few years, the inherent energy consumption and latency overhead caused by the transfer of data from the memory to the processing units (Von-Neumann bottleneck) is still present. In order to circumvent this problem, new hardware architectures that emulate the human brain´s biological computation have been proposed. Two-terminal resistive switching devices, memristors, have been studied not only due to their fast pulsing time and low operating voltages, but also for their intrinsic non-linear response. This last property is especially useful when aiming for systems based on reservoir computing. Reservoir computing architectures excel at processing temporal/sequential data by having a fixed reservoir space and only requiring its readout layer to be trained, leading to considerable savings both in time and energy expenditure.

Amorphous oxide semiconductors (AOS) have been recently studied for their use in neuromorphic systems, as they are compatible with cheap, easy and low temperature fabrication processes, making them prime candidates for applications that take flexibility and transparency into account (e.g. System-on-panel applications, wearables)[1]. In this work we present memristive devices that utilize Zinc–Tin–Oxide (ZTO) as their active resistive switching material. By choosing ZTO instead of more heavily studied AOS´s, such as Indium-Gallium-Zinc-Oxide (IGZO), we avoid the use of rare elements, resulting in a more sustainable alternative.

The devices are studied in terms of their materials, fabrication processes, and electrical performance. Quasi-static I-V characteristics, pulse measurements analysis and synaptic performance are analysed, with special focus on their performance towards reservoir computing.

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Characterization of Anodized Aluminum Oxide Thin Films for Device Applications.

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This technique has been widely used in the devices such as transistors and quite novel in resistive memories. The thin anodized layer was characterized using UV-VIS, FTIR, Raman spectroscopy, four-point collinear probe to determine sheet resistance, and AFM. UV-VIS analysis revealed that parameters such as time and applied voltage during the growth process of the anodized aluminum oxide (AAO) layer altered the transmittance values, rendering the films more transparent with the growth process. In addition to these analyses, spectroscopic techniques such as FTIR and Raman revealed the amorphous nature of the anodized films. Furthermore, with four-point probe measurements, it was possible to observe an increase in material resistance with increased oxide thickness [1]. Images obtained by AFM were analyzed using software developed by the research group, student João Guilherme Vaz Duarte, where first and second-order statistics were performed. As a result, it was observed that higher anodization voltage led to higher roughness, reaching 30 nm at 30 V. At low voltage and with anodization time minimized to 2 minutes, the root mean square roughness was 6.8 nm. It was observed that the produced films exhibited surface relieve isotropy and correlations around 132 nm. Finally, the fractal dimension was determined, and we found values around 2.2 indicating that the surface is close to two-dimensional.

CNPq, CAPES, FINEP, FAPESP, FAPEPI, UFPI, INEO

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CYCLE ENDURANCE AND FAILURE IN ITO/MEH-PPV/AL RESISTIVE SWITCHING DEVICES

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Improving resistive memory reliability requires understanding some bottlenecks, i.e., control and stability of the memory parameters during endurance cycling and physical degradation that shows up in memories that contain metal oxides. The physical degradation of indium tin oxide/ MEH-PPV /aluminum (ITO/MEH-PPV/Al) devices was studied through I–V sweeps and cycle endurance with different compliance currents (□□), in addition to scanning electron microscopy (SEM), energy dispersive X-Ray spectroscopy (EDS), and Raman spectroscopy. The devices showed a dependence of the conductance quantization □0 in current compliance □□, i.e., the □0 histogram shows different distribution shape after changing □□. After many cycles, the devices presented partial destruction in the active area (physical alteration) followed by memory parameter degradation and finally failing (no commuting anymore). SEM/EDS measurements in the deteriorated region showed that the aluminum electrode was removed and only remnants of the polymer remained. The Raman spectroscopy analyses focused on changes in the polymeric structure caused by the endurance cycle, such as changes in chain planarity, which is related to the band around 966 cm-1 that was shifted to lower wavenumbers (965 cm-1) together with the increase in intensity which indicates less planar conformations when compared to the non degraded area. Alteration of the conjugation length was evidenced by the contribution around 1581 cm-1. In this case, we can see a shift: of 1581 cm-1 to 1584 cm-1, for the non-degraded area and degraded area, respectively. Both results indicate a decrease in the conjugation length. All these changes show fragmentation of the polymer chain as a result of the endurance cycle.

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Electrical contact influence on the analysis of memristive behavior in ZnO:Na thin films

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The advent of memory resistors (memristors), postulated by Leon Chua in 1971 [1] with a functional device demonstrated in 2008 [2], focus the research of semiconductors on new materials that behave as a memristor. The memory effect is observed in oxide semiconductor materials, whose intrinsic defects, charge transport, and superficial effects are the main ingredients to achieve this state. In addition, the stable characteristics of the memristive response in thin films of oxide semiconductors allied to the integration with CMOS technology [3], favor the development of new computational technologies, such as artificial neurons, neural networks, non-volatile memories, chaotic systems, and many others applications and devices. This study aims to evaluate the role of electrical contact symmetries over the memristive effect in a thin film of sodium-doped zinc oxide (ZnO: Na). Symmetrical (Au-Au) and asymmetrical (Au-Ag) contacts were deposited on top of film surface emulating memristive devices. Current-voltage characteristic curves (I-V) are obtained by cyclic sweeps of stair-like amplitudes from 20V to 40 V over periods of 1 and 5 minutes. The memristance is calculated by the area inside the I-V curve and the influence of the step's height of the applied staircase signal is evaluated. Asymmetrical contacts present a Type-I characteristic memristor while symmetrical contacts show a Type-II behavior for measurements conducted at room temperature and open air atmosphere.

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Exploring resistive memory properties of sodium-doped zinc oxide thin films

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The advent of resistive memory effect in electronic devices holds the promise for various applications such as neuromorphic computing [1], non-volatile memories [2], and biomedical implants [3]. Memristors, in particular, have garnered attention for their capability to modulate resistance via an external electric field, enabling configuration into multiple distinct states. Traditionally, materials showcasing the resistive memory effect are engineered utilizing a metal-insulator-metal (MIM) structure, wherein a layer of semiconductor oxide is sandwiched between two metal electrodes. Nonetheless, resistive memory has also been observed in devices employing lateral planar electrical contacts. This study is focused on investigating the resistive memory characteristics of thin films of sodium-doped zinc oxide (ZnO:Na). These films were synthed using the spray pyrolysis technique, and their electrical properties were evaluated through cyclic current-voltage sweeps. Our research endeavors to delve deeper into the electronic transport phenomena inherent in ZnO:Na thin films, particularly those deposited on glass and ITO substrates. Employing planar electrical contacts for the sample grown on glass substrate and vertical (MIM) electrical contacts for the sample grown on an ITO substrate, we aim to unravel the distinct transport behaviors and discern the underlying mechanisms driving them. We anticipating that the memory response evaluated through our approach could serve as a pivotal characterization tool for nanoscale electrochemical processes, potentially advancing our understanding of complex electrochemical phenomena.

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Resistive memory devices with anodized aluminum oxide thin films

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Resistive memory devices with Al/MEH-PPV/AlOx/Al structure were built and underwent electrical characterization in order to identify the electroforming and operating parameters of the device. This structure, when compared to those already established by the group, was facilitated by the oxidized layer, requiring only a single sweep from zero to 8. Thin films of aluminum oxide grown by anodization were used in the construction of resistive memory devices, before the construction of the devices, the thin films of anodized aluminum oxide (OAA) underwent characterization through the techniques of UV-Vis, AFM, Raman, 4-tip and FTIR, in order to understand the optical, morphological and electrical properties of this layer, which helps in the understanding of the physical and functional properties of the device [1]. These results demonstrate that the anodization process is a good choice for growing oxide films for device applications. The electroforming process of this type of structure, when compared to those already established by the group, was facilitated by the oxidized layer, requiring only a single sweep from zero to 8 V for electroforming. Moreover, the structure with Al/MEH-PPV/AlOx/Al showed an average ON/OFF ratio of 1.7x10^2 (two orders of magnitude), rendering the different resistive states easy to distinguish [2].

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Understanding Resistive Switching in Al/MEH-PPV/ITO Organic Memory Devices through Temperature Variation

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The devices known as Resistive Random Access Memory (RRAM) are devices that exhibit resistive switching. Despite advances in studies on the switching mechanisms of polymer-based RRAM devices, there are still difficulties in understanding the fundamental concepts of resistive switching. In this work, an Al/MEH-PPV/ITO device was characterized as memory. The study of the electroforming process and the characterization of the device as memory were conducted under temperature variation regime. Initially, the study of the electroforming process was carried out at room temperature. After samples were showing well defined resistive states at room temperature - Low (LRS) or High (HRS) - temperature variation was carried avoiding voltages to commute. The Quantum Point Contact (QPC) model was used for data analysis. We propose that conduction occurs through conductive filaments formed by oxygen vacancies, with the presence of a potential barrier of 1.51 eV[1]. Through temperature variation, when the device is already a memory, it was confirmed that charge carriers tunnel through the potential barrier. As the device cools, the height of the potential barrier decreases and its width increases. Under temperature variation, in the range of 200 K to 300 K, the current obtained in the HRS and LRS states does not vary with increasing temperature, only small oscillations in the current value are observed. Thus, we suggest that conduction occurs through the tunneling mechanism. However, when switching is forced under decreasing temperature, the barrier widens, reducing the tunneling probability along with the intensity of the transmitted current. Finally, at around 100 K, switching between the low-resistance state (LRS) and high-resistance state (HRS) does not occur, and the region of negative differential resistance is not observed.

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EP03-XIV BRAZILIAN ELECTROCERAMICS SYMPOSIUM

Driving Innovation in Biomass and Greenhouse Gas Transformation: A Journey with ISI Biomass

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Founded in 2013, the ISI Biomass has emerged as a beacon of excellence in applied research in Três Lagoas/MS. Renowned for its substantial contributions to the development of novel products, and innovative processes in biomass transformation, ISI Biomass has cultivated a strong reputation through the execution of over 80 projects across various industrial sectors. These projects align with different core focus areas, such as Circular Bioeconomy, Bioprocess and Biotechnology, Energy and Sustainability, and Decarbonization Technologies. Among its notable client and partner roster are esteemed companies such as Suzano, Galp, and Exxon Mobil, underscoring ISI Biomass's ability to address industry-specific demands promptly and efficiently. Collaborative ventures with producers of renewable raw materials have played a pivotal role in driving technological advancements focused on the characterization and transformation of solid, liquid, and gaseous biomasses, and GHGs, with a keen emphasis on decarbonization and facilitating the energy transition of the Brazilian industry. Endorsed by EMBRAPII in CCUS Technologies, ISI Biomass is unwavering in its dedication to innovative and sustainable solutions. Projects such as 'DeCarbon' and 'TUPÃ' exemplify this commitment. 'DeCarbon' strives to develop a sustainable, cost-effective, and highly efficient technology for capturing CO2 emitted by the steel industry, while 'TUPÃ' focuses on advancing catalytic and electrochemical conversion technologies to transform CO2 and CH4 emissions from the oil & gas sector into clean fuels. ISI Biomass features advanced facilities like the Decarbonization Technologies Laboratory, focusing on gas conversion for renewable hydrogen and hydrocarbons, and the SOFC/SOEC technology system for single cells and stacks testing. Such resources highlight ISI Biomass's dedication to pioneering research and innovation in biomass transformation.

In operando Diffuse Reflectance Infrared Fourier transform (DRIFT) Spectroscopy for Metal Oxide Based Electrochemical Cells

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In DRIFT spectroscopy, the sample is illuminated by an infrared (IR) beam, and the scattered (rather than transmitted) light is collected using the appropriate optics. Not only does this configuration lend itself to *in operando* measurements, DRIFT spectroscopy has also been found to be more surface sensitive than other IR techniques.[1] The usefulness of DRIFT spectroscopy for studying the metal oxide-gas interface is clear from the work in metal oxide based gas sensors and high temperature catalysts.[2] Critical insights into different surface processes, ranging from the influence of humidity on the oxygen reduction reaction in fuel cell cathodes to anodic coking mechanisms when using hydrocarbon fuels, could surely also be gained. The use of DRIFTs, however, for metal oxide electrochemical cells is still in its infancy. Only a few near operando studies have been reported and cell optimization is still required.[3, 4] In this presentation, we will discuss the bottom up design of our measurement set-up. We will present results on different high temperature metal oxide based electrochemical systems from our lab.

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Ordered Mesoporous Ceria and Cerium Gadolinium Oxide Prepared by Vacuum-Assisted Nanocasting

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Four ceria-based mesoporous oxide materials were prepared using a new Vacuum Impregnation (VI) templating method developed by the authors, Vacu-um-Assisted Nanocasting (VAN). Two hard templates (SBA-15 and KIT-6) were employed and products of composition CeO2 and Ce0.9Gd0.1O1.9 (CGO) were made with each. The desired Fluorite phase and composition were confirmed by powder XRD and EDS. Product structures were characterised by XRD, TEM, gas physisorption and SAXS. All products contained ordered mesoporous material in high yields. The specific surface areas (SSAs) and pore volumes of the products were determined to be high and the pore and pore spacings related well to the templates from which the materials were synthesised. TEM studies con-firmed that the samples had a 3D pore structure, this being the negative of the original template. The target materials were not only produced in high yields, but also displayed porous single crystal morphology, with non-linear lattice planes. The highest SSA values and pore volumes were reported for materials im-pregnated using the KIT-6 template, and with the CGO composition. The results suggest that VAN is an excellent and reproducible method for producing or-dered mesoporous cerias and also has considerable potential for wider application. All the mesoporous products showed dramatically increased reducibility in TPR experiments compared to a high SSA nanoparticulate ceria reference. This is very promising for their potential applications in oxidation catalysts and in fuel cell components.

Shedding light on exsolution mechanisms using PAINEIRA beamline at SIRIUS

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Exsolution is the mechanism whereby a doping metallic element is incorporated in a host oxide lattice, forming a solid solution. Upon heat treatment and a reducing atmosphere, the lattice contracts while the doping element migrates to the surface segregates as crystalline nanoparticles and is socketed to the matrix. This technique has opened opportunities for materials design with relatively simple synthesizing pathways leading to higher stability and activity. The socketed nature and crystallographic alignment induce strain within the NPs, potentially affecting catalysis and electrochemistry application. The host matrix's chemical composition and structural properties are fundamental to induce the exsolution mechanism. The perovskite structure is the most favorable material for hosting exsolved NP due to its flexibility in presenting a variety of cations with different s, allowing cation, ion oxides, and electron transport and structural defects. Based on that, the structural characterization of the perovskite is essential to determine distortion and defects, probe the stoichiometry, and obtain the average particle and strain. Thus, a high-quality X-ray diffraction analysis, uniquely obtained in the in-situ experiment during the exsolution formation in a synchrotron facility, is a powerful technique to shed light on the exsolution mechanism. In this work, we have explored the PAINEIRA beamline capabilities at the SIRIUS synchrotron laboratory to the structural characterization of LaCrxRu(1-x)O3 perovskite ex-situ and in-situ with a controlled flow of 3%H2/He and temperature variation up to 8500C. The beamline energy was 19.5 keV in the transmission, and the high-resolution detector was used to acquire the XRD patterns. Rietveld refinement was carried out using GSASII software. We identified the distortion from the regular perovskite, especially since the determination of stoichiometry gave rise to the quantity of exsolved Ru nanoparticles that formed.

Thermal diffusivity in Barium Bismuthate

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Perovskite-type complex oxides are a family of compounds that have attracted growing interest because of the variety of tunable physical properties, which makes them attractive for technological applications in different areas [1]. In this talk, I will present and discuss our recent investigations of thermal diffusivity in a representative of this class of oxides: the Barium Bismuthate BaBiO3 (BBO) [2]. BBO exhibits an insulating ground state with a still debated origin and a superconducting state upon hole-doping, besides being predicted to host a topological insulating (TI) state upon electron doping [3]. A complex relation between electronic and lattice degrees of freedom has been called into question in an attempt to explain the electronic states of this compound [4]. Our thermal conductivity experiments found a remarkably low value at room temperature (~1W/mK), a plateau at intermediate temperatures, and an unexpected ~T2 power law at low temperatures (T < 5K), reminiscent of a glass-like behavior [2]. Our specific heat measurements at very low temperatures support this scenario. The analysis of the mean free path, which is of the order of the atomic distance at room temperature, suggests the presence of additional scattering mechanisms that impede an efficient heat flow.

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Bridging Ceramic Superconductors with UN Development Goals: Perspectives and Applications

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Ceramic superconductors exhibit remarkable properties such as zero resistivity and diamagnetism above the boiling temperature of liquid nitrogen, making them promising candidates for various applications including electrical engines, energy generation, storage, and high-tech devices like single photon detectors. In this overview, we explore the correlation between ceramic superconductors and the United Nations (UN) Development Goals, emphasizing their potential impact on sustainable development. Through bibliometric analysis, we underscore the significance of ceramic superconductors in addressing global challenges outlined by the UN. Additionally, we discuss the application of supermagnets and second-generation tapes in healthcare systems, particularly in MRI devices for diagnostic imaging. Furthermore, electric superconducting motors offer a clean alternative to highly polluting diesel engines in maritime transportation. Magnetic levitation technology holds promise for developing zero-emission public transportation systems. At the nanoscale, superconducting nanowire single photon detectors (SNSPDs) enable real-time monitoring of environmental health, exemplified by applications in plant physiology. Within this context, the Superconductivity and Advanced Materials Group is dedicated to advancing the production and enhancing mechanical properties of ceramic superconducting nanowires. Our research aims to harness the potential of SNSPDs for in situ applications, explore bulk ceramic materials for energy storage, and investigate emerging nickelate superconducting ceramics.

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CH_4 conversion into value-added products by catalytic processes assisted by electrochemical reactions in solid oxide cells

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Methane (CH_4), the major constituent of natural gas and biogas, is an abundant source to obtain value-added hydrocarbons. The oxidative coupling of methane (OCM) is a direct catalytic route to convert CH_4 towards C_2 hydrocarbons (C_2H_6 and C_2H_4). The use of electrochemical devices such as solid oxide fuel cells (SOFC) as a reactor for OCM is possible, providing synergistic control of electrochemical oxidation/reduction reactions to energy production with in-situ catalysis [1]. In this context, the use of mixed oxide $La_{0.5}Ce_{0.5}O_{2-\delta}$ (LCO) was studied as an additional catalytic layer on the Ni/YSZ anode of a SOFC for the operation under CH_4 as fuel. The presence of surface oxygen vacancies in single-phase LCO, which may benefit the OCM reaction, was evidenced by Raman spectroscopy [2]. The catalytic properties of LCO at 800 ºC were investigated in a fixed-bed catalytic reactor, resulting in a C_2 selectivity and yield of 41% and 8%, respectively. The modified SOFC with the additional LCO-catalytic layer was fabricated and tested under H_2 and CH_4 [2]. The electrochemical properties were studied during online gas analysis of the anode outlet. The experimental data revealed that CH_4 conversion and product distribution are closely related to operational conditions such as reactant concentration, anode feed flow rate, current output, and operating temperature. In addition to C_2, products of internal methane reforming (CO and H_2) were detected in all evaluated conditions. The SOFC showed stable behavior, maintaining a stable current of 20 $mA\cdot cm^{-2}$, 10% of CH_4 conversion, and 14% of C_2 selectivity throughout 30 h. The combined catalytic and electrochemical reactions described are considered a promising approach to producing valuable chemicals and electrical energy.

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Dielectric properties of TiO_2 co-doped with yttrium and niobium

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The effects of small contents (up to10 mol%) of Y_2O_3 and Nb_2O_5 on the microstructure and dielectric properties of TiO_2 were investigated, aiming to identify the underlying mechanism in the colossal permittivity of co-doped specimens. Sintered materials were prepared by the solid state reaction method and characterized by X-ray diffraction, scanning electron microscopy, and electrochemical impedance spectroscopy. All sintered specimens exhibited the characteristic tetragonal TiO_2 rutile phase. Secondary phases were detected at the grain boundaries, independent on the sintering temperature. The mean grain increased with both sintering temperature and co-dopants content. The higher electric permittivity was obtained for specimens with 5 mol% of co-dopants, sintered at 1480ºC, and the lowest value of the dissipation factor for samples with 10 mol%, sintered at 1500ºC. The dielectric properties of co-doped TiO_2 were attributed to the internal barrier layer capacitance and electron-pinned dipole defect mechanisms.

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Effect of lanthanum doping on the ceria fluorite structure and its relationship with transport properties

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Doped ceria and its solid solution are popular materials widely investigated in energy conversion and electrochemical devices. It has a cubic fluorite structure and doping with La^{3+} changes to a disordered fluorite and a C-type structure. Moreover, the doping level offers a path to tune the defect chemistry for applications in several fields.[1] In this work, we investigate solid solutions of La-doped ceria ($La_xCe_{1-x}O_{2-x/2}$) with x from 0 to 50 at.% compressed into pellets to investigate the electrical properties and its correlation with defect chemistry and crystal structure. The transport properties were studied via electrochemical impedance spectroscopy in air and different p_{O2}. The findings show that electrical conductivity increases from 0 to 5 at.%, and then remains constant up to 15 at.%. However, beyond 20 at.%, it starts to decrease. This trend can be explained by the formation of vacancies formation.[2] For lower levels of lanthanum doping, the creation of vacancies improves conductivity. However, at higher concentrations (>20 at.%), the increase of oxygen vacancies leads to the formation of dopant-vacancy clusters. This process arises from the Coulomb interaction between vacancies and local lattice relaxation in the crystal. The increase in activation energies above 20 at.% indicates higher resistance to defect migration. X-ray powder diffraction indicated the presence of only one phase with increased strain and expansion of lattice parameters, as determined through Rietveld refinement. Raman spectroscopy indicated structural changes in the fluorite structure, including the emergence of a C-type phase. Additionally, it detected local symmetrical breaking and vibrational changes in the structure due to the formation of oxygen vacancies.

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Enhancing piezoelectricity in poly(vinylidene fluoride): the role of reduced graphene oxide synthesis in potential sensor.

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Polymeric materials like poly (vinylidene fluoride) (PVDF) have been extensively studied for their piezoelectric properties, making them ideal for sensor applications. The development of a composite material has demonstrated enhanced piezoelectricity. It has been observed that the synthesis method of reduced graphene oxide (RGO) significantly influences the increase in the electroactive β crystalline phase, which is responsible for generating piezoelectricity. Various synthesis techniques for RGO were explored, including thermal treatment reduction (RGOT), hydrazine reduction (RGOQ), and microwave-assisted plasma reduction (RGOP) using Ar/N2 gas mixtures. Among these, the PVDF/RGOT composite, reduced at 500°C, exhibited superior piezoelectric capacity. This was verified through polarization tests and the measurement of its dielectric constant. The material displayed a remanent polarization of 1.4 μC/cm² and a relative permittivity of 18.3 at 1.2 Hz, highlighting its potential for sensor applications, such as pressure sensors. A specific architecture was developed to organize the composite material into a sensor with remarkable piezoelectric capabilities, capable of generating electrical signals under mechanical pressure—known as the direct piezoelectric effect.

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Exploring the Mechanism of Copper Nanoparticle Exsolution from Perovskite Oxides: A Multi-technique Approach

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The exsolution of copper nanoparticles (Cu NPs) from perovskite oxides (POs) presents a promising avenue for producing highly stable catalysts for several applications [1]. However, despite its potential, a significant research gap exists in understanding the fundamental mechanisms underlying the exsolution process and its associated morphologies [2]. Given that exsolution involves multi-scale dimensional and compositional aspects, we employed a range of techniques to probe these dimensions comprehensively. By integrating Raman Spectroscopy, X-ray Diffraction (XRD), Scanning and Transmission Electron Microscopy (SEM and TEM), X-ray photoelectron Spectroscopy (XPS), and X-ray Absorption Spectroscopy (XAS), our ongoing research aims to unravel the intricate effects that dictates the exsolution process. Herein, we conducted a comprehensive analysis of Sr(Ti,Fe,Cu)O_3 PO before and after NPs exsolution at various temperatures in a 5% H_2/Ar atmosphere and evaluate its potential applications, including the thermal valorization of CO_2. The microscopy findings indicate distinct exsolution mechanisms among the POs' crystal facets, driven by discrepancies in interfacial energy affecting nanoparticle nucleation and growth [3]. Raman, XPS, and XRD analysis suggested atomic level alterations, while XAS unveiled Cu oxidation state variation before and after the exsolution at different temperatures. Our ongoing in situ analysis seeks to uncover the reduction, nucleation, and growth stages of the process. Ultimately, our goal is to develop a quantitative model to regulate particle and population, critical for controlling activity and selectivity in catalytic applications.

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Growth and characterization of a Cu-modified (K, Na)NbO3 single crystals obtained by the Bridgman-Stockbarger method

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Lead-based single crystals are well known for their superior electrical properties. However, environmental concerns about the effects of the continued use of Pb-based materials worldwide are encouraging research into alternatives to their use. Single crystals of (K, Na)NbO3-based compositions are one of the most promising materials for substituting Pb-based ones [1]. This work reports the growth and the structural, chemical, and dielectric characterization properties of Cu-modified (K, Na)NbO3 lead-free single crystals grown directly from the melt by the Bridgman-Stockbarger method. To our best knowledge, it's the first time that the growth of this composition by the Bridgman route has been reported. The as-grown crystal was cut to proceed with the characterization. The results of the XRD patterns showed high-quality single crystals of an orthorhombic structure, with similar cell parameters of its polycrystalline form. The EDS analysis showed a composition deviation, especially for the K and Na elements, which is expected due to the large incongruence of the KNN-Cu. The temperature dependence of the dielectric constant showed two dielectric anomalies, around 201 °C and 381 °C, corresponding to the ferroelectric-ferroelectric transition and ferroelectric-paraelectric transition, respectively, which is in agreement with XRD.

Impedance spectroscopy analysis of percolation of ions within alkali salt- solid electrolytes ceramic membranes

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Electrochemical impedance spectroscopy (EIS) analysis was applied to evaluate the carbon dioxide ionic conductivity at the interfaces of porous solid electrolytes impregnated with alkali salts. An impedance analyzer was connected to an alumina sample holder with gold electrodes and platinum terminal leads, inserted in a programmable tubular furnace. Yttria-stabilized zirconia, samaria- and gadolinia-doped ceria, tungsten-doped lanthanum molybdenum oxide porous solid electrolyte ceramic pellets were prepared by using either a polymer or graphite as thermally removed sacrificial pore formers. Molten eutectic compositions of sodium-potassium and/or lithium-sodium-potassium carbonates were impregnated into the porous solid electrolytes. The collected [-Z"(f) x Z'(f)] impedance data showed the evolution from oxygen ion conductivity to carbon dioxide ion conductivity when the temperature of the ceramic pellets reached the melting point of the carbonates. Endurance tests were performed to evaluate the lifespan of the composite ceramic pellets in the molten state of the carbonates for either carbon dioxide capture or sensor device evaluation.

Nickel immobilization aiming improved electric conductivity on silicon oxycarbide (SiOC) matrices

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Silicon oxycarbide (SiOC) ceramics are polycrystalline materials that contain a semiconductive, conductive phases together insulating fraction. The addition of transition metals can enhance the formation of silicon carbide (SiC) and graphitic carbon domains [1]. Research has shown that SiOC electrodes interact favorably with hexacyanoferrate(II) and (III), resulting in higher electroactive areas compared to glassy carbon (GC) electrode [2]. This study explores the effect of incorporating nickel into SiOC ceramic structures and assesses their electrochemical properties using $Fe^{2+}/^{3+}$ as a probe. Polymer precursors were formulated with 60 wt.% poly(methylhydrosiloxane) and 40 wt.% divinylbenzene, in the presence of 20 wt.% polyethylene, and different amounts of NiCl2 (0, 1, 3, 5, 10, and 20 wt.%) followed by pyrolysis at 1400 °C for 1 h, under static argon atmosphere, giving rise to Ni-modified ceramics. Paste electrodes were prepared using a certain ceramic:mineral oil proportion, and the electrochemical behavior of the $Fe^{2+}/^{3+}$ probe was examined via cyclic voltammetry. Ni-modified ceramics showed reduced electrical resistivity compared to pristine SiOC, with values of 5.20 and 0.44 Ωcm for SiOC 3 and 5 wt.% Ni, respectively, compared to 154 Ωcm for pristine SiOC. The improved conductivity was attributed to presence of SiC and nickel silicides within ceramic matrix. Ceramic electrodes outperformed GC electrode in terms of response to the electrooxidation of the $Fe^{2+}/^{3+}$ pair, with SiOC 3 wt.% Ni demonstrating the best performance. This is associated to the enhanced electroactive areas of the Ni-modified ceramics. Impedance spectroscopy revealed that the low resistance of the semiconductive phase and minimal diffusional resistance in SiOC/Ni ceramics facilitated a more effective interaction with the $Fe^{2+}/^{3+}$ pair, resulting in improved current response.

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Oxygen ion conductivity in ceria-based electrolytes co-doped with samariumand gadolinium

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In a systematic study, two compositional series of ceria-based oxides, both co-doped with Sm and Gd, were
synthesised using a low temperature method and evaluated as oxygen ion-conducting electrolytes for
Intermediate Temperature Solid Oxide Fuel Cells (IT-SOFCs). Series one, Ce1-2x$Sm_xGd_xO_{2-x}$, had equal concentrations of Sm and Gd but varying total dopant concentration. Series two, $Ce_{0.825}Sm_xGd_{0.175-x}O_{1.9125}$, had a fixed total dopant concentration but the Sm:Gd concentration ratio was varied. The materials were characterised using scanning and transmission electron microscopy, inductively coupled plasma mass spectrometry and X-ray diffraction. Impedance spectra were recorded on dense pellets of these materials. From these, total, bulk and grain boundary conductivities and capacitances along with activation energies, pre-exponential constants and enthalpies of ion migration and defect association were obtained. These gave a detailed insight into the fundamental conduction processes in the materials. $Ce_{0.825}Sm_{0.0875}Gd_{0.0875}O_{1.9125}$ had the highest total ionic
conductivity at temperatures of 550 °C and above and also demonstrated an enhanced conductivity with respect to its singly-doped parent compounds, $Ce_{0.825}Sm_{0.175}O_{1.9125}$ and $Ce_{0.825}Gd_{0.175}O_{1.9125}$, at 400 °C and above. This compares favourably with previously-reported values and has promising implications for the development of IT-SOFCs.

Solid state synthesis of Er-Yb-doped PMN-0.30PT and their characterization for photoluminescent properties tuned by BIAS electric field.

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The crystal structure of most ferroelectric materials can be locally distorted by changing the temperature, and pressure or by applying a magnetic and/or electric BIAS field. When these external factors are applied to rare-earth-doped ferroelectrics (RE-F), the resulting modification in the local symmetry around the rare-earth dopant sites may result in a tuning of the photoluminescence properties of the doped ferroelectric compound. Such behavior opens great potential for optical applications of RE-F in photonic displays and medical ultrasonic imaging transducer. This work reports the synthesis of Er-Yb-doped PMN-0.30PT ceramics and the characterization of their physical properties, mainly the photoluminescent one, aiming at the investigation of the potential applications of such compounds for piezo-photonics and ferro-photonics applications. The room temperature up-conversion photoluminescence spectrum of the as-sintered ceramic bodies revealed two emissions at about 553 nm and 669 nm corresponding to the transition from $^4S_{3/2}$ to $^4I_{15/2}$ and $^4F_{9/2}$ to $^4I_{15/2}$ of Er^{3+} ions, respectively. Then, it was verified that the emission intensity is proportional to the ^{n}th power of the excitation intensity ($I \propto P^n$), as proposed by theoretical models. The dependence of the $I \propto P^n$ behavior on the applied electric BIAS field was investigated and the results discussed based on the photoluminescent properties driven by changes in the local crystal field around the RE ions.

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SUPERIONIC CONDUCTOR GLASS-CERAMICS FOR IONIC SELECTIVITY OF ALKALINE METALS

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The growing use of lithium-ion batteries has intensified the demand for lithium, projected to reach 2.4 Mton by 2030. However, land-based lithium reserves are insufficient to meet long-term demand. As a solution, extracting lithium from seawater, which holds nearly five times more lithium than land sources, has emerged. This project focuses on creating glass-ceramic membranes using Li1.5Al0.5Ge1.5(PO4)3 (LAGP) composition to extract lithium from seawater via electrodialysis (ED) or dialysis (DD). The synthesis involved preparing the glass, which involves calcining the precursors for two hours at 700°C and melting at 1250°C for 30 minutes. Further, crystallization was achieved through a two-step heat treatment, nucleation, for 1, 2 and 3 hours (N1, N2 and N3), and grain growth, for 3 and 4 hours (C3 and C4). Material characterization included density measurement and impedance spectroscopy, revealing high relative density (97%) for N1C4 and N3C4 samples and achieving the highest ionic conductivity (5.22x10−4 Scm−1) at room temperature (RT) for the latter sample, which is promising for lithium extraction. This is particularly noteworthy given that literature reports the highest LAGP ionic conductivity as 7.25x10-4 Scm-1 [1]. Determination of ionic selectivity on water solution is under investigation using an electrochemical H-cell along with ED or DD and results will be discussed at the conference.

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Tunning the optical and photovoltaic properties in (K,Ba)(Nb,Ni)$O_{3-б}$ perovskite by polymorphic niobium pentoxide precursors

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(K,Ba)(Nb,Ni)$O_{3-б}$(KBNNO) is an important multiferroic material that has intrinsically coupled ferroelectric, optical and photovoltaic properties, which in turn are related to the structural characteristics of the host system. In this work, to understand how structural modifications can induce changes in the optical and photovoltaic properties of the KBNN ceramics, the effect of polymorphic phase of Nb_2O_5 precursors (i.e. monoclinic and orthorhombic ones) on the crystalline structure of the host system was investigated. X-ray diffraction studies revealed structural differences in terms of lattice parameters and bond lengths for the two batches of KBNNO ceramics. Raman spectroscopy also showed subtle differences in the intensity and broadening of some peaks between the two ceramics. Optical absorption results and the related change in the bandgap for the two batches of KBNNO ceramics were correlated with changes in tilting angles, bond lengths, octahedral distortions, and oxygen vacancy formation. Photovoltaic measurements carried out in ceramic samples poled at room temperature showed a significant difference in the photocurrent generated and power conversion energy for each batch. In summary, our results revealed a significant impact of the polymorphic phase of Nb_2O_5 on the physical properties of KBNNO.

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Characterization of Na2O-Al2O3-SiO2 glass system and in situ crystallization of BaTiO3 phase

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Glass-ceramic are polycrystalline materials with presence of residual amorphous phase, obtained from the controlled crystallization of glasses. These materials have a high dielectric constant, mechanical strength, chemical durability, low coefficient and high resistance of thermal expansion. In order to further enhance their properties, the strategy of incorporating perovskite phases into glass-ceramics has been adopted. In this work, a glass, named NAS-BT, was prepared by the melting-quenching technique, with a chemical composition (in mol%) of 20% SiO2, 17.5% Na2CO3, 16.7% Al2O3, 13% TiO2, and 32.5% BaCO3. The glass was melted at a temperature of 1450°C for 30 min. The viscous liquid was poured into a ceramic jar containing distilled water to obtain the vitreous frits. The frits were ground and sieved through a 170 mesh sieve. The glass powder was characterized by the DSC technique to determine the Tg and Tc. Pellets of 1 cm diameter with 500 mg glass powder were prepared, and thermally treated at temperatures of Tc1 = 650°C and Tc2 = 700°C for 1 hour. From the XRD of the pellets, the growth of BaTiO3 (JCPDS 74-1964) and the nepheline phase (JCPDS 35-424) were observed in the pellet thermally treated at 650°C for 1 hour. In the pellet treated at 700°C, an increase in the intensity of diffraction peaks was observed, resulting from crystal growth. The microhardness of the glass-ceramic pellet treated at 950°C for 1 h was 454 MPa, a typical value for silicate-based glass-ceramics. Archimedes test was also performed on the pellet treated at 950°C, with results of 0.23% water absorption, 0.67% apparent porosity, and density of 2.97 g/cm3. Surface images of the pellet, attacked with 5% V/V HF solution for 5 min, were analyzed by SEM, revealing the presence of morphologies in the form of rods and rounded particles, which characterize the present crystalline phases.

Comparative gas sensor response of SnO_2, WO_3, and ZnO to NO_2 and potential interferents

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Gas sensors are important devices for environmental monitoring and safety applications. Semiconducting metal oxides (SMOx) are currently the leading materials in sensing technology due to their capability to interact with gaseous species through adsorption and desorption. Sensors based on SMOx usually exhibit high sensitivity, fast response time, and long-term stability [1]. SMOx-based gas sensors have been investigated to detect oxidizing gases, particularly nitrogen dioxide (NO_2). NO_2 is a pollutant and toxic gas released into the environment mainly through combustion at chemical plants and by automobiles [2]. In this work, a comparative study of the gas sensor properties of SnO_2, WO_3, and ZnO is presented. The sensing performance toward the detection of NO_2 and potential interferents, including CH_4, H_2, and CO, was also investigated at multiple operating temperatures using interdigitated electrodes arrays on substrates. From the electrical measurements, it was observed that WO_3 exhibits the behavior of n-type semiconductor, with sensitivity and response time dependent on both the gas concentration and the operating temperature. Gas sensor measurements showed that the sensor based on WO_3 exhibits the highest response to 50 ppm NO_2 at 300 ºC, with an approximately 450-fold increase in electrical resistance. Moreover, at this operating temperature, WO_3 displayed the highest selectivity to NO_2 relative to H_2, CH_4, and CO. Advanced operando analysis on the WO_3 sensors can provide additional information about the gas/surface interaction and its impact on the NO_2 sensor response.

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Comparison of the photocatalytic activity between Ag-doped SrTiO3 and BaTiO3.

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Photocatalysis represents an advanced oxidative process (AOP) reliant on hydroxyl radicals (OH-) as primary oxidizing agents for environmental decontamination and treatment of contaminated water. It is categorized into homogeneous and heterogeneous systems. In homogeneous systems, there is an absence of solid catalysts, while in heterogeneous photocatalysis, a material, often a semiconductor, acts as the oxidizing agent. Photocatalytic reactions utilize photons to induce an electronic excitation process and facilitating exciton formation. Semiconductors such as SrTiO3 and BaTiO3 are commonly employed in heterogeneous photocatalysis. This study focused on the preparation of Sr(1-x)Ag(1-x)TiO3 and Ba(1-x)Ag(1-x)TiO3, with x varying from 0 to 5% in mol of Ag, utilizing microwave-assisted hydrothermal synthesis. Synthesis involved a heating rate of 10°C/min, reaching 140°C for 40 minutes in a modified domestic microwave adapted for hydrothermal syntheses. Characterization of ceramic powders was conducted through XRD, SEM and FTIR. XRD analysis revealed a secondary carbonate phase. These ceramic powders were then applied in the photodegradation of Rhodamine B (RhB) dye. Results demonstrated that Ag-doped ceramic powders exhibited accelerated dye degradation. The best results was to SrTiO3:5%Ag (< 3h30). Conversely, undoped samples required approximately 10 hours for BaTiO3 and 7 hours for SrTiO3 for complete dye photodegradation. These findings underscore the effectiveness of SrTiO3 in RhB photodegradation, with silver doping further enhancing dye degradation kinetics.

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Discovering new single-phase stable high-entropy oxides using machine learning

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High-entropy oxides (HEOs) represent a burgeoning category of materials noted for their broad utility, including in fields such as energy conversion and storage technologies. These materials have attracted substantial attention for their distinctive architecture, intricate stoichiometry, and the synergistic benefits stemming from their high entropy. Despite the increasing number of studies reported on HEOs in recent years, there is still a lack of compelling explanations for their structural properties, electrochemical activities, and the effects related to high entropy [1]. In the present work, a methodology for studying the formation of stable HEOs phases based on machine learning is proposed. Initially, data on single-phase stable HEOs and their compositions were mined. Once the raw data were collected, the feature engineering stage was performed based on descriptors related to the physical, chemical, and thermodynamic properties of the atoms and oxides comprising the system. In total, more than 250 features were generated and underwent different selection methods for the trained models. Four machine learning models were trained, including two architectures of direct artificial neural networks and two decision tree architectures. Following a critical combinatorial analysis of atoms, a study on the synthesis of materials with the fluorite crystal structure was conducted, and an adapted version of the hydrothermal synthesis method was executed. The theoretical results obtained were models with accuracies close to 90% with confidence interval lower bounds near 75%. Regarding the experimental part, two compositions suggested by the models as fluorite were unprecedentedly synthed: (Ce,La,Nd,Mg,Zn)O and (Ce,La,Nd,Mg,Al)O. The X-ray diffraction pattern predominantly confirmed the fluorite phase in both cases.

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Effect of Ag Concentration on YBCO Ceramic Pellets from powders obtained via Solution Blow Spinning

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This research focuses on the incorporation of different concentrations of silver into the YBCO precursor solution [1], through a chemical approach using the one-pot method [2]. The resulting solution is used to produce fibers by the solution blow spinning (SBS) technique, which are then subjected to heat treatments to achieve the desired phase, i.e., ($YBa_2Cu_3O_{7-\delta}$ or YBCO) and other samples with 0.5, 5 and 20 wt% of Ag, which corresponds to a superconducting material when cooled to a temperature of ~90K. After the formation of this phase, the fibers were stacked and compacted into pellets. The YBCO pellet underwent heat treatment at 925 ºC for 1 hours, whereas the Ag samples reached a maximum temperature of 985 ºC for the same duration. Density estimation and hardness measurements indicate that the presence of Ag enhances the mechanical properties of the samples. XRD analysis reveals the formation of YBCO along with detectable peaks attributed to metallic Ag. This outcome suggests the potential for the development of mechanically robust ceramic nanofibers suitable for applications such as single photon detectors.

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Effect of Silver addition by Chemical route on $YBa_2Cu_3O_7$ ceramic nanowires

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The advancement of nanotechnology aims to improve existing applications and sustainably and economically create new materials. High-temperature superconductors hold significant promise in this domain, particularly in novel devices like nanowire superconducting single-photon detectors (SNSPDs). Typically, the manufacturing of SNSPD devices involves complex and costly techniques for producing nanowire materials for the technological field. The solution-blown spinning (SBS) technique has emerged as a cost-effective and sustainable alternative for the SNSPD production. Unfortunately, ceramic nanowires produced via SBS are still highly fragile. Hence, we studied the effects of Silver (Ag) on YBCO ceramics to improve their mechanical and superconducting properties using both theoretical and experimental approaches. In the theoretical section, some periodic DFT calculations were employed to investigate the doping of Ag into the periodic lattice of YBCO in its orthorhombic phase. Specifically, we incorporated an effective on-site Hubbard parameter (Ueff= 9 eV) to accurately model the localized Cu d orbitals. In the experimental section, Ag acetate was added to the precursor solution containing Y, Ba, and Cu acetates with polyvinylpyrrolidone [1] as a reducing and stabilizing agent. The results indicate that Ag significantly affects the phase formation temperature of YBCO, reducing it up to 895 °C. At theoretical level, the electronic structure calculations on pristine YBCO revealed its metallic nature, with lattice parameters of a = 3.825 Å, b = 3.865 Å, and c = 11.594 Å, demonstrating excellent agreement with experimental observations. Furthermore, the formation energies of Y, Ba, Cu, and O vacancies, and Ag substitutional defects at different lattice sites, were determined.

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Effect of sintering condiction on ion selective membranes

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Lithium is a metal of extreme relevance to the current technological scenario, due to its use in the growth of battery industries. With the growing demand for the use of lithium in this sector, specifically points out that by the year 2050 around 1/3 of this sector's reserves of metal on land will be consumed[1]. In this context, the search for new sources is crucial, with the ocean emerging as an alternative to meet the demands of this industry. Thus, the objective of this work is to prepare a superionic conductive ceramic material from NASICON family, which presents physical properties that support applications linked to lithium extraction[2]. Furthermore, the effects of sintering parameters, such as plateau time (2, 6, 10, and 12 hours) and sintering temperature (1000 °C, 1050 °C, 1100 °C, and 1150 °C) were studied to obtain a ceramic material with composition Li1+xAlxTi2-x(PO4)3. Besides that, the conductivity of the samples was evaluated, as a function of the sintering parameters to optimize the choice of the sample with greater conductivity and lower porosity for application as a membrane[3]. Preliminary results indicate that the membranes achieved high conductivity values of 2.15x10-3S/cm indicating great potential for application as ionic selective membranes.

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Effects of sintering conditions on the properties of magnetoelectric ceramics of KNN:Fe and KNN:Co

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Using materials with magnetoelectric properties has attracted increasing interest in the scientific and technological fields. However, most of these materials still have Lead (Pb) in their composition, which limits their use due to high toxicity. Using sodium and potassium niobate (KNN) systems to prepare ferroelectric materials has to be an alternative effort for replacing materials with Lead as the main component. KNN is a promising candidate due to its high Curie temperature, good ferroelectric properties, and appreciable electromechanical coupling coefficients, becoming a bright material for applications in electronic devices with ferroelectric and magnetoelectric properties. In this work, ceramics of the (0.5)KNbO3/(0.5)NaNbO3 system doped with 0.1% wt. of Fe2O3 and CoO oxides were prepared by the conventional route of oxide mixing. Samples were densified by conventional sintering (CS), spark plasma sintering (SPS), and uniaxial hot press sintering (HPS). Effects of the sintering conditions were observed in the densities and structure signature of the materials. The impact of oxygen vacancies due to the dopping process, and also the sintering conditions, could be identified in the microstructure and ferroelectric properties and become a rule for the magnetoelectric properties.

Effects of temperature and electric field on the formation of electroactive phase, and its influence on their dielectric, piezoelectric, and ferroelectric properties, in ceramic-polymeric composites of PVDF/KNN

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This study investigates the effects of temperature and the application of an external electric field during the formation process of electroactive phases (β and γ) in the polymeric matrix of ceramic/polymeric composites of Potassium Sodium Niobate (KNN) and Poly(vinylidene fluoride) (PVDF). Such study aims to maximize the formation of these electroactive phases to optimize the electrical coupling between KNN and PVDF, resulting in a system with highly sensitive piezoelectric properties, combined with high flexibility, low weight, and control over its dielectric and piezoelectric characteristics (by adjusting the proportions between KNN and PVDF). The formed composites were analyzed by Fourier-transform infrared spectroscopy (FTIR), allowing the identification and quantification of the formation of β and γ phases in detriment to the non-polar α phase, revealing a significant increase in the quantity of electroactive phases under specific conditions of time, temperature, and electric field intensity. Concurrently, the performance of the electrical coupling was evaluated through dielectric, piezoelectric, and ferroelectric properties, revealing a significant improvement as the proportion of electroactive phases increases.

Gas Sensing Response of Zn2SnO4/SnO2 Heterostructures

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While semiconducting metal oxide sensors show reasonable sensitivity, achieving an enhanced lower detection limit and/or selectivity could significantly broaden their applications in real-time monitoring. This study works on the growth mechanism and gas sensing capabilities of zinc tin oxide-based structures synthed via a microwave-assisted hydrothermal method. The synthed materials were characterized using techniques such as X-ray diffraction (XRD), Raman spectroscopy, Fourier-transform infrared (FTIR) spectroscopy, scanning electron microscopy (SEM), scanning transmission electron microscopy (STEM), X-ray photoelectron spectroscopy (XPS), and nitrogen adsorption/desorption experiments. Gas sensor evaluations revealed that ZnSnO3 exhibited an exceptional lower detection limit for nitrogen dioxide (NO2), with an anticipated tenfold increase in electrical resistance upon exposure to just 1 ppb NO2 at an operating temperature of 150 °C. Furthermore, the Zn2SnO4/SnO2 heterostructure demonstrated superior selectivity to NO2 over hydrogen (H2) and carbon monoxide (CO), boasting a sensor response approximately 1500 times higher for the oxidizing gas. This study underscores how engineering the growth of nanostructures can achieve lower detection limits and enable the development of highly selective gas sensor devices. This achievement is attributed to the increased surface area and enhanced contact potential barriers facilitated by the engineered nanostructures.

Glass-ceramic materials containing ZnO and Ag:ZnO nanocrystals for dye photocatalysis

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Current studies indicate that photocatalysis processes are being widely employed for activities related to environmental preservation, as they can degrade dyes in water. Photocatalysis is a method of breaking down molecules with the formation of hydroxyl free radicals (OH^-), acting as an oxidizing agent. The process can be divided into two types: Heterogeneous (with a semiconductor material as the catalyst) and Homogeneous (without a catalyst). In heterogeneous photocatalysis, certain types of glass-ceramic materials have begun to be used as a new and alternative way to improve the process.[1] Associated with the functionality of semiconductors in these reactions, which break down molecules using UV light, two glass-ceramic materials containing the semiconductor ZnO and Ag-doped ZnO were developed. Initially, glasses of the SiO_2-Al_2O_3-Na_2O system were prepared using the melt-quenching method. Using the resulting glass, before spraying and bulk cutting, and then thermally treated to obtain the Nepheline phase containing ZnO and Ag:ZnO nanocrystals (prepared using the Pechini method, employing Citric Acid, Zinc Nitrate, Silver Nitrate, and Ethylene Glycol, with the solution calcined at 300°C and 700°C). The glasses obtained were thermally treated based on data obtained from thermal analysis to obtain the glass-ceramic. The material were characterized by X-ray diffraction and employed in photocatalytic processes for the degradation of the dye Rh-B. The results showed that the glass-ceramics have the desired phases. Photocatalysis tests demonstrated that the glass-ceramic material containing Ag-doped ZnO exhibited better performance in dye degradation. Acknowledgments: Laboratório de Caracterização e Gestão de Resíduos Sólidos; FCT-Unesp; FAPESP (MPF/MPSP/CESP process CEF 2023/14546-7)

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Growth and characterization of structural and optical properties of potassium aluminum sulfate dodecahydrate single crystal

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Potassium Aluminium Dodecahydrate ($K(AlSO_4)_2 \cdot 12H_2O$), also known in the literature as KAS, belongs to the alum family, which has a cubic structure with a Pa3 space group. KAS single crystals have been used in the cosmetic industry as skin care products, food additive and recently as antimicrobial. Recently, $K(AlSO_4)_2 \cdot 12H_2O$ single crystals have been investigated for optical applications and switching due to their large energy band gap and high transmittance. In this work, KAS single crystals were grown by the slow evaporation technique of supersaturated solution. The growth process duration was 15 days, approximately one week less than reported in the literature. Just after few days, the spontaneous nucleation process produced several tiny crystals of KAS at the bottom of the beaker. The x-ray diffraction results from the as-grown crystals confirmed their monocrystalline nature with a cubic structure. The optical transmittance of KAS single crystals showed a transmittance larger than 80 % in the entire visible spectrum. The direct optical band gap obtained ranges from 5.6 – 5.9 eV, as reported in the literature, confirming the potential application of $K(AlSO_4)_2 \cdot 12H_2O$ in optoelectronic devices.

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Influence of temperature on the properties of Nb_2O_5 films grown by RF-Magnetron Sputtering.

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In recent years, niobium pentoxide (Nb_2O_5) has garnered attention for its potential applications in solar cells and non-volatile memories [1,2], the latter due to its negative resistance characteristic. To enhance device efficiency, a deeper understanding of the film growth process and its influence on properties is crucial. In this study, we investigated the impact of substrate temperature on the growth of Nb_2O_5 thin films using RF-magnetron sputtering, as well as the thermal treatment of the films on their structural, optical, and electrical properties.

Films were deposited on substrates at room temperature, 300°C, and 400°C. Samples deposited with substrate temperatures up to 400°C remained amorphous, necessitating either a higher temperature or post-heat treatment for crystallization. In terms of optical properties, samples exhibited approximately 80% transmittance (on fused silicon substrates), with a slight increase in refractive index following heat treatment. Films deposited at 300°C and 400°C demonstrated lower Urbach energy; however, heat treatment led to a significant increase, indicating greater disorder.

Electrical measurements revealed lower resistivity in samples deposited at 300°C and 400°C. However, heat treatment resulted in increased resistivity, particularly for samples grown at 300°C.

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$La_{1-x}Y_xNiO_3$ nanostructures produced by microwave-assisted hydrothermal synthesis

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$RNiO_3$ (R = rare earth) compounds have been extensively studied due to their important physical properties.[1] They present a rich phase diagram, with controllable magnetic and electrical transitions affected by several factors, which make them promisors to applications in catalysis, transistors, biosensors, etc.[2]

In particular, the $LaNiO_3$ compound presents a metallic behavior in a wide temperature range, but the substitution of La^{3+} for Y^3+ promotes changes in the structural and electrical properties. This work focuses on the synthesis and characterization of $La_{1-X}Y_XNiO_3$ ($0 \leq x \leq 0.2$) compounds. They were prepared by microwave-assisted hydrothermal route and were characterized using scanning electron microscopy (SEM), X-ray diffraction (DRX), thermogravimetry (TG), and electrical resistivity as a function of temperature ρ(T).

SEM images revealed cubic nanoparticles of an average of 150nm for $LaNiO_3$ samples. The doped samples present polyhedral-shaped particles with a of 100 to 200 nm. XRD results revealed that samples with $x < 0.15$ are polycrystalline and no additional phase was observed, they crystallize in a rhombohedral-distorted perovskite structure (R-3C). The XRD of the other samples showed additional peaks of NiO and Y_2O_3. Thermal analyses confirmed the phase formation by the thermal treatment, and ρ(T) measurements showed metallic behavior and Y-doped samples ($x > 0.05$) exhibited an increase of ρ(T) at $T < 100K$.

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Nickel-Modified SiOC Ceramic for Electrochemical Determination of TNT

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Silicon oxycarbide (SiOC) ceramic materials exhibit mechanical, chemical, electrical, and optical properties that enable various applications such as their use in semiconductor devices, protective coatings and voltammetric sensors [1]. Their potential as electrode materials can be employed in the detection of 2,4,6-Trinitrotoluene (TNT), due to the strong interaction of silicon-oxygen bonds with nitro groups [2]. The detection of TNT is relevant because it is primarily used as an explosive material in demolition processes, leaving harmful residues in the environment [3]. SiOC material with 3wt.% nickel (SiOC/3Ni) was obtained by pyrolysis at 1400°C for 1h under static argon atmosphere from a ceramic precursor consisting of 40wt.% poly(methylhydrosiloxane), 60wt.% divinylbenzene, and 20wt.% polyethylene, with 3wt.% $NiCl_2$ incorporated. Characterization of the SiOC/3Ni ceramic using XRD, Raman, SEM and EDS showed the presence of conductive phases of graphitic carbon and nickel silicide, and the semiconductive phase of silicon carbide. These phases are essential for establishing communication between electrode and potentiostat. Besides, SiOC/3Ni exhibited homogeneity in the distribution of elements, which is important for producing paste electrodes. These electrodes were prepared by mixing the material with mineral oil in an 80:20 ratio. Electrochemical analysis was performed using cyclic voltammetry and square wave voltammetry techniques in 0.01 mol.L^{-1} hydrochloric acid with 200 µmol.L^{-1} of the analyte TNT. The applied potential, pre-concentration time, and pH were analyzed. The best conditions for analyte detection were by applying a fixed potential for a certain pre-concentration time within a potential range of 0.0 to 0.7 V.

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Obtaining barium ferrite from niobium mining tailings: a potential technology for manufacturing permanent magnets

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Mining activities are extremely important for the Brazilian economy, but various problems such as contamination of the soil and the aquatic ecosystem [1] are caused by the large volume of tailings generated. Brazil is the largest producer of niobium in the world and its extraction generates two types of tailings called magnetic tailings and barite. Due to their high iron and barium content, these tailings have chemical compositions that, after processing, allow for the production of barium ferrites commonly used in the manufacture of permanent magnets. As a result, these tailings have the potential to be used as inputs in the manufacture of magnetic ferrites, transforming them into high value-added products.In this context, both magnetic tailings and barite were used in the synthesis of barium ferrite via solid-state synthesis, using two different milling times (2 and 4 hours) and heat treatments at 1100ºC, 1200ºC and 1300 ºC for comparison purposes. In addition, 100% commercial sources of iron and barium were used, where commercial iron oxide and barium carbonate were used, and 100% non-commercial sources, i.e. using 100% of the tailings as a source of these elements. X-ray diffraction (XRD) in conjunction with the Rietveld method and magnetic characterizations were used to characterize them. The XRD results showed that all the materials synthed had the phase of interest. As for the magnetic measurements, it was possible to obtain a material with relevant properties, reaching values of Magnetic Remanence and Maximum Energy Product equal to 1.190 kG and 0.29 MG.Oe respectively, demonstrating that the ferrites obtained from the tailings have great potential for application in the permanent magnet market.

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On the photovoltaic interaction dynamics with ferroelectric and magnetic domains

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Every year, new electrical generation technologies are introduced to supply the growing energy demands. On the other hand, attention to environmentally cause has led to an increased focus on clean and renewable energy sources, with solar cells emerging as a biggest potential among these sustainable alternatives. In this sense, ferroelectrics and magnetoelectric oxides, with a perovskite structure of the ABO3 type, have garnered significant attention in the field of photovoltaic (PV) applications with a new technology, known as ferroelectric photovoltaics. In this study, we investigate the photovoltage response to light in BiFeO3 thin film photovoltaic devices. We manipulate the photovoltage responses through electric poling and magnetization techniques. Piezoelectric and magnetic force microscopy responses indicate significant surface changes with the application of external magnetic and electrical fields. Additionally, Kelvin force microscopy under induced illumination reveals intense photovoltaic activity in the magnetized and polarized surface regions. Finally, more intense photovoltaic responses are also observed in conventional photovoltaic characterizations.

Optimization of dielectric properties of composites films of PVDF/xKNN50

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Using materials with high ferroelectric properties has attracted increasing interest in the scientific and technological fields. However, most of these materials still have Lead (Pb) in their composition, which limits their use due to high toxicity. Using sodium and potassium niobate (KNN) systems to prepare ferroelectric materials has to be an alternative effort for replacing materials with Lead as the main component. KNN is a promising candidate due to its high Curie temperature, good ferroelectric properties, and appreciable electromechanical coupling coefficients, becoming a bright material for applications in electronic devices with ferroelectric and magnetoelectric properties. The use of ferroelectric polymers in devices also has increased due to their flexibility and good mechanical properties. However, improvements in the electric properties of the films can become then more attractive to the applications. In this work, we synthed composite films of poly(vinylidene fluoride) (PVDF) and KNN50 ceramics, and their ferroelectric properties were analyzed as a function of the content of ceramics in the polymer matrix. The films were synthed by the dissolution of the PVDF matrix in DMF and the dispersion of the KNN ceramic powders. The polymerized solutions were dried at 90°C for 48 h. The films show good dispersion of the ceramic in the polymer matrix, allowing up to 80 wt.% dissolution of the ceramic while maintaining the base characteristics of the polymer system (flexibility and mechanical strength). A significant increase in the relative dielectric permittivity values up to frequencies of 1MHz at room temperature of the composites was observed as the ceramic concentration increased. However, even at low concentrations of KNN, there is a change in the polarization response of the composite films due to the formation of a major electroactive crystalline phase in the polymer activated by the ceramic incorporation, when the ferroelectric hysteresis curv

OUT OF EQUILIBRIUM VORTEX DINAMYCS: interaction of vortices with triangular defects and transport currents

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This research focuses on studying the influence of triangular defects, produced as blind-holes and dots, in a superconducting sample [1]. Three different orientations were use, e. g., left, right, and down triangle comparing with a current density flowing from left to right, simulating either a 3D or 2D materials using Fortran-90 language. The simulations were carried out in the time-dependent Ginzburg-Landau framework [2], considering a situation with zero applied magnetic field, where the vortices are known as kinematic vortices [3], and a varying transport current density. The results show that the symmetry and the type of defect are crucial to the electrical properties of the material, as well as the dynamics presented by the vortices. In particular, the current crowding effect plays an important rule on the vortex dynamics and the installed resistive state. As general conclusion, the knowledge of vortex dynamics are essential for development of future superconducting devices, mainly the ceramic ones, where defects are intrinsically present due to its multigranular character.

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Photocatalytic Activity of CaTiO3 doped with 3% and 5% Ag

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Environmental pollution in its various forms has become a significant concern for both the scientific community and society at large. Industries such as textiles, leather, and food production utilize dyes, yet their disposal is often inadequately managed. In an effort to address this issue, this study proposes a ceramic material capable of decontaminating water and effluents containing organic dyes through the process of heterogeneous photocatalysis. Heterogeneous photocatalysis, an advanced oxidative process (AOP), efficiently degrades organic compounds using involved electrons, with semiconductors serving as catalysts in the reaction. Among various catalysts, TiO2 and ZnO are well-documented in the literature. This study investigates the photocatalytic potential of Ca(1-x)Ag(x)TiO3, where x varies between 0, 3%, and 5% in terms of silver mole fraction. Ceramic powders were synthed using the microwave-assisted hydrothermal method (MAH), with a heating rate of 140°C/min, held at 140°C for 40 minutes, and a pressure of 4bar. The ceramic powders were characterized using techniques such as X-ray Diffraction (XRD), Fourier Transform Infrared Spectroscopy (FTIR), X-ray Fluorescence (XRF), Scanning Electron Microscopy (SEM), and Raman Spectroscopy. In the heterogeneous photocatalysis experiments, the material was mixed into a 10ppm Rhodamine B (RhB) solution and exposed to UV light for 2 hours. Regular intervals were utilized to collect aliquots of the solution for UV-Vis absorption analysis. The results from XRF, XRD, and Raman techniques confirmed the presence of crystalline titanate phase and incorporated silver within its structure. The RhB photocatalysis results demonstrated that the sample containing 3% Ag degraded the dye within 90 minutes. Ackowledgements:(MPF/MPSP/CESP Process CEF0404094-74/2011) References: CERVANTES, T. N. M.; ZAIA, D. A. M.; SANTANA, H. DE .. Estudo da fotocatálise heterogênea sobre Ti/TiO2 na descoloração de corantes sintéticos. Química Nova.

Precipitation in Hydrogen Peroxide: An Easy Route for Nanoparticles and Thin Films of Perovskite Ceramic Oxides

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Ceramic oxides with perovskite structures such as $BaSnO_3$, $BaTiO_3$, and $SrTiO_3$ and their doped counterparts have physicochemical properties of technological interest like unusual electronic mobility, ferroelectricity, piezoelectricity, and pyroelectricity.[1,2] These properties of perovskite-based components are essential for high-tech devices such as solar cells, energy storage, lasers, and photovoltaic catalysis.[1,2] Traditional methods for synthesizing these oxides, such as solid-state, sol-gel, or solvothermal processes, require high temperatures, pressures, or time.[1] Such harsh conditions are required for complete perovskite phase crystallization and often lead to poor control of the particle's morphology, distribution, and stoichiometry, which affect the quality of the grain boundaries and reflect the physicochemical properties of the processed materials and devices.[1,3] Besides having similar properties when compared to water, hydrogen peroxide solutions in acidic conditions can complex some metal salts or alkoxides that normally hydrolyze in water and stabilize some metallic cations in a higher oxidation state.[2] By changing the chemical equilibrium conditions, peroxo nanoparticles can be precipitated with the addition of base.[2] These nanoparticles can be converted to perovskite upon heating and form stable colloidal solutions with oxygenated solvents, making them promising compounds for thin film applications via colloidal deposition techniques.[3]

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Preliminary study of the influence of UV radiation on the synthesis of YBCO ceramic nanofibers

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Nanofibers constitute a special group of 1-D nanomaterials of great interest due to their important medical, environmental, and technological applications, among others [1]. Many nanofibers are used as intermediates in the production of superconducting materials, which are those whose resistance to the passage of electric current is abruptly suppressed when cooled below its critical temperature (Tc) [2]. One of the most studied compounds among cuprate superconductors is YBa2Cu3O7-δ (YBCO). In addition, one technique applied to producing nanofibers is solution blow spinning (SBS) [3]. YBCO ceramics were produced using a precursor solution consisting of yttrium, barium and copper acetates, acrylic acid, ammonium hydroxide, methanol, and polyvinylpyrrolidone (PVP). The viscosity of the solution was (69±3) cP. This solution was taken to the SBS system, obtaining polymer fibers, then subjected to heat treatment at 600°C and sintering at 925°C with oxygen flow. The influence of UV radiation was carried out through three experiments: applying UVC light for one hour to the polymeric fibers (1), to the solution in the absence of PVP (2), and the precursor solution (3). TG-DTG, FTIR, and UV-vis analyzed possible alterations. A slight increase in the degradation temperatures of PVP and a decrease in the crystallization temperature of YBCO were preliminarily observed in DTG analysis. FTIR and UV-vis also observed some changes in the bands in experiment 3, and in solubility tests, the appearance of insoluble products was observed in experiments 1 and 3, which could be attributed to the degradation or cross-linking of PVP.

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Preparation and Characterization of Ceramic Targets and Thin Films of ZnO and Al-doped ZnO

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ZnO is a semiconductor material with optoelectronic properties, allowing various applications. When arranged as thin films, ZnO can be used as transparent conductive oxides in optical devices such as energy converters[1]. Among the methods for preparing thin films, magnetron sputtering is emphad, highlighting the importance of the ceramic target preparation for thin film production. ZnO and ZnO containing 3mol% Al (AZO3) ceramic targets were produced using two methods: solid-state reaction (SSR) and ceramic powders obtained by the Pechini method (PEC). The targets were uniaxially pressed with compaction pressure varying at 65, 255, and 400 MPa, sintered from 950-1200°C, and characterized by X-ray diffraction and apparent and relative theoretical density. The results showed that the targets prepared by both methods have ZnO (wurtzite) as crystalline phases. The AZO3 targets exhibited ZnAl2O4 as the secondary phase. Density results showed that both targets prepared at 65 MPa by SSR, sintered at 950°C present the best density conditions, reaching values greater than 93% of the theoretical density, compared to the targets prepared via PEC, whose best density was around 80% of the theoretical density. Based on these results, ZnO and AZO3 targets prepared by SSR (65 MPa-950°C) were used for thin film deposition via magnetron sputtering for 30 minutes on glass substrates to evaluate their optical characteristics. The films, characterized by XRD, showed oriented growth in the (002) plane of the wurtzite phase, without the secondary phase found in the AZO3 targets. The films presented a band gap of 3.2eV for ZnO and 3.4eV for AZO3, with transparency above 80%, at wavelengths from 400 to 800nm, obtained by UV-Vis absorption spectroscopy. The results show that the produced films have potential for applications in optical devices, including those used as transparent conductive oxides for energy converters.

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Preparation of n-type semiconductor Bi2WO6 to investigate photocatalytic properties

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Bismuth tungstate is a n-type semiconductor with the respective band gap around ≈ 2.7 eV. Here, the promising photocatalytic material was obtained using the combustion method, i.e., bismuth vanadate in orthorhombic phase Bi2WO6 [1]. To achieve this compound, bismuth oxide (Bi2O3) and sodium tungstate (Na2WO4.2H2O) raw materials were mixed, after subjected to temperatures between 600-700 °C for two hours, in the presence of stoichiometric amount or excess of urea (CO(NH2)2). The urea combustion process is a promising technique for the synthesis of materials because it efficiently converts precursors into final products of high purity and homogeneity [2]. The samples were visually analyzed and then subjected to structural characterization by X-ray diffraction, infrared spectroscopy, Raman spectroscopy and Scanning Electron Microscopy. Characterization measurements by XRD indicated the presence of the main phase of orthorhombic Bi2WO6 in the compositions BW4-600, BW4-700. The results of Infrared Spectroscopy showed the presence of bonds attributed to the vibration of W-O-W and stretching of W-O and Bi-O, respectively, for the two different compositions. Similarly, Raman spectroscopy measurements showed typical modes of orthorhombic bismuth tungstate, in agreement with the literature. The microscopy technique indicated nanometric particles with characteristic morphology of tungstate-based materials. In conclusion, the urea amount was essential to obtain Bi2WO6 phase as here synthed and future studies may indicate its photocatalytic potential.

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Preparation of silicon carbide (SiC) ceramics from pyrolysis of rich-organosilane precursor aiming electrochemical applications

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Silicon carbide (SiC) is a widely used material as in the production of resistance heating elements in the electric furnace, development of high-strength composites and as power electronics devices. SiC has been used as compound in manufacturing of modified electrodes for determining different analytes [1]. Now, apart from SiC bonds, the microstructure contains a residual carbon phase embedded within matrix, whose proportions depend on polymer chemistry and processing conditions. This study aims to obtain SiC ceramics from carbon-rich polymer precursor and evaluate their potential as electrode materials in voltammetric measurements. Polymer precursor was prepared by hydrosilylation reaction between 50 wt.% diphenylsilane and 50 wt.% divinylbenzene and heating to 1300 and 1500 °C under Ar atmosphere, resulting in the respective SiC ceramics. Paste electrodes were prepared with 80 wt.% ceramic and 20 wt.% Nujol to record the electrochemical behavior of ferri-ferro probe at the ceramics and glassy carbon (GC) electrodes by cyclic voltammetry. Typical bands related to the vibrational mode of SiC bonds were evidenced with higher intensities for ceramic at 1500 regarding to 1300 °C. Diffraction peaks of SiC confirmed the more effective crystallization of sample at higher temperature. Morphology of ceramic at 1500 °C was composed of sintered globular particles, typical of SiC materials, whereas at 1300 °C a flatter surface was obtained. SiC electrodes displayed better response for electrooxidation of $Fe^{2+/3+}$ pair compared to GC electrode and this result was corroborated with electroactive area (Ae) values. At 1500 °C, this value was three times greater than that for sample at 1300 °C, indicating that SiC ceramic fabricated at higher temperature is promising for determining analytes with different interests.

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SiOC Ceramic-Based Sensor for Methyl Parathion Determination in River Water Samples

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Silicon oxycarbide (SiOC) ceramics are materials with high corrosion resistance, thermal stability and composition consisting of semiconductive and conductive phases, facilitating the electric current flowing. SiOC materials find wide applications in electrochemical studies, including molecule identification through electroanalytical techniques [1,2]. This study aims to apply SiOC ceramic as electrochemical sensor in methyl parathion (MP) identification, an insecticide banned in Brazil since the early 2010s but still found in water samples. SiOC was obtained by pyrolysis at 1400°C for 1 h, under static Ar atmosphere, of a polymer composed of 60 wt.% divinylbenzene and 40 wt.% poly(methylhydrosiloxane). The paste electrode was formulated using 80 wt.% of ceramic and 20 wt.% Nujol® mineral oil. Ceramic was characterized by FT-IR, XRD and XPS and further submitted to voltammetric experiments for analytical method development. SiOC exhibited superior oxidation currents compared to vitreous carbon electrode, allowing MP oxidation to near-zero values. Voltammetric behavior of MP was evaluated through pH, electrolyte support and electrolyte concentration. The electrochemical technique was selected via multivariate analysis of parameters and their results were analyzed by variance analysis with a 95% confidence level. The electroanalytical method was compared to an established chromatographic method for MP determination in Paraná River waters. The paste ceramic proved to be a novel sensor in MP determination, with a quantification limit of 27.4 nmol L–1, presenting advantages in relation to modified sensors, due to simplicity on electrode preparation and handling, reduced reagent consumption, and shorter analysis time compared to the chromatographic method.

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Strategic application of NASICON-type Ceramics as Ion-Selective Membranes

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The current global need for sustainable practices and the increasing scarcity of strategic minerals have driven research into crucial processes such as the exploration of raw materials beyond traditional mining techniques [1]. In this context, the development of ion-selective membranes may perform an important role in extracting metals from aqueous solutions, including seawater and liquid battery systems. Among the promising materials for this application are superionic conducting ceramics with NASICON structure [2]. In this sense, with the main goal of achieving high ionic conductivity, high lithium ion selectivity, and chemical stability in aqueous environments, this study focuses on the obtention and characterization of ceramic membranes with a composition of $Li_{1.4}Al_{0.3}Ti_{1.7}Si_{0.1}P_{2.9}O_{12}$. Preliminary results demonstrate the efficiency of obtaining the rhombohedral NASICON crystal structure through solid-state reaction synthesis of oxide mixtures, as well as structural maintenance and high densification of 95% after sintering for 6 hours. Additionally, excellent ionic conductivity values in the range of $5.0\text{x}10^{-4}$ – $2.0\text{x}10^{-3}$ $S.cm^{-1}$ indicate the strategic relevance of studying the application of these materials as ion-selective membranes for lithium prospecting.

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Study of protonic anode-supported SOFC obtained by co-pressing method

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Researchers around the world have increasingly turned their focus to fuel cells as promising alternatives to conventional energy sources due to their numerous benefits, including reduced or negligible CO2 emissions, increased efficiency, and minimal environmental impact [1]. Among the range of fuel cell technologies, Solid Oxide Fuel Cells (SOFCs) stand out for their notable advantages such as fuel and heat recycling (cogeneration), compatibility with diverse fuel sources, and superior conversion efficiency. Among materials for solid oxide fuel cells studied, the ABO_3 type perovskites stand out, which are composed of barium cerates and zirconates, for applications in proton conduction. It is a fact that both cerates and zirconates have high acceptability of aliovalent dopants in their crystalline structure, thus generating oxygen vacancies that favor the increase in proton conduction in the cell [2]. Obtaining solid oxide fuel cells involves advanced manufacturing techniques that aim to take advantage of the unique properties of these devices. A frequently employed method involves the co-pressing and co-sintering of cell components in layered structures, aiming to enhance both the efficiency and longevity of the cells. This approach is feasible thanks to its effectiveness, simplicity, and scalability in large-scale production. The present work aims to obtain cells supported on the anode using $BaZr_{0,4}Ce_{0,4}Y_{0,1}Gd_{0,1}O_{3-\delta}$ as electrolyte, layers of $BaZr_{0,4}Ce_{0,4}Y_{0,1}Gd_{0,1}O_{3-\delta}$-NiO as anode and BSCF-$BaZr_{0,4}Ce_{0,4}Y_{0,1}Gd_{0,1}O_{3-\delta}$ ink as cathode. The cells supported on the anode were successfully obtained for 5 layers by co-pressing and co-sintering, after studying the effect of grinding on the starting powder obtained by the Pechini method. The samples were tested using synthetic air and H_2 as fuel. The measurements were carried out using the impedance spectroscopy (EIS) technique, and Open Circuit Voltage (OCV), and IxV curves were obtained.

Superconducting vortex dynamics influenced by a star-like blind defect

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Abstract:

The study of vortex dynamics and resistive states is crucial for both scientific understanding and technological applications, as the ability to transport electrical current without dissipation is directly influenced by these phenomena. To gain better control over vortex dynamics, various models of defects have been investigated extensively [1,2]. In this work, we present a theoretical study conducted via computational simulations of two-dimensional mesoscopic superconducting samples with star-shaped geometries of blind holes. The computational sample is represented by a rectangular shape with dimensions 30x20 $\xi(0)$, featuring a central star-shaped defect, formed by two opposite equilateral triangles with sides measuring 10 $\xi(0)$. By employing the generalized time-dependent Ginzburg-Landau theory, we apply a current to the system and analyze the temporal evolution of the order parameter [1]. Our findings reveal that the presence of the star-shaped defect induces non-conventional Phase-Slip events and enhances current crowding effects along certain borders of the star, thereby guiding vortex motion. This study sheds light on the intricate interplay between defect geometry and vortex dynamics in mesoscopic superconductors, offering valuable insights for future research and technological advancements.

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Synthesis of perovskites $BaZr_{0.4}Ce_{0.4}Y_{0.1}Sm_{0.1}O_{3-\delta}$ and $BaZr_{0.1}Ce_{0.7}Y_{0.1}Sm_{0.1}O_{3-\delta}$ by Pechini method and characterization for application as electrolytes of proton-conducting solid oxide fuel cells

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Proton-conducting solid oxide fuel cells (P-SOFCs) are devices that convert chemical energy into electrical energy through the oxidation of fuel gas at the cell's anode, generating water as a by-product after conducting the generated protons from the anode to the cathode [1]. In this study, the synthesis and characterization of two perovskites for P-SOFCs electrolytes was carried out, one being a new composition (BaZr0.4Ce0.4Y0.1Sm0.1O3-δ) and another already studied in the literature (BaZr0.1Ce0.7Y0.1Sm0.1O3-δ), but synthed by a different method. The objective of this study is the synthesis and characterization of the mentioned materials, in order to investigate their applicability in P-SOFCs. The samples were synthed by the Pechini method, using nitrates as precursors. The calcination temperature was determined using TGA, and both compositions were calcined at 1300 °C. Temperature at which mass loss becomes constant in TGA measurements. XRD was performed for each calcined sample, and these results were compared with diffractograms of similar cubic compositions available in the ICSD. Dilatometric analysis of the two samples were carried out, obtaining the temperatures of maximum densification rates; with the values of these temperatures, isothermal dilatometry was carried out to determine the sintering time. Pellets were pressed from each sample using uniaxial pressing, and these were sintered at 1400 °C for 1 h. Platinum electrodes were deposited on the parallel flat surfaces of the BaZr0.1Ce0.7Y0.1Sm0.1O3-δ pellet and the sample was analyzed by impedance spectroscopy, obtaining an activation energy of 0.7 eV and conductivities of the order of 10^-4 to 10^-3 S/cm in the range of 400 to 700 °C in synthetic air. In the future, the other perovskite will also be analyzed by impedance.

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The electrical behavior of thin films of ZnO and Al:ZnO

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ZnO is a transparent conducting oxide (TCO), n-type semiconductor, presenting optical and electronic properties that allow for various applications. In thin films, ZnO can be utilized, for example, in UV-resistant coatings, UV photodetectors, gas sensors, or photocatalysis, among other applications1. However, ZnO exhibits inferior electrical properties compared to ITO, commonly used as TCO, thus requiring processing techniques that enhance or highlight its electrical conductivity without compromising its high transparency. In this context, this study presents the results of an investigation into the potential of thin films of ZnO and Al-ZnO doped with 1 mol% (AZO1) for energy conversion applications. The films were prepared using the magnetron sputtering deposition technique, employing ceramic targets, and deposited onto interdigitated glass electrodes with gold. The films were characterized by X-ray diffraction (XRD), UV-Vis spectroscopy, and photoconductivity measurements. XRD results demonstrate that both pure and Al-doped films grow oriented on the (002) plane of the hexagonal wurtzite structure of ZnO. UV-Vis results show transmittance above 80% for ZnO films, increasing up to 90% for the Al-doped film in the 400 to 800 nm range. Photoconductivity results indicate that conductivity increases in the presence of light and also with doping, reaching values of 1.927x10-7 S.m-1 for the ZnO film and 8.517x10-3 S.m-1 for the AZO1 film in an illuminated environment.

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Thin films of Al-doped ZnO to application as ozone gas sensor

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ZnO is a ceramic material semiconductor with multifunctional properties, enabling various applications in microelectronics and optoelectronics. When arranged in the form of thin films, ZnO can be used, for example, in resistive coatings and UV photodetectors, gas sensors, photocatalysis, and also as transparent conductive oxides for photovoltaic cells [1]. For applications such as toxic gas sensors, the structure of ZnO can be altered to increase efficiency and enhance selectivity. This study proposes an investigation of thin films of ZnO and Al-doped ZnO, deposited via magnetron sputtering, for applications in ozone gas sensors. The films were deposited on glass substrates using ceramic targets of ZnO and ZnO doped with 1, 2, and 3 mol% Al. The ceramic films deposited over 30, 60, and 120 minutes without substrate heating were characterized by X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), profilometry, scanning electron microscopy (SEM), and atomic force microscopy (AFM). The results revealed preferential growth in the (002) Wurtzite crystalline structure (ZnO) plane. XRD results did not identify the presence of Al in the doped films, but XPS results confirmed the presence of the dopant in the ZnO lattice. The film thickness increased with deposition time, along with the of the spherical morphology particles observed by SEM. On the other hand, with the increase in the percentage of the dopant in the ZnO lattice, the particles decreased, and the film roughness increased. The films were subjected to ozone (O3) gas sensitivity tests at a temperature of 250°C. The results showed that the films exhibited a decrease in sensor properties according to the percentage of Al in the ZnO structure. However, all films are sensitive to O3 gas, including low concentrations of 50 ppb, a limit considered for a maximum daily average of 8 hours of human exposure, as established by the WHO.

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TUPÃ project: Solid Oxide Electrolysis Cell and Fischer-Tropsch Reactor Integration for CO2 and CH4 Valorization in Brazil

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Brazil stands as a cornerstone in advancing decarbonization technology, boasting abundant biomass production and a variety of renewable energy sources. Recognizing the potential for further advancements, collaborative efforts between ISI Biomass and LIPCAT/UFRJ aim to create a pioneering prototype. This prototype involves the study of Solid Oxide Electrolysis Cells (SOECs) assisted by CH4, combined with the co-electrolysis of H2O and CO2 for the dual production of syngas at both electrodes. The goal is to integrate the prototype into a Fischer-Tropsch reactor to utilize the produced syngas for industrial additive production. At the heart of this approach is the aspiration to harness the potential of syngas production by CO2 and CH4, problematic gases emitted by various industrial processes. This process will not only enhance energy efficiency but also highlight the transformative power of sustainable technologies. This study explores viable methods to maximize syngas production at both electrodes of the SOEC. We are using solid oxide cells supported on Ni/YSZ electrodes, YSZ electrolyte, GDC barrier layer, and LSCF oxygen electrode. Eventually, we will test the cell with a bimetallic Ni-M/CeO2 (M = Fe, Co, etc) catalyst layer for the methane conversion. Preliminary results indicate that the syngas production rate, even without the catalyst, is about 40%. As we develop this solution, we highlight Brazil's pioneering role in fostering sustainable practices that can inspire change across South America. Acknowledgments:

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Unveiling the Structure and Stability of Silver Species at the Grain Boundary of YBCO-based Ceramic Nanowires. An ONIOM-DFT study

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The superconductor based on YBCO ceramic holds potential for disruptive applications, spanning from supermagnets in the medical field to efficient wind power generators. We recently synthed certain YBCO ceramic nanowires, demonstrating that the addition of silver (Ag) could significantly enhance both the mechanical and superconducting properties [1]. The ability of Ag to modify its aggregation states creates incertitude about the species present, and their location during any synthesis. Hence, we investigated the structural and energetic properties of Ag species and their interaction in the confined environment of grain boundaries in our YBCO nanowires using an ONIOM methodology (PBE:UFF). Based on structural models for Ag-free YBCO systems generated at the periodic PBE level, we developed a cluster model for YBCO. This YBCO model was characterized by a stoichiometry of $Ba_{54}Cu_{160}H_{564}O_{448}Y_{27}$, and various cuts in the [100] zone axis were simulated. Finally, we separated some YBCO cluster pairs at a distance of 2 nm and relaxed Ag clusters ($Ag_nO_m^l$, n=1,...,10; m=0,...,10, and l=-1,0,1) to simulate the confinement effect between the grains of Ag-YBCO nanowires. Similar to the results published by McKee *et al.* [2], the cohesion energy values for neutral Ag clusters increase as the cluster (n) increases. This increase reflects the larger gain in energy due to the formation of multiple new bonds formed by numerous atoms (from -144.0 kJ mol^{-1} to -82.4 kJ mol^{-1}). To date, the interaction of Ag_8 clusters with CuO-planes in Ag-YBCO models has been the most exergonic among all the interactions studied.

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EP04-Organic Near-Infrared Materials and Emerging Applications

Near Infrared dyes for Photovoltaics, Green Photonics and Biological Applications

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Significant efforts have been dedicated to develop near-infrared (NIR) dyes for both biological and optoelectronic applications,[1] such as imaging, photodynamic therapy (PDT), solar cells[2] and biological sensors. Among many, polymethine dyes can be considered as interesting photosensitizers due to the easy and low-cost synthesis along with remarkable absorption property in the far-red NIR region.[3] Squaraines and cyanines are notable for their high molar absorption coefficients, remarkable brightness, fluorescence and photostability, especially in organic media.

This contribution focuses on the design and synthesis of various series of NIR absorbing polymethine dyes. A preliminary structure-properties relationship is presented to highlight the most relevant molecular features for the interactions with light and biomolecules. Among the different applications, results on their use as photosensitizers in Dye-Sensitized Solar Cells (DSSCs), PDT, and “turn-on” fluorogens for the quantitative detection of proteins will be discussed. Additionally, the encapsulation of these dyes in organic and inorganic nanomaterials to enhance their optical properties, photostability, biocompatibility, and efficient cellular internalization will be examined. Finally, the first application of these dyes as solid-state emissive materials in sustainable lighting based on emissive proteins will be presented.

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Shortwave infrared-sensitive, narrowband all-organic optical upconversion devices with a gain

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Organic upconversion devices (OUCs) made by integrating an organic shortwave infrared (SWIR)-sensitive photodetector with an organic light-emitting diode (OLED) offer a low-cost, pixel-free route to see images taken in the infrared light region. OUCs emerge as a promising addition to the current inorganic compound-based SWIR cameras, with many applications in bio-medical imaging, machine vision systems, or in industrial and environmental monitoring. In this talk, I will introduce the OUC concept and summarize recent advances to fabricate such devices entirely from solution or to increase the SWIR sensitivity, both in terms of a high infrared-to-visible photon conversion efficiency or a low dark current. In the second part of this talk, I will present OUC results that were obtained within a joint Brazilian-Swiss research project. Polymethine dyes with an exclusive, very narrow absorption in the infrared range were synthed for the fabrication of devices that are visibly transparent. An analysis is presented of the surprisingly slow and unusual OUC response speed, which denotes the ability to accurately detect in the visible a rapidly changing infrared signal. Finally, OUCs are introduced that combine a photomultiplication photodetector with an OLED. A photodetector with a gain generates many more than one electrical charge per incident SWIR photon and boosts the OUC photon conversion efficiency.

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Upconversion nanoparticles and infrared activated processes

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Lanthanide-based upconversion nanoparticles (UCNP) have been used in several different applications, since IR pumping and emission covering the UV-Vis region up to infrared are very attractive from a technological point of view. We will show examples where light-activated processes, such as photocatalysis and temperature measurements, can benefit from the spectral properties of UCNPs.

Regarding photocatalysis, new organic-inorganic hybrid aerogels have been prepared based on bacterial cellulose (BC) aerogels and inorganic photocatalysts such as TiO2, BiVO4 and MoS2 [1]. These innovative materials bring together the properties of BC aerogel, such as mechanical stability, flexibility and microporous structure, together with the unique photocatalytic and surface properties and mesoporous structure of the inorganic counterpart.

When it comes to temperature measurements, sustainable smart tags have been manufactured. These tags feature a two-step verification for anti-counterfeiting triggered by the photothermal response of upconverting nanoparticles [2]

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Charge generation in single-component organic thin films: squaraine dyes for shortwave infrared light detection

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Organic Photovoltaic (OPV) devices are traditionally constituted by blends where charge separation occurs at the interface between a donor and an acceptor material. As a consequence, the efficiency of the device strongly depends on the morphology and stability of the blend, making their engineering, optimization and fabrication a very delicate task. The idea of a simpler functioning device constituted by a layer of a single component is therefore very appealing. Sensitivity in the shortwave infrared (SWIR) window is possible with inorganic semiconductor-based devices, but their use is limited due to high production costs, complex processing, and scarce biocompatibility. The possibility to sense SWIR light with an organic-based device would open the way to a wide number of applications ranging from biomedical imaging to optical telecommunications. The task is challenging due to the scarcity of organic dyes absorbing in the SWIR region and the even more difficult pairing with a suitable complementary component to realize an efficient donor-acceptor heterojunction. Squaraine dyes are excellent candidates for this task. A family of properly functionalized squaraines has been employed for the fabrication of single-component SWIR-sensitive photodiodes, also in combination with organic light-emitting diodes in upconversion photodetectors[1]. In this work, a joint experimental and theoretical study is presented towards the rationalization of the behavior of these devices and their optimization. Special attention is devoted to elucidate the mechanism of charge separation in single-component squaraine monolayer films.

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Design and synthesis of shortwave infrared-absorbing squaraine dyes

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The availability of organic dyes for optical sensing and imaging in the infrared wavelength range is essential for advanced applications such as deep-tissue imaging, optical communication or industrial and consumer product identification. 1,3-squaraines have been established as an important class of dyes with strong and narrowband absorption in the near-infrared range up to around 900 nm. Here, we report the design and synthesis of a series of new squaraine dyes with peak absorption extending to beyond 1100 nm, which is in the shortwave infrared range. The dye absorption can be modulated by tailoring the donor side chains as well as the central acceptor unit. The acceptor strength of the squaric acid core was increased by its functionalization with dicyano- and rhodanine electron accepting groups. For the side chains, we opted for extended aromatic systems such as benz[cd]indoles and dimethoxydiphenylamine-benz[cd]indoles, resulting in dyes with a pronounced donor-acceptor-donor structure. By considering the case of a dicyano-rhodanine substituted squaraine, we discuss possible limits of the "strong donor – strong acceptor" approach to bathochromically shift the absorption. We compare the merits of squaraine dyes with other classes of infrared dyes, such as cyanines and BODIPY's.

Acknowledgements:
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NANOTHERMOMETER BASED ON POLYCHLORINATED TRITYL RADICALS SHOWING TWO-PHOTON EXCITATION AND EMISSION IN THE BIOLOGICAL TRANSPARENCY WINDOW

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Perchlorotriphenylmethyl radical (PTM) are organic radicals chemically stable with inherent magnetic spin. PTMs exhibit other appealing properties such as a rich electrochemistry, electronic and optical properties (absorption and emission)[1] and chirality.[2] Here, we will review recent developments employing trityl-based radicals as organic radical nanoparticles (ONPs). Such ONPs having inside isolated radical molecules and dimeric excimers, can be two-photon excited showing optimal properties for NIR temperature sensing with excellent thermal absolute sensitivity of 0.6–3.7 %·K−1 in the temperature range of 278 to 328 K using a ratiometric approach. Individual ONPs are able to sense temperature changes at the nano-microscale. In vivo thermometry experiments in Caenorhabditis elegans (C. elegans) worms and ex-vivo with enucleated pig eye sclera, as a real tissue model, show that such ONPs can locally monitor internal body temperature changes with spatio-temporal resolution and high sensitivity, demonstrating their potential as NIR nanothermometers for bio applications.[3]

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Quantitative imaging of physiology in freely-moving mice

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The study of physiology in living animals is often constrained by the need for physical restraint, anesthesia, or euthanasia. These procedures introduce confounding factors in the interpretation of physiological measurements [1,2].

Here, we propose utilizing the optical properties of shortwave infrared (SWIR, 1000-2000 nm) for imaging biological processes. Recently, we have achieved record-breaking speeds in SWIR fluorescence imaging (<3 ms, 300 fps), enabling the resolution of features such as blood vessels even in fast-moving mice [3, 4].

One challenge in quantifying fluorescence intensity in moving animals is the reliance on their pose, position, and proximity to the detector. To overcome this challenge, we developed a ratiometric approach, which involves measuring the emission of two orthogonal fluorescent dyes: the sample fluorophore, which serves as a well-established probe for physiological activity in the organs of interest, and the reference fluorophore, which provides a stable signal in the same organ and acts as a reference point for comparison.

After validating this ratiometric strategy in vitro and ex vivo, we applied it in vivo by measuring the clearance of indocyanine green (ICG), a clinically-used assay for liver physiology [4]. ICG clearance kinetics was quantified in both blood vessels and liver compartments using imaging, tracking, and intensity extraction. Chrom7, an orthogonal cyanine dye to ICG, was used as the reference probe. Our SWIR ratiometric imaging successfully reproduced the results observed in isoflurane-anesthetized mice for ICG blood half-life and liver clearance, consistent with findings in clinical literature.

This work opens avenues for researchers to study organ physiology in freely-moving mice without the confounding effects of anesthesia, enabling quantitative measurements in a more natural state.

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Resonance energy transfer in micelles: optical spectroscopy in suspension and two-photon microscopy in *ex vivo* tissues

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Resonance energy transfer (RET) is a fascinating phenomenon in fluorescence microscopy, offering benefits such as an increased Stokes shift, the ability to shift emitted light towards the red/near-infrared spectrum, and to monitor the integrity of nanocarriers in bioimaging applications.[1] When both the energy donor and acceptor dyes are loaded onto the same nanoparticle, a RET signal can be observed. However, upon nanocarrier disaggregation, the dyes are expected to separate, leading to a decrease in RET efficiency. In this work, TPGS (d-α-tocopheryl polyethylene glycol succinate) and CTAB (cetyltrimethylammonium bromide) micelles loaded with two indocarbocyanines compatible for RET: DiI (green emitter, the energy donor) and DiD (a red/near infrared emitter, the energy acceptor), were spectroscopically characterized above and below the critical micellar concentration (CMC) and then tested in ex vivo permeation experiments using porcine scleral tissues. In aqueous suspension, RET is observed above the CMC for both surfactants: selective excitation of DiI leads to a sizable emission from DiD, in the red/far-red spectral region. Below the CMC, the RET efficiency decreases for TPGS micelles, while a surprising RET efficiency boost is detected in presence of CTAB. This latter counterintuitive phenomenon has been explained with the formation of aggregates containing both dyes.[2] The distribution and integrity of the two nanocarriers is probed by two-photon microscopy after permeation in the scleral tissue, exploiting the deep penetration of the NIR excitation source. Monitoring the RET efficiency variations at different depths confirms the different behavior of the two surfactants and demonstrates the importance of robust spectroscopic characterization of nanocarriers to employ RET as an integrity test for nanoparticles.

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comparison of reactivity between dimethylhexane conformers using the density functional theory

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Octane rating is a measure of a fuel's anti-knock properties, especially in gasoline, where it is closely linked to the concentration of octane, one of the main components responsible for ensuring efficient fuel combustion. The search for new additives that improve octane rating has been a growing area of research in the scientific community. In this context, dimethylhexane emerges as a promising isomer of octane, belonging to the class of alkanes, saturated hydrocarbons consisting exclusively of carbon and hydrogen atoms. In this study, we performed calculations on the electronic density and vibrational properties of the 3D structure of 2,2-DMH and 3,3-DMH isomers by DFT [1]. The 3D molecular geometry was acquired from PubChem and optimized. In our calculations, we utilized a hybrid functional (B3LYP) [2], def2-TZVPP basis set, and a method for minimizing gradient noise. For 2,2-DMH, we observed a stabilization energy at -315 Eh, HOMO -8.196 eV, LUMO 0.795 eV, a band gap of 8.99 eV and dipole moment 0.05 Debye. Conversely, for 3,3-DMH, the stabilization energy was also -315 Eh, with HOMO at -8.206 eV, LUMO at 0.802 eV, a band gap of 9 eV and dipole moment 0.11 Debye. We have obtained similar values for the vibration frequency and observed differences in the polarities and electronic densities in the LUMO of the molecules. Our findings underscore the importance of further studies to elucidate and compare the reactivity of different DMH conformers. Acknowledgments: This extension project was carried out with the support of the Proex, Proext-PG Capes, involving graduate students, PIBIC/UFVJM, CNPq, BIOSEM-LESMA, FAPEMIG, and Capes, and undergraduate programs in Science and Technology, Engineering Physics, and Materials Engineering. References:[1] MOUATARIF, S.; VAN ALSENOY, C.; ABOULMOUHAJIR, A. Spectroscopy Letters, v. 41, n. 2, p 87-99, 2008. [2] MUNIZ-MIRANDA, Francesco et al. Theoretical Chemistry Accounts, v. 135, p. 1-9, 2016.

EP05-Sustainable Development of Printed Electronics: from Materials Processing to Devices Implementation

Biomass-derived carbon materials: understanding the correlation between atomic structure and electrochemical properties using in-situ techniques

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Carbon-based electrodes have received considerable attention due to their low cost, tailorable morphology and microstructure, and the possibility of processing them by direct carbonization of eco-friendly and naturally available biomass resources. In energy storage applications, several material parameters need to be optimized, such as surface area, pore or crystallinity, which requires a profound understanding of structural evolution of carbon during carbonization and heat treatment, as well as the effect that graphitization catalysts will have on the final structure. For instance, hard or amorphous carbon represents the material of choice for sodium-ion batteries, whereas highly crystalline carbon (i.e. graphite) is required in the case of lithium-ion batteries.

In this presentation we will review preparation and modification approaches to obtain carbon materials from biomass-precursors, providing a sustainable pathway to advanced electrodes in energy storage applications such as supercapacitors and lithium- and sodium-ion batteries. Activation and graphitization strategies will be reviewed, with emphasis on catalytic graphitization, a process that yields graphitic nanostructured carbon using transition metal catalysts at mild processing conditions. The correlation between processing parameters, degree of structural ordering and electrochemical properties will be highlighted with novel results from our group using state-of-the art in-situ characterization methods such as environmental TEM or synchrotron X-Ray diffraction and Pair Distribution Function determination. It will be shown that biomass offers a wide menu of precursors from which carbon materials with tailored structural ordering and porosity can be readily processed.

The effect of this structural ordering will be highlighted in three energy storage applications. In the case of supercapacitors, it will be shown that biomass-derived carbon monoliths can be used as three-dimensional scaffolds for deposition of oxide nanostructures with improved cycle stability. In the case of sodium-ion batteries, we will show that control of processing parameters can result in disordered carbons with optimized interplanar spacing that favors sodium adsorption and intercalation. In the case of lithium-ion batteries we will show that under controlled conditions biomass-derived graphite with capacities comparable to synthetic graphite can be obtained at lower processing temperatures, providing a sustainable route to more environmentally friendly anodes.

Environmental Sensing with Printed and Flexible Sensors

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Soil nitrogen (N) exists in various forms, such as nitrate (NO3-), ammonium (NH4+), nitrite (NO2-), organic N, and gaseous compounds like dinitrogen gas (N2), ammonia (NH3), nitric oxide (NO), and nitrous oxide (N2O). Among these, NO3- and NH4+ are crucial for plant growth and are commonly found in agricultural fertilizers. Monitoring their concentrations is vital for efficient fertilization and preventing environmental pollution, including NO3 leaching, which leads to water and groundwater contamination, and increased emissions of particulate matter and N2O, a potent greenhouse gas. We present a cost-effective platform for real-time monitoring of greenhouse gas (GHG) emissions and soil data, specifically tailored for biofuel agriculture. Our approach uses a sensor array to measure key soil chemical species influencing GHG fluxes, including NH4+, NO3-, O2, moisture, temperature, pH, CO2, and denitrification enzyme concentrations. Sensors, including a soil N2O sensor, are deployed in replicate sensor bundles placed at depths of 10, 20, and 30 cm below ground. An above-ground electronics platform facilitates data collection and transmission via a mesh network to a gateway for analysis. Validation methods include continuous surface flux chambers using cavity ring-down spectroscopy (CRDS), eddy covariance, and laboratory assays. Our wireless sensor network provides a novel solution for real-time monitoring, empowering farmers to manage emissions effectively.

Exploring the Terrain of Printed and Organic Electronics through Artificial Intelligence and Natural Language Processing

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The emergence of large language models, such as those employed in tools like ChatGPT, has made it possible the expansion of natural language processing to extract data from literature in unprecedented ways. This lecture will provide a bird's-eye view of the field of printed and organic electronics through the analysis of tens of thousands of papers. This overview was obtained by initially constructing a citation network for the papers under analysis, from which subareas were determined. The methods employed involve predominantly community detection in complex networks and natural language processing. The most significant subareas (communities) in printed and organic electronics include inkjet printing and organic solar cells. While the majority of subareas focus on applications, as expected, some communities feature materials such as perovskite, graphene and metal-organic frameworks (MOFs), along with characterization techniques utilized in fundamental studies. Due to the strategy employed for the landscape, only statistically relevant topics are captured, and thus recent developments in the field could not be identified. To address this limitation, a detailed analysis of the temporal evolution of the topics was conducted, allowing for projections to be made for the near future. In particular, emphasis will be placed on the expected impact of artificial intelligence tools in the coming years.

Inkjet-printed devices and circuits for ultra-low frequency applications

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The detection of ultra-low frequency electrical oscillations holds significant relevance across various applications. These include the detection of (bio)chemical substances and devices to detect microorganisms, cells, and plants in sensing applications. Microorganisms such as bacteria, microbes, algae, plants, and non-excitable biological cells use electrical signals that last for several minutes and width periods that can last for hours. To effectively detect these signals, the sensing device needs to have low intrinsic electrical noise. Particularly relevant is the 1/f noise which dominates frequencies below 1 Hz. Remarkably, the use of printing conductive and semiconductive inks in porous substrates such as paper creates nanostructured electrical interfaces. These surfaces, when interfaced with wet or liquid environments, have an electrochemical sensing layer with very low intrinsic electrical. Compared to inorganic-based devices, inkjet printed devices using conducting polymers have an unbeatable low noise level, typically two orders of magnitude lower than their inorganic counterparts. This ultra-low noise property opens up a diverse range of applications. Printed devices covering relatively large areas (millimetre square) can monitor bioelectrical signals in plants and microorganisms or use microorganisms such as algae for sensing purposes or even for microenergy generation purposes. In healthcare applications, low-frequency sensing devices play a crucial to monitor electrical fields involved in tissue regeneration and wound repair. Additionally, therapeutic electrical devices are emerging to impede cancer cell migration and proliferation. Some microorganisms can also be seeded in hybrid devices by inkjet. Devices fabricated using printing techniques in natural substrates such as paper are fully disposable and environmentally friendly. In this contribution, we discuss the design and fabrication of ultra-low noise devices by inkjet printing.

Manufacturing of Li-ion battery electrodes by 3D printing: Pros, cons and technological perspective.

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In the last years, with the rise of the Internet of Things (IoT), there has been a huge rise of affordable free-form sensors, antennas, and other electronics to cover the demand for information and digitalization of the world. The necessity to power up these devices has created a demand for energy storage devices that can power them without sacrificing their new functionalities, such as flexibility, printability, or sustainability. One of the key factors needed from these energy storage devices is to adapt to the miniaturized and non-standard shapes that the new generation of printed electronics brings. In this regard, the interest in printed energy storage devices, and more specifically batteries, has boomed in the last few years. The printing strategies not only provide the batteries with the miniaturisation and free-form capabilities but also the high resolutions achievable open new possibilities in regard to their architecture, allowing the formation of non-planar structures. [1] The interest in these ad-vanced, or 3D structures, for batteries, comes from their capability to significantly overcome the areal capacity of 2D electrodes without compromising power density. [2] This translates into an effective decoupling of the energy and power density which was impossible until now and provides an extra asset to the batteries to adapt to the specific application.

In this presentation, I will provide an overview of the printing techniques covering their impact on the material arrangement of the end device and its impact on the device performance. I will show examples of how 3D printing strategies can allow us to improve the different metrics we want in battery elec-trodes while simplifying the prototyping process. Additionally, it will be shown how 3D printing can be used to implement more sustainable active materials in battery manufacturing.

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Materials for Eco-Design Strategies for an Innovative Industry

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Printed electronics technologies draw tremendous attention because of their ability to overcome the limitation of traditional high-cost manufacturing approach, mostly based on silicon. Printing technology can be used to fabricate devices on various kind of flexible substrate such as paper, textile, bendable polymers even on human skin. On the other side, it has also a great potential to offer biodegradable and recyclable solutions, by choosing substrates that can be recycled and/or naturally degraded in nature. This is a way forward to minimize the electronic waste (e-waste) caused by the ever-increasing number of disposable electronic devices as it is the case of paper electronics, whose performances will depend on the ink's properties selected for the different building blocks that constitute the device or system to be fabricated. A long list of functional materials can be chosen, going from conductive polymers, ionic liquids, and carbon nanostructures to metallic nanoparticles, and metal oxide nanostructures with conductive, semiconducting, or dielectric properties, can be used to formulate these inks. The development of stable, cost-effective, non-toxic, and eco-friendly printable inks with desired printability is crucial to deposit and pattern these materials onto a substrate to enable the production of a new class of devices for electronics and energy purposes that are extremely lightweight, affordable, readily customizable, thin, flexible, and recyclable. All these challenges are addressed in the present presentation.

Sustainable and Tunable Synaptic Electrolyte-gated organic field-effect transistors (EGOFETs) for Light Adaptive Visual Perceptive Systems

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The recent advances in optic neuromorphic devices have led to a subsequent rise in the development of energy-efficient artificial-vision systems. Whilst the energy consumption of such devices is known to be much lower than conventional vision systems, it is known that manufacturing accounts for the largest share of the climate impact in microelectronics, dominating over the product use phase. Thus, there is a need to develop sustainable manufacturing processes and to adopt low impact materials for hardware solutions of the future. In this study, an Electrolyte-Gated Organic Field-effect Transistor (EGOFET) is experimentally demonstrated for the implementation of a high performing synaptic optical sensor using sustainable materials that degrade to benign products at the End of Life (EoL). The device shows remarkable light response with maximum Paired-Pulse Facilitation (PPF) of up to 151% at a light power density of 38 µW cm-2, which enables artificial synaptic applications with an average power consumption as low as 2.4 pJ for each training process, representing one of the best among the reported results. Moreover, the results suggest that much longer spike times are achievable due to the ability of the 'honey' electrolyte to retain a greater number of residual charges prior to the second spike, ultimately producing a better synaptic response. A benefit of our approach is that the selected active layer can absorb across the entire visible spectrum and responds to blue, green and red light. To demonstrate the tunability of our vision system, an ensemble decision tree has been used to enable the EGOFET to distinguish between different primary colours at different power densities with 95.6% accuracy. This study provides a new concept towards the design of sustainable adaptive vision systems.

Sustainable processes to produce metal oxide devices: from coating to printing

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Nowadays, the number of electronic waste (e-waste) that each person generates is quite impressive and it tends to increase exponentially in the next 30 years. This will lead to a high quantity of e-waste accumulation that will not be recycled and will most likely end in landfills of developing countries. To overcome this serious societal problem, it is necessary to rethink the

production process of some electronic devices and to reconsider their life cycle assessment, more specifically their environmental footprint. Coating and printing materials can be a solution for electronics and its market is expected to have a compound annual growth rate of 21.5 % from $9.9 billion in 2021 to $23 billion by 2026. By adopting more sustainable materials and processes, electronics waste is reduced, leading to the reduction of the carbon footprint, and paving the way for green electronics. In this presentation, we report suitable processes (spray coating; inkjet, screen, and flexographic printing) to deposit solution-based materials (InOx, IGZO, ZTO, AlOx, MoO3) and ensure the possible scale-up of metal oxide-based devices, such as thin film transistors, diodes, and memristors. These devices will lead to great societal impact since they can power up the speed and efficiency of lighter and thinner wearables, as well as smart windows applications highly needed for the emergent IoT.

Capacitance in Electrolyte-Gated Transistors Extracted from Gate-Source Current Measured Simultaneously with the Transfer Curves Analysis

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Electrolyte-gated transistors (EGTs) exhibit high on-currents at low voltages, enabling low-power operation of such devices since an electrolyte presents very high capacitance due to the electrical double layer formed at its interface with the semiconductor. Printed EGTs employing organic semiconductors or metal oxide semiconductor nanoparticles deposited on flexible and biodegradable substrates, such as paper, or other porous flexible materials have a rough semiconductor-electrolyte interface, resulting in high area-specific capacitance. In these examples, capacitance may depend on the interface morphology and applied voltage, making it insufficient to consider the typical electrolyte double-layer capacitance solely for device parameter analysis. This work demonstrates that EGTs capacitance can be obtained during transfer curve measurements, leveraging the gate-source current measured simultaneously with the drain-source current. The gate-source current analysis is performed using an equivalent circuit. In the accumulation regime, the circuit can be approximately modelled as a resistance (R) in parallel with a capacitor (C) from the electrolyte, both in series with another resistance (r) from the semiconductor. The fitting of the current flowing through this equivalent circuit when a linearly time-varying voltage is applied to the transistor, to the experimental Ig x Vg data, allows for determining the electrolyte capacitance under measurement conditions. This method has been used to various devices, comparing the effects of substrate morphology, semiconductor materials, and electrolytes on the capacitance value and, consequently, on other transistor parameters such as saturation current, semiconductor mobility, and more. The results demonstrate that this method is a simple yet powerful tool for improving the accuracy of EGTs parameter determination.

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Designing fullerene-based polymers for a sustainable future

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Main-chain fullerene-based polymers are still rare, however, they are gaining interest for their use in photovoltaics and organic electronics. For examples, recent work has demonstrated their use as interlayers in perovskite solar cells to give efficiencies around 23% [1] and exceptional stabilities in organic solar cells [2]. They might also find use in ammonia sensors [3] and in drug delivery systems. The key properties that these materials exhibit is their combination of fullerene's extraordinary ability to accept electrons, and their polymeric capability to make thin films from solution that are smooth compared to films from fullerenes alone. This said, the methodology used to make these polymers can impact extremely heavily on its final physico-chemical properties. Therefore in this presentation we quickly review the various types of poly(fullerene)s and their structures, and disclose two new methods of making them. This work then focuses on methods of making these novel materials using biocompatible, sustainable routes, and exploring their application in solar cells. In particular we look at ways of making amphiphilic poly(fullerene)s which are not only sustainable but also have properties tailored for solar cell and drug delivery technologies.

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Flexible 3D-Nanomembranes: from Hybrid Electronic Devices to Molecular Interfaces

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In the last decade, research has focused on utilizing flexible 3D nanomembranes in electronic devices to transform device architectures and functionalities. This presentation provides a comprehensive overview of recent advancements, from integrating surface-supported metal-organic frameworks (SURMOFs) into hybrid electronic devices to exploring molecular interfaces in nanoscale junctions and bio-functional thin films.

Incorporating SURMOFs into electronic devices has notably enhanced electrical conductivity through intelligent integration strategies. By employing in situ polymerization techniques, the electrical conductivity of HKUST-1 templates has been boosted, enabling the development of innovative hybrid electronic-optoelectronic devices. Integrating ultrathin HKUST-1 SURMOF films into device architectures has facilitated the accurate determination of dielectric properties, establishing them as robust low-k dielectrics for novel electronics.

The discussion dives into molecular interfaces in nanoscale junctions, elucidating charge transport mechanisms and electronic properties. Engineering hybrid capacitors with mechanically compliant nanomembranes have enabled the reliable determination of dielectric constants of ultrathin molecular ensembles, guiding practical device design.

Moreover, flexible 3D nanomembranes facilitate the fabrication of high-performance organic thin-film transistors (OTFTs) with smaller footprints and enhanced mechanical flexibility. Utilizing rolled-up nanomembranes as drain electrodes has led to OTFTs with ultra-low operating voltages and resilience against mechanical deformations, showcasing their potential for rugged electronics.

In conclusion, the versatile application of flexible 3D nanomembranes spans various electronic devices, offering promising avenues for future nanoelectronics and molecular electronics advancements.

Liquid Phase Exfoliation of Graphene on Cyrene for the Sustainable Production of Microsupercapacitors

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The isolation of graphene for the fist time, along with other two-dimensional (2D) nanomaterials has generated a revolution on the development of energy storage devices, namely supercapacitors.[1] However, most of the times these materials are isolated on harmful solvents, such as N-Methyl-2-pyrrolidone (NMP). On these regards, dihydrolevoglucosenone (cyrene) has become a suitable sustainable solvent for the processing of 2D materials by liquid-phase exfoliation.[2,3] In this work, it is shown a full description of the processability of graphene in cyrene by liquid phase exfoliation and its subsequent application as a supercapacitor electrode. The obtained dispersions will be characterized in terms of TEM, AFM and UV-Vis. A proper comparison with NMP and other conventionally used solvents is also addressed. Finally, the application of these "inks" will be demonstrated by spray coating supercapacitors onto sustainable substrates. As an outlook it will also be discussed the use of cyrene to process other 2D materials. To sum up, this work will demonstrate a sustainable methodology for the processing of nanomaterials and eco-friendly methodologies for energy storage applications.

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Paper-based SERS platform functionalized with ZnO nanorods for pesticide detection

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Paper substrates have generated interest in electronic applications and Surface-Enhanced Raman Spectroscopy (SERS) technique due to their flexibility, versatility, cost-effectiveness and environmentally friendly nature. In this work, we present the functionalization of Whatman Grade 1 paper (WP) substrates with zinc oxide nanorods (ZnO NRs) to detect environmental contaminants. ZnO NRs were grown by hydrothermal synthesis assisted by microwave irradiation on WP substrate and subsequently decorated with silver nanoparticles (AgNPs), deposited by temperature assisted electron-beam evaporation. WP substrates functionalized with ZnO NRs/AgNPs were used as a SERS platform to detect the thiabendazole (TBZ) pesticide. TBZ is one of modern agriculture's most widely used benzimidazole fungicides, mainly for pre-harvest and post-harvest protection against fungal diseases in fruits and vegetables. WP substrates with ZnO NRs/AgNPs exhibited superior SERS activities compared to WP substrates with only AgNPs, for TBZ detection. The improvement in detection with the use of ZnO NRs can be attributed to their large surface area, providing an ideal platform for the adsorption of target molecules, thereby increasing the probability of interactions with incident light and, consequently, enhancing sensitivity. Additionally, ZnO exhibits a prominent ability to provide an efficient charge transfer pathway, contributing to the SERS chemical enhancement mechanism. The enhancement factors (EF) and limit of detection (LOD) for TBZ using ZnO NRs/AgNPs were 9.8×10^{6} and 5.0×10^{-10} mol/L, respectively. The results are promising and superior to other substrates reported in the literature. The paper substrate is an abundant, non-toxic, cost-effective and flexible platform that, after appropriate functionalization, can be used in field analysis with portable Raman spectroscopy.

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Study of an Impedimetric Immunosensor Based on the Sensorial Platform of Poly(o-phenylenediamine)-AuNPs and 5-methylCytosine Antibody

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Recently new electrochemical methodologies for detecting the methylation of nitrogenous bases have been developed, due to the relation between methylated DNA and cancer. The electrochemical impedance spectroscopy (EIS) technique stands out as a transduction model for immunosensors due to its high sensitivity to interfacial changes, reaching detection limits on the picomole scale. In most cases, ferrocene is used as a redox probe to increase the signal of the antibody and antigen interactions, however, the excess of these redox species can cause problems associated with false-positive sensor responses. This work is an alternative methodology for an electrochemical immunosensor, based on a single-step sensory platform of poly(o-phenylenediamine)-AuNPs, to determine the global levels of 5-methylcytosine (5-mC), utilizing dissolved oxygen as a redox probe. The immunosensor was developed by immobilizing the 5-mC antibody to the surface of the modified electrode. No secondary antibody was used. The platform performance was evaluated by EIS in different concentrations of 5-mC in a PBS solution containing atmospheric oxygen. The EIS reveled that the presence of dissolved oxygen decreased the Rct value, and the system impedance increased with the addition of 5-mC in solution as a function of increasing antigen-antibody binding, hindering the permeation of molecular oxygen to the redox sites of the polymer.

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Water Based Inks for Active Layers in Organic Photovoltaics

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Semiconductive inks, used for the production of organic photovoltaics, are commonly made with organic solvents such as chloroform and chlorobenzene. The organic solvents pose high health risks and are also highly harmful for the environment, which shows the importance of the search for new sustainable eco-friendly inks. The main goal of this study was the production of donor, acceptor and donor:acceptor nanoparticles in a stable suspension in water, which is a non-toxic and not harmful to the environment solvent. This study also compared the use of both fullerene and non-fullerene acceptors in the nanoparticle solutions. Homogeneous depositions were successfully obtained in many coating techniques including spin coating, slot-die coating and blade coating, both in glass-based substrates and flexible substrates. These water based inks were also applied as active layers of organic photovoltaics (OPVs). The nanoparticles of the donor and the acceptor materials, and also the nanoparticles with both donor:acceptor materials inside the same nanostructure were all successfully produced, stabilized and characterized. The morphological analysis of the nanoparticles film depositions presented homogeneous nanoparticle distributions and showed that the polymers were spherical-like shaped. The optical characterization with the absorbance and photoluminescence analysis showed that there was a charge transfer between the donor and acceptor materials inside the nanostructure. The OPVs produced were analyzed using the open circuit voltage (Voc) and the short circuit current density (Jsc) parameters. Stability studies of both the nanoparticle films and the complete OPVs were also made comparing organic solvents and the water-based nanoparticle inks, showing that the nanoparticle inks are more stable than the organic solvent ones. Therefore this study demonstrates the possibility of obtaining flexible water based organic photovoltaics, which can be coupled to a roll-to-roll printer.

Anionic Influence on Electrochemically Synthed Poly(Azo-DAB) Thin Films: Exploring Conductive Polymer Performance

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The conducting polymers have been extensively researched for their potential applications in electronic devices and sensors [1]. Direct deposition by electropolymerization of thin films can form conjugated polymers efficiently onto conductive substrate surfaces. In this work, we study of the influence of different counter-anions on the formation and electrochemical performance of polymer films of 3.3′-diaminobenzidine (DAB). The films poly(azo-DAB) were electropolymerized using inorganic acids such as HCl, HNO_3, H_3PO_4, and H_2SO_4, respectively.The characterization of poly(azo-DAB) films was conducted using cyclic voltammetry and electrochemical impedance spectroscopy in an inert supporting electrolyte (0.5 mol L^{-1} KCl). The CV recorded at FTO modified with poly(azo-DAB) shows a quasi-reversible redox couple (Epa = -0.14 V; Epc = -0.37 V vs. SCE), which is attributed to oxidation and reduction of the azo group. The EIS analyzes showed a linear correlation between counter-anions and charge transfer resistance of polymer. The electropolymerized film in solution H_2SO_4 exhibited lower charge transfer resistance values, which is associated with higher electronic conductivity. Furthermore, counter ion HSO_4^- acts in stabilize the amine radical cation of poly(Azo-DAB) [2].Thus, when comparing the coefficient values obtained for active species (Γ) on the electrode surface with the low resistive values for each counter-anions, a better electrochemical performance is attributed to the HSO_4^-.

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A study of the thermoelectric effect on screen-printed disordered material

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The development of thermoelectric materials based on conductive polymers has gained great prominence in recent years. In this research field, the conductive inks allow the fabrication of printed thermocouples and thermoelectric cells [1]. Therefore, several studies regarding thermoelectricity in conducting polymers have been published recently [2]. However, these conducting materials are disordered in contrast to crystalline metallic materials. Therefore, this research focuses on studying the influence of the conductive phase concentration on the electrical and thermoelectric properties of a multiphasic conductive paste. The transparent conductive paste (TICON) (Patent BR102019026350-4)[3] has been produced with different concentrations of its conductive phase, and the Seebeck coefficient and electrical conductivity have been obtained. To measure the Seebeck coefficient, an apparatus was developed, automated, and evaluated by performing Seebeck coefficient measurements for known metals such as chromel, constantan, iron, cooper, and alumel. We performed electrical conductivity measurements from current vs. voltage curves obtained for films produced with different aspect ratios for each material composition. Finally, the material disorder influence on the Seebeck coefficient has been interpreted taking into account the disorder influence on its electrical conductivity.

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A Study Regarding Silver Reaction With Sulfur-Based Compounds Toward Preventive Measures

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Silver particles have a wide range of applications, such as conductive pastes, sensors, wearable technology, and antibacterial agents [1]. However, silver is susceptible to corrosion by various agents, among which sulfur-based compounds are the most studied. Due to sulfur high affinity for silver, sulfur-based compounds spontaneously produce a darkened layer on the silver surface [2]. Even though several studies regarding silver reactivity with sulfur compounds have been reported, the development of strategies to prevent silver reactions with sulfur remains a scientific and technological lack. For this purpose, reaction control and quantitative tarnish measurements are the main challenges. Therefore, our research focuses on the investigation of silver compounds and chemical processes obtained by the controlled interaction of sulfurous gases with silver coatings. We have obtained silver coatings by screen printing a silver paste onto glass substrates and sintering at 550 °C. For reaction control and tarnish quantification, we have developed a reactor comprising an air flow and a sulfur heater controller. In addition, we have performed large-area energy dispersive X-ray spectroscopy measurements. Sulfurous compounds have been characterized by X-ray diffraction. As main results, we have evaluated reaction reproducibility, performed controlled reactions, and identified Ag2S as the main compound produced by the interaction of silver coatings with sulfurous gases.

Cathodic Performance of Polyaniline-Based Hybrid Materials in Biofuel Cells

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The effectiveness of the cathode in catalyzing electrochemical reactions can directly impact the overall efficiency of the biofuel cell, determining the amount of electrical energy generated from biological substrates [1]. So, in this work, hybrid materials of polyaniline (PAni) with 2% of graphene oxide reduced with hydrazine sulfate (rGO SH), were fabricated and applied to hand-made screen-printed electrodes (SPE) [2] as modified cathodes for use in biofuel cells with Saccharomyces cerevisiae. The materials were characterized using scanning electron microscopy (SEM), Raman spectroscopy, attenuated total reflectance Fourier transform infrared spectroscopy (ATR-FTIR), and X-ray diffraction (XRD). Followed by evaluation through cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS). The bioelectrochemical system was characterized and studied using CV, EIS, and polarization curve. The incorporation of PAni-rGO SH onto the screen-printed electrodes (SPE) resulted in higher current intensity as observed in cyclic voltammetry (CV) analyses, indicating improved electron transfer kinetics and efficiency. Moreover, the use of PAni-rGO SH as modified cathodes decreased the charge transfer resistance (EIE) within the biofuel cell, facilitating faster electron transfer processes and thereby enhancing overall cell performance. Additionally, the hybrid materials underwent thorough characterization providing insights into their structural and chemical properties.

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Characterization of Electrolyte-Gated Transistors Employing Honey-Based Electrolyte on Flexible Substrates with Laser-Induced Graphene as Electrodes

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The study of flexible devices is important due to their versatility of applications, including wearables, electronics, smart packaging, and Internet of Things (IoT). Additionally, other benefits across several fields include weight and volume reduction, integration on irregular surfaces, user comfort, and damage resistance. In this context, printed electronics and laser engraving methods, when combined, address the need for this field in manufacturing such devices. This study investigated the preparation and characterization of electrolyte gated transistors (EGT) using a variety of flexible substrates (kraft, watchman paper, and polyamide) and graphene electrodes formed by laser. The semiconductor employed was zinc oxide (ZnO) in nanoparticle form deposited by spray coating, while the chosen electrolyte was honey, due to its intrinsic properties such as the formation of a double electric layer, a very important factor for EGT performance. The main objective of the study was to evaluate the influence of the substrate both on the preparation of the electrodes and on the transistor performance. For the electrodes, the variation in resistance as a function of the substrate was investigated. For the transistors, the influence of the substrate on their electrical properties, such as transconductance, hysteresis, Ion/Ioff ratio, threshold voltage, and mobility, was evaluated. Preliminary studies showed that changing only the substrate causes significant variation in the device. While the EGT on kraft paper presented threshold, Ion/Ioff ratio, and mobility of 3.2 V, 8000, and 14.15×10^{-3} cm^2 V^{-1} s^{-1} respectively. The EGT on polyimide exhibited threshold, I_{on}/I_{off} ratio, and mobility of 0.75 V, 115000, and 340×10^{-3} cm^2 V^{-1} s^{-1} respectively. This change is due to both the resistance of the electrodes and the substrate/semiconductor interface. However, the results underscore the importance of the surface on which the device is manufactured.

Charge transport mechanisms in composite materials based on silver microparticles dispersed on conductive media.

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Material based on silver micro or nanoparticles dispersed in polymeric media represents one of the most important commercial products in the printed electronic field. This type of paste is an electronic composite with high electrical conductivity, with applications in the fabrication of automotive glass defoggers, antennas, and membrane keyboards [1]. Alternatively, composites produced using conducting polymers and carbon-based materials, such as graphene, are suitable for these applications [2]. Thus, the present research regards the comparison between the charge transport mechanisms of graphene and silver-based composites with different concentrations of their conductive phases. Samples have been produced by the screen printing method, and DC and AC electrical characterizations have been obtained for different concentrations of the conductive phase and temperature. We have obtained silver-based composites with electrical conductivity from (2.5 ± 0.9) x 10^{-2} to (2 ± 0.7) x 10^{4} S/cm and graphene-based composites with conductivity from (2.2 ± 0.1) x 10^{-9} and (1.0 ± 0.5) S/cm. The percolation concentrations have been obtained as (65 ± 5)% and (39 ± 5)% for silver-based and graphene-based composites, respectively. In addition, AC characterization and conductivity temperature dependence have shown metallic-like behavior for both materials. As a main conclusion, we have shown charge transport in silver-based and in graphene-based composites is quite similar. Therefore, the composite electrical conductivity is mainly affected by the raw material conductivity.

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Charge transport mechanisms in graphene-based composites

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In the electronic field, there is a growing demand for materials that achieve the requirements of fast processing, low cost, and reduced environmental impact. In this context, we investigated the charge transport in graphene-based composites [1]. In this study, we produced films using conductive composites with graphene concentrations ranging from 20% to 70%, deposited by screen printing. These materials electrical conductivity has been obtained by direct current (DC) characterization at room temperature, at different temperatures, and by impedance spectroscopy (using alternated current AC). We have shown all samples exhibited ohmic behavior, with electrical conductivities ranging between (2.2 ± 0.1) x 10-9 and (1.0 ± 0.5) S/cm. The electrical conductivity showed an exponential correlation with the conductor phase concentration below the percolation concentration of (39 ± 5) %. For concentrations higher than percolation, a linear dependence of conductivity on conductive phase concentration was found. Impedance spectroscopy results have been modeled with the Randon Free Energy Barrier model, showing most compositions have exhibited metallic-like behavior [2]. On the other hand, only samples produced with composites comprising 20%-wt of graphene have exhibited an insulating-like behavior with a γ_min of about 5 Hz.

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Conductive ink application toward smart textile technology

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Smart textiles are fabrics able to react to external conditions, such as heat, magnetism, electricity, chemicals, and light [1]. Currently, some studies have been pushed by applications in healthcare, sports, automotive, etc. In this study, we have coated different natural and synthetic fabrics with a commercial conductive ink [2], PCT 2.2 TICON. The conductive coatings have been characterized in terms of their sheet resistance in comparison to that of coatings on glass (100 Ω) and polyethylene terephthalate (150 Ω). The coatings on polyester fabric and polyamide fabric have exhibited sheet resistances closest to references, 80 Ω and 120 Ω respectively. In addition, we have evaluated the coating stability on polyamide fabric by sheet resistance evaluation after an ultrasonic bath for 30 minutes. This experiment resulted in a 1.5 times increase in conductivity. In summary, we have shown polyamide fabric is suitable for coating using the commercial conductive paste PCT 2.2 TICON.

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Development and application of screen-printed conductive materials as electrodes in perovskite solar cells.

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Currently, perovskite solar cells, with the highest energy conversion rates, are constructed using electrode materials that are expensive and produced by thermal evaporation or sputtering techniques.[1] Carbon-based electrodes and silver-based conductive paste deposition by printing techniques are alternatives to thermal evaporation elimination. Similarly, low-cost transparent conductive printing materials have already been developed and could be applied as perovskite solar cell electrodes. Therefore, our work focuses on developing new silver-based paste formulations, carbon nanomaterial-based pastes, and transparent conductive pastes for application as electrodes in perovskite solar cells. Films obtained with these materials have been characterized in terms of morphology (optical microscopy and profilometry), electrical properties (electrical conductivity and sheet resistance measurements), and transparency (UV-Vis measurements). In addition, the materials have been employed in the fabrication of solar cells, which were characterized in terms of efficiency and fill factor. As a preliminary result, we have shown screen-printed transparent conductive material also acts as a hole-transporting layer. However, film wettability, uniformity, and sheet resistance have negatively impacted the open-circuit voltage, short-circuit current, and fill factor. Thus, solar cell efficiency has been obtained at 3%, while its conventional counterpart has achieved 18%. During the conference, we aim to present our project perspectives and strategies, as well as further improvements on the transparent conductive material, film fabrication, and preliminary results obtained with the application of other printed materials.

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Development of a low-cost ecofriendly MWCNT modified paper screen-printed chitosan-based electrode derived from shrimp shells for sensitive electrochemical detection of bisphenol A

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Although the use of portable and disposable electrochemical sensors increasingly brings numerous benefits to the society, the increase in demand for its production can lead to an environmental problem, given that such devices are generally made of non-recyclable materials, tend to be counted as e-waste soon [1]. At the same time, while the chitosan (CS) is one of the most environmentally friendly biomaterials, the primary source of biomass for its industrial production are discarded, constituting a potential source of environmental pollution. In parallel, it is well-known that Screen-Printed Electrodes (SPEs) has attracted the attention of researchers due to the easy production, low-cost and suitable for industrial-scale production. In this work, due to the unique ability to form stable films on solid substrates, the CS was extracted from shrimp waste and used as an eco-friendly hydrophobic barrier material for the development of paper as substrate of a carbon based SPE, composed of three electrodes and modified with Multi Walled Carbon Nanotube (MWCNT). With the purpose to analyze the redox characteristics of the paper based SPEs, the Cyclic Voltammetry (CV) and Electrochemical Impedance Spectroscopy (EIS) techniques were employed in the redox system Fe^{II}/Fe^{III} (10 mmol L^{-1} de $K_3[Fe(CN)_6]$ em 0,1 mol L^{-1} KCl), with the scan rate of 10 mV s^{-1} in the potential range of -0,4 a 1,0 V. The raw materials and their respective composites formed was characterized by MEV, FTIR, RAMAN and DRX techniques. The findings suggest that the paper based SPE can be applied as an environment-friendly and sustainable electrochemical device in sensor applications for the determination of bisphenol A (BPA), a potential endocrine disruptor, in bottled mineral waters.

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Development of conductive elastomeric pastes for electronic textiles

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Electronic textiles (e-textiles) are an advancement of wearable electronics and presupposes the integration and manufacture of electronic devices directly into clothes or ordinary textile objects, giving them new functionalities [2]. Thus, the creation of electronic circuits and conductive paths through printing techniques is seen as essential for the advancement of e-textiles [1]. In this sense, fabric-compatible inks and conductive pastes are essential elements for the feasibility of applications in textile electronics [3]. In this work, we describe the development of elastomeric conductive paste formulations using graphite powders and carbon black as conductive load materials and different elastomeric polymer additives like EVA, SBR and PVA. Conductive tracks were fabricated on spandex™ fabric substrates using stencil printer and then thermal annealed at low temperature by different techniques. Under optimized conditions, the developed pastes produced tracks with very good conductivity showing an average sheet resistance of Rsq = 17-30 Ω/□ depending on the polymer type and good adhesion to the fabric substrate. The electric properties associated to the low-cost place such elastomeric pastes as prospective candidates for e-textile applications.

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DEVELOPMENT OF DISPOSABLE ELECTRODE WITH WATER-BASED CONDUCTIVE PAINT

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The advancement of simple, affordable, and disposable electrochemical sensors has significantly increased in recent years due to their easy manufacturing, versatility, and low cost. The key to developing these sensors lies in the ink formulation, typically comprising a conductive material, a binding agent, and a solvent. Achieving the right proportion of these ingredients is crucial for efficient electrochemical systems. The binding agent, or polymeric base, is dispersed in a solvent until the desired viscosity for the printing technique is attained. Among solvent types, organic solvents generally offer low flash points, promoting quick drying and low viscosity, thus aiding in paint processing [1]. However, due to the toxicity and safety hazards posed by organic solvents, water-based paints emerge as a compelling alternative to address these environmental concerns. Various formulations were tested, incorporating different components such as binding agents like scratch, carboxymethyl cellulose, chitosan, polyvinyl alcohol and water-based acrylic resin. Surfactants and alcohols were also added to enhance adhesion, viscosity, and consistency. The optimal water-based conductive paint composition, achieving superior electrochemical response and substrate adherence, was obtained by blending water-based acrylic resin, graphite, and glycerol in a 1:1:0,4 mass ratio. The substrate utilized was polyethylene terephthalate (PET) from soda bottles [2]. Characterization of the electrode via cyclic voltammetry and impedance yielded results comparable to those of solvent-based conductive paints.

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Development of flexible magnetic films by the incorporation of Ni/Ni3C nanoparticles in a matrix of Amazonian tannic extract (Myrcia atramentifera).

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The development of nanostructured magnetic materials based on Ni and its compounds (Ni/Ni3C) has been the objective of scientific research due to the versatility of applications that these materials. In this context, magnetic films can be applied in a variety of technologies such as data storage, flexible spintronics, chemical detection, and magnetic sensors.[1] Additionally, the growing prospect of obtaining environmentally eco-friendly materials has promoted the use of vegetable matrices for film synthesis, such as tannins, for example. In this work, we report the fabrication of flexible magnetic films on paper substrates by adding Ni/Ni3C nanoparticles to the tannin extract matrix of the Amazonian species Myrcea atramentífera.[2] The tannin extract solution was obtained by processing the species' bark through grinding, sieving, and water extraction for 8 hours at 70°C, followed by filtration and concentration. After this step, a tannin extract suspension containing 0.1% Ni/Ni3C was prepared by dispersion in an ultrasonic processor. The suspension was dispersed onto a paper substrate and dried at 30 °C for 10 minutes. The films were characterized by XRD, SEM, AFM, and TGA/DSC measurements. The structural and morphological results indicate the formation of continuous films with dispersed nanoparticles. Thermal analysis results suggest that the nanoparticles dispersed in the films maintain structural stability up to 350 °C. The films present macroscopic magnetic response at room temperature, which can be attributed to the presence of nanoparticles with a coercive field of 100 Oe and saturation magnetization of 26 emu/g. [3]

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Exfoliated Graphite-based Ink from Sustainable Feedstocks for Inkjet Printing of Conductive Platforms on Paper

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Printable conductive inks have been widely used for manufacturing compact and flexible electrodes using techniques such as inkjet printing. Liquid-phase exfoliation (LPE) of graphite materials in organic solvents has emerged as one of the most investigated methods for the production of printable inks due to its scalability, high yields of few-layer graphene or exfoliated graphite, and low costs of raw materials. However, exfoliated graphite dispersions with mass concentration and colloidal stability suitable for applications are typically achieved using highly toxic organic solvents with significant environmental and human risks, such as N-methyl-2-pyrrolidone (NMP)[1,2]. In this context, we have prepared an environmentally-friendly and conductive ink from renewable components and deposited this formulation by inkjet printing. Graphite powder was exfoliated in terpineol using sonication (average of 730 nm), and the conductive ink was obtained mixing the dispersion with an ethyl cellulose solution in ethanol. This conductive formulation has colloidal stability (several weeks) and mass concentration (~4 mg/mL) suitable for inkjet printing on paper substrates. The printed patterns were used as working electrodes in electrochemical sensing since they have compatible electrical resistance for such applications. Spectroscopic techniques have revealed the formation of exfoliated graphite particles, with typical thickness and distribution, and microscopies demonstrated the morphological features of exfoliated graphite deposited on the paper substrate. Electrochemical characterizations probed that the printed electrodes can be used as multifunctional platforms for electrochemical sensing applications, which has opened new perspectives for achieving more sustainable systems.

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Fabrication and characterization of ohmic contacts utilizing LIG/Zn for eco-friendly transistors applications

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Graphene, discovered in 2004, boasts unique properties essential for electronic applications. Laser-induced graphene (LIG) offers a cost-effective method for graphene production, enabling diverse electrode designs and compatibility with biodegradable substrates. Semiconductor films based on zinc nanoparticles (ZnO-NPs) provide low-temperature fabrication without substrate degradation, aligning with sustainability goals. However, ZnO forms a Schottky contact with LIG. To address this, we deposited Zn by electrodeposition onto the LIG surface to create an ohmic contact with ZnO, thereby facilitating electron transport through the channel. Our study focuses on optimizing biodegradable resistors and transistors using LIG/Zn electrodes on kraft paper substrates and ZnO semiconductors. LIG electrodes were initially engraved on 300g kraft paper using a homemade laser machine. The LIG was immersed in a 0.2M zinc acetate solution, and a 10 mA current induced zinc growth via electrodeposition (LIG/Zn). A 10% weight ZnO-NPs solution in a 1:1 water-ethanol mixture was then spray-coated onto the substrate. A drop of honey was placed on the channel region and the transfer curves were acquired, yielding an on/off ratio of approximately 1000 times for both configurations. The preliminar results show that the threshold voltage in LIG/Zn was lower than that in LIG electrode, at 1.39 V against -0.14 V, respectively. We can attribute this improvement to the presence of Zn on the LIG surface, thanks to the Ohmic contact with the ZnO. A comprehensive characterization of EGT with LIG source-drain electrodes covered with Zn by electrodeposition will be shown. This process enhances the electrode contacts by utilizing biodegradable and biocompatible materials. In summary, we have showcased eco-friendly transistors with good characteristics and parameters, thus advancing cleaner and more sustainable electronics.

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Flexible conducting material based on starch and PEDOT:PSS

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Advances in electronics have transformed modern life, and several new electronic devices are made available on the market every year. Thus, one of the most important challenges is the reduction of electronic device lifespans due to their rapid obsolescence and the constant cycle of new model launches. At the same time, bioelectronics emerges as a potential solution to these challenges, and it opens up new opportunities for electronic material application. In this research field, the combination of organic electronic materials with natural ones is promising to achieve short-lasting and biocompatible electronic devices [1].

For this reason, water and starch, both abundant resources, are chosen for manufacturing electronic materials [1]. In this work, we have synthed a starch-based conductive material with a conducting phase composed of poly(3,4-ethylenedioxythiophene): polystyrene sulfonate (PEDOT:PSS). We created starch-based gels according to the procedures described in the reference, and we used the drop casting method to produce thick films.

Through the application of this technique, we were able to make 15 ± 2 μm thick films with mechanical properties comparable to the pristine starch film and containing 20, 40, or 60% w/w of PEDOT-PSS. The resistivity (ρ) of the films ranged from 129 kΩ to 0.053 kΩ. As a result, we have presented a preliminary investigation regarding the introduction of a conductive material based on starch with potential applications in biodegradable and biocompatible electronics.

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Fully Printed ZnO-based Electrolyte-Gated Transistors Fabricated on Different Paper Substrates for Sustainable Electronics

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The pursuit of sustainable devices has unveiled new applications, mainly addressing electronic waste issues. It is crucial to fabricate devices endowed with properties such as biodegradability, particularly in areas tailored for short-life applications, where devices are discarded after use, as seen in smart packaging, for example. Printed devices represent one such niche, offering opportunities for sustainability due to their low cost and compatibility with large-area manufacturing. Our work focuses on the sustainable production of printed transistors, emphasizing substrate material. Traditional substrates like silicon and glass lack the flexibility and recyclability of alternatives like paper. To combine paper electronics proposition with low power consumption, we fabricated printed electrolyte-gated transistors (EGTs), which operate at low bias. Materials used for the EGTs consisted of water-based solutions, with carbon as electrodes, nanoparticle layer of ZnO serving as active layer, and commercial honey electrolyte. Both ZnO and carbon were deposited via screen-printing. Three different paper substrates were used: sulfite, kraft and butter paper. Several transistors were characterized via output and transfer curves, from which the main parameters were calculated along with their errors. Despite challenges associated with producing devices on paper, including impurities and surface roughness, the devices exhibited similar behavior and low error, indicating that our EGT's operation depends more on ZnO/honey than ZnO/paper interface. Other characterizations performed included evaluation of materials morphology by scanning electron microscopy, mobility and sheet resistance by Hall effect, and stability at different scan rates. Our findings evidence that our EGT can adapt to various paper surfaces and, consequently, can be printed on different types of packaging without significant performance losses.

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Impedance-Based Sensor Array for Detection of Thermotolerant Coliforms in Potable Water

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Ensuring the quality of potable water, treated water, rivers, and affluent from coliforms is imperative for public health preservation and the sustainability of aquatic ecosystems. Coliforms, specifically thermotolerant coliforms (fecal coliforms), are widely recognized as an indicator of water microbiological safety. Their presence suggests potential risks to human health, ranging from gastrointestinal disorders to more severe diseases, such as waterborne pathogen infections. Various techniques are currently employed for detecting thermotolerant coliforms, including Immunological Detection Methods (ELISA), Polymerase Chain Reaction (PCR), among others. However, these techniques require laboratory-scale equipment and trained staff for sample handling. In this study, we present a portable and user-friendly alternative for detecting thermotolerant coliforms in potable water. We developed arrays of electronic sensor units using metal oxide thin films as active layer which can be integrated to a portable impedance analyzer for field analysis. These metallic oxides include zinc Oxide (ZnO), indium zinc oxide (IZO), aluminum-doped zinc oxide (AZO), and indium tin oxide (ITO) deposited by RF magnetron sputtering. Electrical impedance measurements were performed by mimicking a medium containing Escherichia coli (E. coli), with the addition of a bacterial culture medium and an enzyme known as β-Galactosidase to mimic bacterial behavior. β-Galactosidase plays the role of simulating thermotolerant coliforms by breaking down sugars present in the culture medium. Through the analysis of impedance and capacitance spectra changes, it was possible to discriminate samples containing β-Galactosidase (simulating E. coli) from samples containing only the culture medium (without E. coli). (The authors acknowledge the financial support from FAPESP, CAPES and CNPq).

Influence of carbon allotropes on the electrospun matrix of PVDF-HFP, for application in optoelectronic devices

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Nanostructured optoelectronic devices have become, in recent years, a technology with scalable potential in both academic and commercial contexts [1], [2].This work aims to present the results obtained from various characterizations performed from the electrospinning of PVDF-HFP nanofibers, dissolved in DMF, with the addition of carbon allotropes, such as cold plasma-induced graphene (Graf) and its reduced graphene oxide derivative (rGO), in concentrations ranging from 0% (pure sample) to 5% mass of additives relative to the polymeric matrix, aiming to analyze the electrical, optical, and morphological behavior of these samples, aiming at their use in TCEs for hybrid OSCs that simultaneously exploit the piezoelectric effect of the copolymer. Thus, the samples were morphologically characterized by Scanning Electron Microscopy (SEM); structurally by Fourier Transform Infrared Spectroscopy - FTIR; in addition to electrical characterization in DC mode, which served to evaluate the quality of the produced nanofibers and the formation of the beta (β) crystalline phase. Thus, electrospun nanofibers of rGO/PVDF-HFP with an average diameter of 320 nm and 210 nm for Graf/PVDF-HFP were produced, as verified by SEM. FTIR spectra for both rGO/PVDF-HFP and Graf/PVDF-HFP samples showed a greater presence of the beta phase with increasing rGO or Graf concentration. The rGO/PVDF-HFP 5% showed an increase in electrical conductivity by one order of magnitude compared to the other concentrations, and the Graf/PVDF-HFP sample showed an increase of two orders of magnitude for the 1% concentration, with both electrical measurement results performed in triplicate.

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Inkjet-Printed Gold Electrodes on recycled PET: Characterization and Functionalization

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Rapid, sensitive, and specific detection of Salmonella serovars is crucial for ensuring food safety and animal health [1]. This study investigates the utilization of recycled PET substrates for the fabrication of electrochemical electrodes via inkjet printing, aimed at developing a point-of-care device capable of detecting three different Salmonella serovars. 2D PET substrates through extrusion were obtained and modified using O2 plasma etching to enhance surface properties for subsequent use in gold electrode printing via inkjet technology [2]. Recycled PET films were characterized for their wettability, roughness, and physicochemical properties, revealing that increased exposure time to O2 plasma etching promoved its higher surface wettability evidenced by a decrease in contact angle from 80º to 47º. Moreover, average roughness was increased, and the higher carbonyl index corresponding to band at 1720 cm-1 by FT-IR/ATR was confirmed. Preliminary results demonstrate that the physicochemical modification with O2 plasma etching could be an efficient strategy for enhancing the performance of inkjet-printed gold electrodes intended for monitoring microorganisms affecting the sanitary status of animal-derived products. This research highlights the significance of biosensor-based diagnostic devices in enabling rapid, sensitive, and specific detection of Salmonella serovars, thereby contributing to quality management of foods of animal origin. Acknowledgements:We thank São Paulo Research Foundation (FAPESP), grant numbers 2023/10811-8 and 2023/02936-5

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Laser Induced Graphene: formation of electrodes on paper for sustainable electronics applications

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The technological development stemming from silicon makes current technological production not only high-cost, but also with significant impacts on the environment, this, alternative forms of electronics tailored to specific niches are highly desirable, as instance, we can cite in this case the printed electronics applied to the Internet of Things (IoT) and smart packaging. Here we report a study of the parameters for LIG [1] formation on Kraft paper using a homemade recording system, where a diode laser (λ=450) was coupled to an automated XY positioning system. The laser power and scanning speed were adjusted to 625 mW and 11 mm/s, respectively. The induction occurred on 300 mg Kraft paper, in 12 x 12 mm patterns, 20 electrodes were produced at different heights in relation to the paper substrate, the Z positions (heights) ranged from 24,5 to 34 mm above the focal plane. After the recordings, sheet resistance measurements were made for each of the electrodes where we obtained values below 35 Ω/sq for electrodes made at the Z= 30mm. Scanning Electron Microscopy (SEM) images showed characteristic morphology of LIG formation on paper with porous, it is notable that the compaction of these pores is related to the position More uniform and filled surfaces were obtained at the Z = 34 mm position compared to the Z = 30 mm position, which open the possibility of exploring this synthesis parameter to form electrodes with specific structures.The results presented in this work include their comparative use in transistors, specifically Electrolyte-gated Transistors (EGTs) and supercapacitors, showing that for each case, there is a more appropriate method to prepare the LIG electrodes.

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Laser-Processed Electrolyte-Gated Graphene Field-Effect Transistors on Flexible Substrate: Synthesis and Characterization

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Synthesis via laser, in general, has emerged as an efficient method for producing eco-friendly devices due to its simple configuration and effective generation. Laser-Induced Graphene (LIG) can be obtained via direct conversion of substrates into graphene by photopyrolysis processes, while laser-reduced graphene oxide (LrGO) is a material resulting from the reduction of graphene oxide (GO) by laser radiation. Electrolyte-Gated Graphene Field-Effect Transistors (EGGFETs) have demonstrated significant potential in various applications, including sensors and biosensors. In this study, we present the production and characterization of EGGFETs obtained by laser processing on flexible substrates. LIG electrodes and channels containing LrGO were synthed using a homemade system employing a diode laser ($\lambda = 450$ nm) on an automated XY system. GO films with thickness of 0.28±0.05 µm were deposited via spray coating on polyimide. Subsequently, the films were reduced via laser radiation at powers ranging from 12.5 mW to 100 mW and scan speed of 5 mm/s. LIG electrodes were engraved at power of 750 mW and speed of 10 mm/s. Post-laser reduction, the LrGO films exhibited thickness reductions between 20% and 65%, with electrical conductivity of 30.74±1.76 S/m for films reduced at 25 mW. The sheet resistance of the LIG electrodes was 10.97±0.02 Ohms/sq. The transfer curves of the EGGFETs, with organic solvent as electrolyte, showed a drain-source current evolution with gate-source voltage variation, consistent with the ambipolar nature of graphene materials. Operating voltages were below 3V, with output currents in the milliampere range. Dirac potential deviations varied with the oxidation state of the films, being 1.0V for slightly reduced films and 0.5V for highly reduced films. Hole and electron mobilities obtained were $\mu h = 1.86k\ cm^2\ V^{-1}\ s^{-1}$ and $\mu e = 20.50k\ cm^2\ V^{-1}\ s^{-1}$, respectively.

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Long stability study of an EGOFET based on DNTT polymer using honey as electrolyte

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One of the advantages of using organic semiconductors (OS) is the reduced cost in relation to the inorganics, and one application front is in the area of biocompatible devices, which allows the research and development of in-loco disease diagnose [1]. Nevertheless, some characteristics of OS still need improvement, such as those related to ambient stability and degradation over time. In this work, it was studied the behavior of the transistor based on the organic molecule dinaphtho[2,3-b:2′,3′-f]thieno[3,2-b]thiophene (DNTT), in the structure Au/DNTT/honey/Au, over five weeks through electrical characterization measurements. Interdigitated source and drain gold electrodes were deposited by photolithography on a rigid glass substrate and in the sequence, the organic molecule dinaphtho[2,3-b:2′,3′-f]thieno[3,2-b]thiophene (DNTT) was deposited as the semiconductor channel. Honey was deposited on the DNTT surface using the drop-casting technique as the electrolyte, and the gate electrode used was platinum. From the characterization measurements, it was concluded that the transistor operates as an electrolyte-gated organic field effect transistor (EGOFETs), because there was no indication of ionic doping in the channel. Therefore the interaction between honey and DNTT occurred superficially, without effective penetration of the ions present in the honey into the DNTT bulk. The on/off ratio is stable throughout the measurement cycles, but decreases as the weeks go by, as does the threshold voltage and the product of mobility and capacitance. However, transconductance remained stable throughout the measurements and weeks.

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Morphological and electrical characterization of thin films of non-fullerene acceptors

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Due to the search for sustainable alternatives in energy generation and its technologies, there have been significant advances in the advancement of new photovoltaic technologies and the discovery of new materials that have great potential to revolutionize conventional electronics, due to their various applications known today, such as sensors, organic and flexible displays, transistors, and solar cells, also aiming to increase efficiency and reduce production costs. Therefore, non-fullerene acceptors (NFAs) have attracted much interest as potential replacements for fullerenes and their derivatives due to their enhanced light absorption and tunable electronic affinities.[1] Thus, these materials were studied in the form of Langmuir films and transferred to solid substrates through Langmuir-Schaefer (LS) technique, taking advantage of their amphiphilic characteristics, allowing the manufacture of organized films with controlled thickness. For sake of comparison the Drop-Casting technique was also applied to fabricate the films. The work presented through these studies involves obtaining information related to the supramolecular structure of Y6:PM6 thin organic films, using UV-Visible absorption measurements, AFM, and electrical characterization (with and without light). The main purpose is to improve the understanding of the organization of the layers and compare the electrical results obtained between films manufactured using the LS and Drop-Casting techniques under solar radiation (AM 1.5), aiming for future applications of these materials in photovoltaic devices.

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Photoelectrical characterization of fullerene-based oligomer and polythiophenes thin films

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Fullerenes and polythiophenes are materials widely used in organic electronics, due to its properties. Polythiophenes derivatives presents a relatively high electrical conductivity and great chemical stability, while fullerene derivatives are known to be great charge acceptors. Their optical and electrical properties grant these materials a great application potential in the organic electronic field. The materials used in this work were OPCBMMB, a fullerene derivative, P3HT and P3OT, both polythiophene derivatives. These were studied as blending of OPCBMMB:P3HT and OPCBMMB:P3OT. The aim of this work is to perform an optical characterization through UV-vis spectra, electrical characterization in direct current and to verify the photoconductivity of these mixed films, monitoring their electrical response when exposed to light with a solar simulator. In the UV-vis spectra of the mixed films, it is possible to see peaks corresponding to both OPCBMMB and the polythiophenes, indicating the presence of both materials in the film. The DC current characterization showed improvements in the mixed films conductivities, compared to the pristine OPCBMMB. The photoconductivity of OPCBMMB showed a low photocurrent, since fullerenes have a strong light absorption on ultraviolet wavelengths [1]. When mixed with polythiophenes, these can widely improve the electrical conductivity of OPCBMMB. The work presents a characterization of OPCBMMB, OPCBMMB:P3HT and OPCBMMB:P3OT, showing how mixed OPBMMB:P3HT and OPCBMMB:P3OT films have an improved photocurrent, with better recovery when compared with pristine samples [2].

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Printed organic devices applied as Schottky and photovoltaic diodes

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Printable organic electronics have been object of investigation being used in circuitry and devices, as printable organic solar cells (OSCs), then paving the way for the flexible electronics [1-2]. This technology uses electronic inks and offers a promising solution to circumvent limitations imposed by the traditional electronics. In addition, it provides lightweight, flexible and stretchable products, being ecofriendly. The present investigation addresses a study about two flexible organic ultrathin film diodes, which feature the PET/ITO/PEDOT:PSS/active layer/Ca-Al structure. One of them has P3HT:PC61BM as the active layer and the other PTB7-Th:PC71BM. The first showed good performance as a Schottky diode, and the second a good photovoltaic response. Therefore, being flexible electronic devices, which are easy to process at a very low cost, they are candidates as circuit components for electronic packaging: one as a diode element and the other as an energy source for the circuit.

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Production and characterization of metal oxide semiconductor thin film transistor deposited by ultrasonic spray pyrolysis

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Transistors are the foundation of modern electronics, enabling computing as we know it. They function by switching and modulating an electrical current using another electrical signal. This modulation can occur through changes in current flow (junction transistors) or potential difference (field-effect transistors). As such, research to improve transistor characteristics like mobility, flexibility, and transparency, as well as their manufacturing techniques, is highly relevant. This research includes finding more eco-friendly alternatives with the ability to cover large areas.This work analyzed the electrical characteristics of zinc oxide thin films deposited using spray pyrolysis with an ultrasonic tip. The analyzed characteristics included mobility, threshold voltage, and subthreshold swing. Physical measurements, such as film thickness, were also performed. The impact of various parameters on the deposited semiconductor was investigated using variance analysis. These parameters included the solution flow rate through the ultrasonic tip, tip movement during spraying, number of spray cycles on the substrate, and drag gas pressure.

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Project and study of the efficiency of a filament guiding device produced by 3D printing attachable to a filament winding coil

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With the increasing application and accessibility of 3D printing techniques in the fields of technology and science in recent years, there has been a growing number of articles and research in various areas and applications using this technology [1]. To explore new applications in science, new filaments are being produced in laboratories to suit specific applications, such as conductive filaments [2]. Automated and complex devices, equipped with laser or optical sensors, controlled by computerized systems are being studied and used in various filament industries to guide the filament for precise winding [3]. This study presents the design and efficiency evaluation of a device, manufactured by 3D printing, which guides the filament in its winding process. The equipment can be attached to a coil without the need for a complex or motorized system. It demonstrates satisfactory results in filament distribution. Thus, the device proves to be a useful and cost-effective equipment to support filament manufacturing processes on a small scale and in laboratory settings.

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Rheometric and mechanical characterization of polybutadiene and unusable truck tires recovered carbon black composites

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The disposal of used tires has currently reached immense worldwide proportions and its treatment still being a challenge. One alternative is the reuse of its components from the decomposition. Recovered carbon black (RCB) is one of these components that has relevant properties for applications in different areas, such as tire remanufacturing. RCB may exhibit suitable properties to act as a reinforcing filler in elastomers. This sense, this study presents the results obtained from the rheometric and mechanical characterization of polybutadiene (BR) and RCB from unusable truck tires composites. Sets of 12 samples of BR/RCB ranging from 0 to 50 phr (per hundred rubber), with increments of 10 phr between each formulation, were produced. The composites were characterized by rheometric tests (ASTM D2084) and mechanical tests, such as tensile strength (ASTM D412), hardness (ASTM D2240), and abrasion resistance (ASTM D 5963). The results obtained in the rheometry tests indicate that the curing time is inversely proportional to the amount of RCB in the formulation. Furthermore, the cross-linking densities were determined using swelling with toluene and calculating with the Flory-Rehner equation. The results showed that RCB provided reinforcement in the composites when compared to pure rubber (reference sample). It is concluded that this filler can be used as reinforcement in composites, enabling the recycling of unusable tires and mitigating environmental damage.

SENSITIVE PIEZOELECTRIC LAYER WITH ELECTROSPUN NANOFIBERS OF POLY(VINYLIDENE FLUORIDE)

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The beta phase of PVDF is known for its highly ordered and stable crystalline structure, forming a compact and uniform matrix, imparting significant piezoelectric properties, thermal stability, and mechanical strength. PVDF nanofibers produced by electrospinning exhibit a well-defined crystalline structure, predominantly in the beta phase, making them suitable for various applications in nanotechnology, electronics, and biomedicine. Electrospinning allows for the control of the morphology and orientation of the fibers, adjusting their characteristics to meet the specific , such as pressure sensors, energy harvesters, biomedical devices, etc. This study aims to enhance the effectiveness of electrical current storage and/or generation, as well as improve the sensitivity of pressure sensors. The solution was inserted into a 3.0 mL syringe within an infusion pump, with a flow rate set to 0.5 mL/h and a needle positioned at a distance of 15 cm from the collector. The solution was injected into the rotating collector at 300 rpm, maintaining the relative humidity at 70%. The concentration of PVDF and solvents was 15 wt%. The results were analyzed by SEM microscopy, observing the linearity, continuity, and thickness of the fibers. With FTIR spectra, it was possible to calculate the relative percentage of the presence of the most predominant crystalline phase, comparing the proportion between the phases of PVDF in electrospun nanofibers. XRD/XRF indicated the crystalline phases found, along with their elemental analysis. The results of DC electrical conductivity tests demonstrated the piezoelectricity.

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Slot-die printed PEDOT:PSS/graphene composite for active layers of gas sensors

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Early detection of harmful gases and vapors has become increasingly important in many fields, for national defense, monitoring environmental pollution and industrial emission, and for medical diagnosis. In addition to the importance of detection, the manufacturing process has been shown to be important in providing cost-effective routes and simplified processing. In this study, gas sensing devices were developed using slot-die printing of an electronic ink prepared by PEDOT:PSS/graphene dispersion. The sensors were analyzed for the detection of ethanol, carbon dioxide and nitric oxide and were manufactured on glass substrates with prefabricated electrodes. Different proportions of the nanocomposite were studied and characterized by scanning electron microscopy, UV-visible spectrometer and Raman characterizations that confirm the presence of graphene in the PEDOT:PSS polymer matrix. It was revealed that the mixture between the materials presents high uniformity and that the synergistic behavior between the materials allowed high sensitivity and repeatability for gases at room temperature.

Study and characterization of the use of rGO in the manufacture of films for the development of a photovoltaic cell

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The purpose of the work is based on the study of semiconductor polymers regarding their electrical and mechanical properties that allowed the development of films for the production of photovoltaic cells, more specifically from the use of components such as reduced graphene oxide (rGO), PEDOT:PSS, FTO adhered on glass substrates and the polymers P3HT and PCBM, which form the synthesis of the samples. The main objective was to look for ways to characterize films of a solar cell in a practical and low-cost way, using few components, considering the current data and advances that the research insertion area of these materials presents, mainly due to the searches for energy sources sustainability that increase every day. The syntheses of the samples were the basis of the entire study and involved knowledge of chemistry and physics for the preparation of films, in addition to techniques for deposition of solutions and spreading by spin-coating. The blend of the polymeric films was analyzed by optical absorption in the spectral range of ultraviolet-visible (UV-Vis) and photoluminescence (PL) and emission ellipsometry (EE) as a function of sample temperature. The surface morphology of the films was studied by atomic force microscopy (AFM). Such techniques are considered low cost and production simplicity. We observed a high degree of polarized emission of the P3HT films, which varies subtly according to the temperature. For blends with RGO, emission's polarization degree decreases and the surface's roughness increases. As a result, the RGO improves the energy transfer between adjacent polymer chains at the cost of greater surface roughness.

Study of an Impedimetric Immunosensor Based on the Sensorial Platform of Poly(o-phenylenediamine)-AuNPs and 5-methylCytosine Antibody

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Recently new electrochemical methodologies for detecting the methylation of nitrogenous bases have been developed, due to the relation between methylated DNA and cancer. The electrochemical impedance spectroscopy (EIS) technique stands out as a transduction model for immunosensors due to its high sensitivity to interfacial changes, reaching detection limits on the picomole scale. In most cases, ferrocene is used as a redox probe to increase the signal of the antibody and antigen interactions, however, the excess of these redox species can cause problems associated with false-positive sensor responses. This work is an alternative methodology for an electrochemical immunosensor, based on a single-step sensory platform of poly(o-phenylenediamine)-AuNPs, to determine the global levels of 5-methylcytosine (5-mC), utilizing dissolved oxygen as a redox probe. The immunosensor was developed by immobilizing the 5-mC antibody to the surface of the modified electrode. No secondary antibody was used. The platform performance was evaluated by EIS in different concentrations of 5-mC in a PBS solution containing atmospheric oxygen. The EIS reveled that the presence of dissolved oxygen decreased the Rct value, and the system impedance increased with the addition of 5-mC in solution as a function of increasing antigen-antibody binding, hindering the permeation of molecular oxygen to the redox sites of the polymer.

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Study of different configurations of ion-gel transistors and neuromorphic applications.

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The integration of biological synapse principles into electronic devices is pivotal for advancing neuromorphic engineering and artificial neural networks. Metal-oxide transistor-based artificial synapses offer compelling advantages such as biocompatibility, cost-effectiveness, compatibility with flexible substrates [1]. In this study, we demonstrate solvent-free, freestanding ion gels based on poly (vinylidene fluoride- co -hexafluoropropylene), P(VDF-HFP), [and the ionic liquid 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl) amide, [EMI][TFSA] [2]. These ion gels serve as high capacitance gate dielectrics for transistor-gating experiments. Electrolyte gated field-effect transistors (FETs) were used with artificial synapses. The active layer of the transistor consists of Zinc Oxide (ZnO) [3], a material known for extensively researched due to its low toxicity, biocompatibility, and biodegradability. Additionally, we conduct a comprehensive investigation into the interface doping processes of electrolyte ions between the active ZnO layer and ion gels to elucidate the conductivity mechanisms and variations in excitatory postsynaptic current (EPSC) in organic synaptic devices. Furthermore, the difference in the electrical properties of transistors in relation to their structure was studied. The structures studied were top-gate/top-contact and top-gate/bottom-contact.

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Study of the Preparation of an Impedimetric Device for Detection of Troponin

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Immunosensors based on electrochemical impedance spectroscopy (EIS) stands out significantly in the research field, primarily due to the high sensitivity, capable of reaching picomole scale detection limits. A redox probe is used to increase the signal-to-noise response for antigen-antibody interactions on the electrode surface. This study proposes an alternative methodology using dissolved oxygen as a redox probe for the detection of global levels of troponin. The oxygen-sensitive response is possible due to the presence of the redox-conducting polymer based on gold nanoparticles (AuNPs) encapsulated in poly(Bismarck Brown Y) (poly(BBY)) and reduced graphene oxide (rGO). The device was synthed using a one-step electropolymerization technique with an aqueous solution containing BBY monomer, hydrogen tetrachloroaurate(III), and rGO. The immunosensor was developed by immobilizing a primary anti-cTnT antibody on the surface of the device coated with poly(BBY)-AuNPs/rGO. The performance of the immunosensor was evaluated by EIS at different concentrations of troponin in PBS containing atmospheric oxygen.

The voltammograms show an increase in current amplitude at the electropolymerization process for AuNPs and rGO. The poly(BBY)/rGO film shows an increase in the specific capacitance, compared to poly(BBY). EIS reveals that the presence of dissolved oxygen in the platform leads to a decrease in the values of charge transfer resistance, meaning that oxygen facilitates charge transfer.

Study of the remediation of water contaminated with dyes by adsorption on thermoplastic starch and kraft lignin composites

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Disposing of industrial effluent containing dyes has become an important environmental and public health issue. To remove these dyes from effluents, adsorption is an effective technique. Thermoplastic starch (TPS) and kraft lignin (KL) composites are potential bioadsorbents for dye removal, as they can be obtained from renewable and low-cost raw materials. This study prepared TPS and TPS-KL composite films to adsorb methylene blue (MB) and methyl orange (MO) dyes. The adsorption and desorption results of the dyes in the films were obtained by ultraviolet-visible spectroscopy (UV-vis). The films were characterized by Scanning Electron Microscopy (SEM), Fourier Transform Infrared Spectroscopy (FTIR), solubility, and thickness before and after interacting with the dyes. The desorbed dye solutions were photodegraded at 12-minute intervals and analyzed using UV-Vis to monitor the remediation of the dyes in solution by light. The results obtained from the experiment show that TPS-KL has a high removal potential (~95%) for MB, with a maximum adsorption capacity of 175 mg g^{-1}, but a low removal potential (~22%) for MO, with a maximum adsorption capacity of 40 mg g^{-1}, proving its efficiency for use in effluent treatment. Remediation studies using photodegradation to treat water contaminated with dyes have shown promising results in terms of light degradation efficiency, with almost complete elimination of the dye. In addition, adsorption, desorption, and photodegradation kinetics are proposed for both dyes. Therefore, the studied processes have proven to be viable and less harmful to the environment, as they use low-cost materials and techniques without generating polluting waste. They are effective in removing, recovering, and eliminating dyes from textile effluents.

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Sustainable Solutions for Energy Harvesting: Evaluation of Piezo-Photovoltaic Hybrid Devices based on P3HT:PCBM:PVDF

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Recently, we have witnessed a growing awareness of the crucial importance of preserving our planet, driven by an increasingly clear understanding of the intrinsic relationship between socio-economic development and environmental sustainability [1]. In this context, there has been a significant emphasis on the demand for innovative systems that integrate sensors and actuators, particularly for efficient energy capture. A particularly promising approach is the utilization of hybrid devices, which combine materials to optimize the efficiency in capturing both solar and mechanical energy, proving valuable in conditions of limited sunlight, such as rainy days or nighttime. Polymer-based hybrid materials offer a range of advantages, including flexibility, lightweight, and reduced production costs, enabling energy generation from renewable natural sources. [2]. Mixed piezo-photovoltaic devices have been successfully developed, utilizing PVDF for mechanical energy harvesting and P3HT:PCBM for photovoltaic harvesting. These layers were fabricated using electrospinning and the Langmuir-Schaefer techniques and characterized by scanning electron microscopy (SEM), FTIR spectroscopy, and electrical DC measurements.

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Sustainable Synaptic Devices: EGOFETs and Biodegradable Photoresistors with Perylene Derivatives

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Flexible electronics based on natural or degradable materials are a key requirement for the next generation of electronic devices, where sustainability, biodegradability, resource efficiency, and high performance are essential [1]. In this context, optimizing their molecular chemical structures, four different perylene derivatives were utilized as the active layer and their performance to compared. Through electrical and optical characterization, we demonstrated that the addition of a second chain of four carbons at the imide position reduces intermolecular interaction in the active layer electronic devices leading to the non-functionality of the electronic devices. This enabled us to identify the perylene with the best performance and utilize it in the fabrication of Electrolyte-Gated Organic Field-Effect Transistors (EGOFETs) and biodegradable photoresistors for applications as electronic synapse devices. Our results demonstrate that both devices exhibit behaviors characteristic of optical synapse devices, responding to optical stimulation across various visible wavelengths (465 nm, 527 nm, and 665 nm). Additionally, we demonstrate that the EGOFET exhibited superior performance in terms of PPF Index (%) and EPSC current compared to the biodegradable photoresistors. Despite that, it's important to note that the biodegradable photoresistors were fabricated on a flexible substrate (paper), whereas the EGOFETs were fabricated on glass. Therefore, in addition to presenting tools for investigating the most suitable chemical structure for the fabrication of electronic devices, this work also demonstrates the successful fabrication of EGOFETs and biodegradable photoresistors as optical synapse devices.

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Transient Current Analysis of Honey-Gated Transistor and its application as neuromorphic device

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Electrolyte-gated transistor based on honey as electrolyte has already been presented in the literature as a device with potential to be applied as a sustainable device or as a sensor or biosensor [1,2]. This device is named as honey-gated transistor (HGT) and its modulation occurs by field effect, not showing modulation by ionic doping. Even operating as an electrolyte-gated field effect transistor, the response that the HGT output current presents is not an instantaneous response to the voltage applied to the gate. However, it presents a transient current which means that HGTs can operate out of the steady state, bringing another potential application, as a neuromorphic device. The developed HGTs have the following structure: gold source, drain and gate in-plane electrodes, poly(3-hexylthiophene-2,5diyl) (P3HT) channel and honey from *Apis-Mellifera* bees as electrolyte. The analysis was on the transient curve that uses squares waves (pulsed) gate voltage with a constant drain voltage, collecting the transient output current along the time ($I_{DS}(t)$). The $I_{DS}(t)$ curve depicts an exponential increases profile followed by a decrease that is similar to a parabolic profile. Different pulse frequency ranges, between 10Hz and 0.2Hz were tested, obtaining distinct output states equivalent to mimic different synapses of neurons. These results bring a new potential application of HGT not explored before: as a neuromorphic device.

Acknowledgments:
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Transparent glass defoggers: an example of scientific investigation leading to a spin-off in printed electronics field

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It is widely acknowledged the field of printed electronics research began with the synthesis of conductive polymers[1]. However, silver pastes have been introduced and applied in industrial processes much earlier. Amongst several applications, the use of silver pastes for glass defogger fabrication is still one of the most important. An alternative method for fabricating defoggers is to employ metal oxides [2]. However, this technology is not suitable for non-flat glasses. Thus, we have introduced a new technology for transparent defoggers fabrication from research activities pushed by scientific motivation. Although this start point usually results in non-commercial technologies, we have obtained a spinoff as the main result. The technological materialization as patent was a key factor in allowing interaction with the industry. This instrument has allowed us to perform patent license and research and technology agreements with industry. Collaboration with industry was the second key factor, allowing knowledge sharing, market-referenced research, access to private and governmental funding, and improving students's skills toward scientific entrepreneurship. As a result of this collaborative and multidisciplinary environment, students have created a spinoff, assessed FAPESP founding, and are performing research and development activities autonomously. In summary, we aim to share experiences with conference participants in the innovation field, to show the developed technology, as well as some technical and scientific results obtained.

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Utilization of Electrolyte-Gated Transistor Based on Honey Electrolyte Anchored in a Paper Matrix for Sensor Applications

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Honey-gated transistor (HGT) is new class of electrolyte-gated transistor which exploits the potential of honey as an electrolytic layer, showing superior performance when compared to traditional aqueous electrolyte [1]. However, in this work, we aimed to better characterize, to investigate the working principle of HGT to use as a sensor. The transistor structure consists of a gold source, drain and gate in-plane electrodes; poly(3-hexylthiophene-2,5diyl) (P3HT) channel, and honey as electrolyte. The honey was anchored in a bond paper matrix for ease of handling and control of the area. To test its potential as a sensor, lithium perchlorate (LiClO4) salt was used in a blend with honey. Performing the transfer and output curves, the HGT operates in two distinct modes into the gate voltage range of (+2.0V to -2.0V): (i) as an Electrolyte-Gated Organic Field Effect Transistors (EGOFETs), modulated by the field effect when the electrolyte is only honey; (ii) or as Organic Electrochemical Transistors (OECTs), where ions migrate into the channel leading to ionic doping when the electrolyte is a blend of honey with LiClO4. This distinction is also quantified through parameters extracted from the electrical characterization such as transconductance as well as the threshold shift of the cyclic transfer curves. Another novelty presented in this work was the proposal to use a bond paper to anchor the honey, which caused minimal changes in HGT operating modes compared to situations without an anchoring matrix. These findings highlight the potential of HGTs as versatile sensing and biosensing platforms, taking advantage of honey's biocompatibility, antifungal and antibacterial properties.

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Electrochemical paper-based devices functionalized with polydopamine for sensing applications

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Electrochemical paper-based analytical devices represent an important platform for low-cost, portable, affordable, and decentralized diagnostics [1]. Among the different electrode materials, carbon is one of the most used due to its low cost, high chemical stability, large availability, and excellent conductivity. In addition, carbon-based electrodes can be patterned on paper by many different routes. For applications in the sensing field, chemical functionalization plays a pivotal role to ensure high clinical performance by tuning surface properties of the electrodes. In this talk I´ll show some key features of the chemical functionalization of polydopamine (PDA) on carbon electrodes for sensing applications. The polymerization occurs in mild conditions in the presence of dopamine resulting in the formation of simple, biocompatible, and versatile PDA coatings. The film thickness of PDA from nanometer to micrometer scale can be controlled with the proper choice of the reaction time, allowing the preparation of hydrophilic electrodes and immobilization of redox mediators [2]. The later is responsible for detecting nicotinamide adenine dinucleotide (NADH) at low potential in the µM-mM range. In addition, PDA introduces catechol/quinone redox moieties than can be explored in the field of sensors to decrease the overpotential necessary to detect NADH [3]. Finally, the preparation of Au nanoparticles with tunable using PDA will be shown, which is a promising platform for the fabrication of electrochemical biosensors [4].

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Expanding the applications of reduced graphene oxide/polymer based flexible devices

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Carbon and polymers are commonly combined to make structures for biocompatible electronic devices including epidermal electronics. These materials allow creating flexible and chemically stable structures. However, any devices require making well-defined geometrical patterns and providing different material properties that is a big fabrication challenge.

We explore laser processing as an approach to locally create carbon/polymer composite. For that, graphene oxide (GO) dispersion is deposited on the polymer substrate and irradiated with a microsecond pulsed laser. We discuss the mechanism of GO reduction using visible wavelength irradiation. Depending on the laser scanning parameters, we can observe reduced GO (rGO) formation, rGO/polymer intermixing, polymer destruction, and carbonization [1]. Moreover, thanks to the use of laser processing approaches, it is possible to ‘draw’ arbitrary patterns and fabricate a range of devices. This method allows us to create mechanically robust conductive structures working as electrochemical electrodes [2], resistors, capacitive and inductive components. We also discuss the prospects for developing basic logic components - diodes and transistors - using laser fabrication approaches.

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Nanoscale Electrical Characterization of Organic and Hybrid Materials for Energy Applications

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The recent development of alternative sources of energy to fossil ones will play a crucial role in global electricity generation and should be one of the global strategies to reduce CO2 emissions and stop climate change. Organic and organic/inorganic hybrid semiconductors are nowadays applied in a plethora of devices such as thin-film transistors, sensors, light-emitting diodes, thermoelectric generators, photodetectors, and solar cells due to their ease of processing, their lightweight, and their favorable mechanical properties. The dramatic increase in the performance observed for many devices, especially for third-generation photovoltaics based on solution-processable semiconductors, renders them attractive alternative solutions for sustainable energy production in the near future — especially where lightweight, semitransparency and large-area applications are required.

To develop efficient and competitive modern electronics from semiconducting (organic, inorganic, or hybrid) materials for energy conversion and storage (flexible) devices, it is essential to understand the relationships between molecular architecture, supramolecular organization, microscopic morphologies, and optoelectronic properties in detail.
By using AFM-derived techniques (such as Conducting AFM, Kelvin Probe Force Microscopy – KPFM, and Scanning Microwave Impedance Microscopy - sMIM), electrical properties can be measured at the local scale (together with the morphological and mechanical characterization of the samples) helping the optimization of the device performances. For instance, for photovoltaic organic devices, we can spatially resolve by KPFM the surface photo-voltage in high efficiency nanoscale phase segregated photovoltaic blends of conjugated polymers. We show on poly(thiophene)-based organic and hybrid systems how the lateral resolution in KPFM and in photo(conducting) AFM can allow a direct visualization of the carrier generation at the donor-acceptor interfaces and their transport through the percolation pathways in the nanometer range.

Organic solar cells (OSCs): energy transfer and exciton dissociation studies

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he combination of conjugated polymers, oxides and carbon nanostructures can be an interesting way of organizing the nanostruture of thin films and develop new optoelectrical properties. The development of electronic devices based on thin films as electrodes or active layers offers some processing advantages and new possibilities in the manufacture of these devices, such as flexibility and large areas. The use of Organic semiconductors for photovoltaic devices presents advantages in processing and on the development of light and flexible devices, using techniques commonly used in the production of large areas, such as spray coating, roll to roll and jet printing ink. The nanostructure matters to efficient organic solar cells (OSCs) due to the compromise a bulk heterojunction (BHJ) formed by electron donor (D) and acceptor (A) components so that excitons created either at the D phase or A phase can efficiently quench at the D/A interface. For a system with optimized charge transport and extraction, the OSC efficiency is essentially determined by the dissociation of those excitons at the heterojunction. In this work, some examples of these studies on the combination of organic materials in thin films will be presented in the fabrication of photovoltaic devices obtained by simple mixture in a common solvent; generated by interfacial synthesis; and by mini emulsion technique. Using simple mixture, it was possible to study devices from green solvent and in a ternary composition in order to rise the photon extracted number and consequently the power conversion efficiency. The interfacial synthesis allows us to obtain new approach to nanostructure the films, thus obtain new optoelectronics properties and the mini emulsion technique allows organic semiconductor nanoparticles synthesis being dispersed in aqueous medium offering the prospect of overcoming the use of chlorinated, inflammable and toxic solvents from the manufacturing process of the devices.

The avenue to “Green” in Organic Bioelectronics

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Through its appealing avenues of processing the component devices at room temperature and from low-cost precursor materials, organic electronics has a tremendous potential for the development of products able to achieve the goals of production sustainability as well as environmental and human friendliness for electronics.

In an effort to stave off the e-waste growth, the presenter and his research group went further down the path opened by organic electronics research and investigated a large number of biomaterials as substrates, dielectrics, semiconductors and smoothening layers for the fabrication of organic field effect transistors, integrated circuits and organic solar cells. The presentation will focus on the highlights of our recent research, especially with respect to materials investigated, devices fabricated and the immense potential for follow up research: (1) flexible natural and biodegradable substrates; (2) natural dielectrics; (3) bio-origin, H-bonded semiconductors in the families of indigos, anthraquinones and acridones; (4) bio-degradation protocols for organic semiconductors.

These highlights will be placed in the context of the mountain that one has to climb in order to reach the coveted “green” connotation for electronics, sensors and integrated circuits: (1) biocompatibility issue; (2) biodegradability issue; (3) compostability issue; (4) cost of production / energy expanded in production issue; (5) materials choice issue (carbon foot print); (6) toxicity and the environmental impact of the synthetic avenue for component materials.

The potential of follow-up research in the green electronics field is immense, with large area electronics fabrication, biomedical implants, bio-sensing and smart labeling, representing only the tip of the iceberg of many more immediate possibilities of high interest for our group. Natural and nature-inspired materials have the unrivalled capability to create “safe-first” electronic markets for human and environment.

When supramolecular electronics meets 2D materials: taming functional complexity

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The development of multifunctional devices capable to respond to multiple and independent stimuli is one among the grand challenges in hybrid electronics. The combination of multiple components, with each one imparting a specific function to the ensemble, represents a viable approach to confer a multifunctional nature to electronic devices. The controlled combination of such components and their integration in real devices can be accomplished by exploiting the supramolecular approach.

In my lecture I will review our recent works on the combination of low-dimensional nanomaterials, with a special focus on 2D materials, with photochromic molecules (diarylethenes or azobenzenes), in order to fabricate smart, high-performance and light-sensitive (opto)electronic devices such as field-effect transistors and light-emitting transistors and as well as flexible 11-bit non-volatile optical memory thin-film transistor device.

Analysis of electrical transients for enhanced solar cell technologies: a comparative study of PM6:Y6 and polycrystalline silicon solar cells

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This study builds upon the previous work by Cunha et al. [1], which presented a novel method for analyzing the electrical transients in the fourth quadrant of organic photovoltaics based on PTB7-Th:PC71BM active layer blends. This method employs transient electrical measurements along the current-voltage (J-V) curves, via variable load resistance (RL) and variable illumination intensity. By analyzing decay time (τ) across RL variations, this method offers novel insights into charge extraction and recombination dynamics. Our research extends this analytical framework to high efficiency non-fullerene organic solar cells based on PM6:Y6 blends and compares them with the behavior of polycrystalline silicon solar cells. Our findings reveal that while both technologies benefit from the detailed transient analysis, the dynamics of charge carrier behavior exhibit notable differences. In PM6:Y6 based cells, the decay time vs RL shows a similar behavior to the one reported in [1], while for the silicon solar cells, a different behavior is noted in the region related to recombination process, showing the different dynamic processes in both technologies. In this way, extending electrical transient analysis to PM6:Y6 and polycrystalline silicon solar cells, our study not only confirms the universal effectiveness of the method for these advanced photovoltaic technologies, but also highlights opportunities for solar cell design and optimization. This analysis underscores the unique charge carrier dynamics in each technology, emphasizing the technique's flexibility and relevance for future photovoltaic advancements.

Acknowledgements

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Analysis of the transient current regime on the transfer curves of electrolyte-gated transistors

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Electrolyte-gated transistors (EGTs) present a conductivity dependent on a mixed ionic–electronic contribution. EGTs can operate as electrolyte-gated field effect transistors (EGFET) or organic electrochemical transistor (OECT). In both, it is important to analyze the transient current, which is the variation of the output current along the time for a constant voltage on the gate and the drain. However, even knowing this dependence, many works do not take into account the reasons that generate the transient current when the measurements taken are the typical transfer and output curves. In this present work it was performed an experimental e a theoretical work to analyze the dependence of the transient current on the transfer curve. The EGT structure is composed of Indium-tin-oxide (ITO) interdigitated electrodes to form the source and drain; poly(3-hexylthiophene-2,5diyl) (P3HT) as the channel; an ion gel film as electrolyte composed by (P(VDF-HFP) and the ionic liquid [EMIM][TFSI]) and Au foil as gate [1]. Depending on the gate voltage range this EGT operates as EGOFET or OECT. Transfer curves were performed under different scan rates resulting in different intensities of the on-state current and hysteresis width for OECTs. Just as the transient current is usually fitted by an equivalent RC circuit, this behavior was extended to a theoretical model to simulate the transfer curve. The most relevant conclusion is that there is an effective gate voltage ($V_{G,eff}$) acting on the EGT that is not necessarily, nor instantly, the same gate voltage (V_G) value applied to the source meter, but rather, presents an exponential dependence with time until reaching the value of V_G applied on the source meter. This work shows how dependent the EGTs performance can be on the chosen scan rate.

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A unique Correlative Microscopy Platform for Combined Nanoscale Analysis by Combination of AFM and SEM

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We describe the first truly correlative AFM-SEM (Atomic Force Microscopy - Scanning Electron Microscopy) microscopy platform designed from first principles and from the ground up for the study of sample properties under a wide range of magnifications [1-2]. Combining these two microscopy techniques, “in-situ,” into a highly integrated workstation opens unprecedented measurement capabilities at the nanoscale while simplifying experiment workflows to yield a higher level of data throughput. Unlike SEMs, the AFM offers not only true three-dimensional topography images, something SEMs can only provide indirectly, but also allows for the characterization of nano-mechanical properties, as well as for magnetic and electrical characterization of samples which increasingly are of interest in material science, multi-component technologies (i.e., solar cell and battery research), and pharmaceutical investigations. On the other hand, the SEM’s wide field of view is critical in identifying regions of interest with features of less than a micron, which are notoriously difficult to find over large spatial scales in conventional AFM systems. In addition, the SEM’s ability to visualize the AFM tip facilitates its navigation to aid the characterization of samples with challenging three-dimensional topologies. In this paper we describe the major elements of the system design and demonstrate how correlative microscopy can help the characterization of samples of challenging morphologies such as the edge of a razor blade or the nanomechanical analysis of platinum nanopillars.

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Biaryl-dicyanopyridines associating TICT and AIEE: Synthesis, photophysical characterization and application in voltage-dependent blue OLEDs

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Pyridylcarbodinitrile derivatives (PPC) displaying aryl, biaryl, and dimethylfluorenyl groups were synthed. In solution, these compounds exhibit blue to green fluorescence with quantum yields (φ_f) up to 0.70. Large Stokes shifts (153-221 nm), along with significant rotational freedom of the rings and DFT data, indicate twisted intramolecular charge transfer (TICT) excited states [1]. The PPC derivative with dimethylmethoxyaryl substitution (MT-PPC) exhibited distinctive emissive properties, featuring a dual emission max. that is environment-dependent. The band associated with the lower energy transition is favored in less polar solvents, while the higher energy band is more pronounced in highly polar solvents. Additionally, this compound exhibits aggregation-induced enhanced emission (AIEE) [2], with a 15-fold φf enhancement upon aggregation, related to a single-maximum emission around 475 nm, whose profile is very similar to those observed for MT-PPC as a pure thin film (470 nm). However, in SF3PO MT-PPC-doped films, the emission is dependent on the dopant percentage. Films with 5% and 10% MT-PPC exhibit blue-shifted emission (433 and 436 nm) compared to the 20% film (445 nm), and especially compared to the pure film. Interestingly, OLEDs with the same doped films also present environment-dependent behavior, with similar trends regarding the derivative maximum. OLEDs with 5% and 10% show emission maxima at 437 nm, while the OLED with 20% of MT-PPC exhibits electroluminescence max. at 463 nm. These changes shift the CIE chromaticity coordinates from (0.1837, 0.1475) to (0.1768, 0.2148), demonstrating that the emissive properties of MT-PPC are tunable in solution, thin films, and OLEDs.

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CARBON COUNTER-ELECTRODE BASED ON ADVANCED CONDUCTIVE POLYMER COMPOSITE FOR SOLAR CELLS

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Noble metals such as Au and Ag are the most commonly applied counter electrode materials in perovskite solar cells. However, these materials are expensive and not beneficial to commercial applications [1]. Carbon, with a close work function (−5 eV) to silver (−5.1 eV) is mostly known as a cheap and accessible element and was first used in dye-sensitized solar cells [2]. Notably, carbon materials' strong hydrophobicity and chemical inertness can significantly improve the stability of Perovskite Solar Cells (PVKs). In this work, polymer composite carbon paste electrode (CPE) is developed using Ethyl cellulose and Chlorobenzene as the polymer matrix (PM), graphite and Carbon Black as conductive fillers (CF), obtaining an optimum proportion of components, viscosity and the best processability method. One of the challenges comes from the micro fillers, due to the high surface energy and higher reactivity, they tend to agglomerate. Particle size by DLS measurements showed that the best deagglomeration system was using an ultrasonic microprobe of 125W, with a tenfold decrease of aggregate diameter. The effect of CF/PM proportion on the composite film conductivity was evaluated by four-point probe method, exhibiting a sheet resistivity of 14Ω□, 20Ω□ and 34Ω□ for a 3:1, 6:1 and 12:1 fraction, respectively. Furthermore, measurements of the membrane thickness, percolation threshold and SEM transection were conducted. CsPbBr3 as a stable perovskite composition, had been used to evaluate produced material as a counter electrode. Results are promising, highlighting the obtainment of an optimized low-cost carbon paste, which ally properties of ease processing and use, conductivity and potential for photovoltaic application.

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Design, characterization and evaluation of organic thin film transistors for use in electronic noses

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In this study, a bottom-gate/bottom-contact organic thin-film transistor (OTFT) was developed using organic dielectric and semiconductor films for isoborneol (IB) detection in water. This research presents a novel approach as OTFTs on glass with poly(4-vinylphenol) (PVP) dielectric and poly(2,5–bis(3–tetradecyl–thiophen–2–yl)thieno[3,2–b]thiophene) (PBTTT-C14) semiconductor films have not been demonstrated previously for IB detection. The OTFTs were on glass substrate with Ni:Cr/Au films as electrodes. PVP and PBTTT-C14 solutions were prepared and deposited by spin coating. Subsequent thermal treatment favored terrace formation. Comprehensive studies including UV-vis [1], Raman [2], FTIR spectroscopy, AFM [1], profilometry, and XRD [1, 2] were conducted on the organic films. Results pointed to the cross-linking of PVP, such as from peaks in the FTIR spectrum. PBTTT-C14 exhibited well-arranged molecular structure with terrace formation as evidenced by UV-vis absorbance peaks. XRD data revealed enhanced crystallinity (d = 2.1 nm) in PBTTT-C14 films [3]. Thin-films of PVP:PMF at 1:5 ratio displayed a dielectric constant of 5.29 and minimal leakage current. OTFTs with PBTTT-C14 showed favorable characteristics, including charge carrier mobility of $\sim 10^{-4} cm^2/Vs$ and a threshold voltage of 1 V. Gas sensor devices exhibited significant response ($\Delta\mu$ in triode ~ 5%) to IB, with sensitivity up to 0.2% per ppm [3]. For a concentration of 10 ppm of geosmin in methanol, a variation of 5.5 kΩ was observed for chemical sensors.

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Detailed analysis of an organic solar cell from an analytical Photocurrent Model including Second-Order Recombination

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A developed analytical model for the photocurrent (Jph) of organic solar cells by considering a second-order charge recombination [1], having as parameter a figure of merit θo, provided analysis of important device parameters. The entity θo gives a quantitative ratio between the extraction of charge carrier and the bimolecular recombination. From the obtained Jph mathematical expression, it was extracted the fill-factor and α dependence on θo: FF vs θo and α vs θo; α being the exponent of short-circuit current and the lighting intensity (Jsc vs Iα). A correlation between the reduction factor of Langevin recombination (ζ) and the dissociation probability of charge transfer states (P) is also discussed. Experimental photocurrent curves, from an ITO/PEDOT:PSS/P3HT:PC61BM/Ca/Al device, carried out at different temperatures (100–300 K), are fitted by the model, showing that the fitting parameters are in agreement with those of exhibited by the literature.

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Enhancing Methanol Detection Using Graphene Oxide and PEDOT-Based Conductive Polymer Composites: Experimental and Theoretical Insights

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This study explores the optimization of methanol detection using graphene oxide (GO) and PEDOT:PSS conductive polymer composites. Through precise adjustments of GO and PEDOT:PSS proportions, a significant reduction in electrical resistivity is observed, enhancing the suitability of these materials as electrodes in organic devices. The electrical and morphological properties of commercial PEDOT:PSS and chemically synthed aqueous PEDOT ink when combined with GO are investigated. Furthermore, the application of these conductive inks as active layers in flexible methanol sensing devices is explored. The GO:PEDOT:PSS 78% composite achieves a resistivity minimum, while the highest methanol response is attained with GO:PEDOT:PSS 68%. To theoretically underpin these findings and understand the interaction between gases/vapors and nanostructured materials, a model based on Kirchhoff’s Circuit approach is developed. By calculating the equivalent resistivity and response of the systems, confirmation is provided that the positions of minimum and maximum points align with experimental data [1]. Additionally, the influence of PSS in the samples is examined, revealing diverse interaction mechanisms between methanol molecules and the active layer, resulting in varied signals during exposure to alcoholic vapor. The theoretical model is subsequently applied to these systems, demonstrating qualitative and quantitative agreement with experimental results. Furthermore, Density Functional Theory (DFT) is applied to observe the inversion signal during the interaction between active layers with and without PSS. This research contributes to the fundamental understanding of detection processes and paves the way for the development of more efficient devices in this context.

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Evaluating deposition methods on structure-property relationship of polyaniline thin films: implications on pH chemical sensors

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Conducting polymers (CPs), as polyaniline (PANI), polypyrrole (PPY), polythiophene (PTH), have a conjugated structure giving them unique properties advantageous for technological applications. CPs find utility in chemical and biochemical sensors due to reversible chemical, electrochemical and physical properties during doping/de-doping processes [1]. Optical, electrochemical, and piezoelectric transducer platforms are widely used with PANI thin films. We have been studying the correlation between the figures of merit of pH chemical sensors and the structure–property relationship of PANI thin films [2]. The assemble of PANI is crucial for its sensing properties and the effect of the deposition method was evaluated. Spin-coated, drop-coated, and electrodeposited PANI thin films were characterized in their morphology, roughness, optical spectroscopy, and electrochemical response to understand their structure-property relationship. The samples were applied in potentiometric and optical pH sensors and their sensitivity and linearity were analyzed in view of the deposition method. The sensor's parameters presented dependency with the morphology, oxidation state and protonation level. The spin-coated set of films presented average sensitivity of 59.2 ± 2.5 mV/pH, approximately the Nernst sensitivity. It is interesting to note the supernernstian sensitivity of the samples electrodeposited (averaging 73.4 ± 1.3 mV/pH) and drop-coated (maximum of 126 ± 7 mV/pH) samples. Meanwhile, the optical sensitivity increased from 0.09 ± 0.01 up to 0.36 ± 0.01 pH-1 by controlling samples' structure. The results presented may open new possibilities for advancing sensing devices.

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Exploiting the Synergy Between Molecularly Imprinted Polymers, Electrolytic Transistors, and Machine Learning Towards Sensing of Small Analyte Molecules

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The development of Point-of-care (PoC) devices is crucial for achieving rapid and cost-effective diagnoses. However, the detection process can be challenging for some biomarkers, which are small molecules found in complex body fluids, often present in low concentrations. In this work, we introduce a novel approach that combines molecularly imprinted polymers (MIPs), electrolyte-gated transistors (EGTs) based on reduced graphene oxide (rGO), and machine learning (ML) to detect hippuric acid (HA) in artificial urine. HA is a metabolite present in the urine of healthy individuals, but it also serves as a marker for various diseases such as kidney and intestinal inflammation[1].

EGTs offer a promising alternative for HA detection due to their ability to operate in aqueous environments and at low voltages (<1V). Here, rGO was chosen as the active layer for EGT because of its ambipolar operation and high conductivity. The gate electrode was modified with MIP specifically designed to selectively recognize HA molecules, ensuring selectivity even in complex media. We employed machine learning techniques to facilitate multivariate analysis during HA detection. The developed device has advantageous features, including low operating voltages (<0.5V) and rapid response times (≤10s), along with its ability to operate across a wide range of HA concentrations (from 0.05 to 200 nmol/L). Additionally, it demonstrated a remarkably low limit of detection (LoD) of 39 pmol/L. The application of ML multivariate analysis enables a substantial enhancement in device sensitivity (1.007 μA/nmolL−1) compared to conventional human data analysis (0.388 μA/nmolL−1).

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Exploring the Electronic Properties of Strain-Engineered Biphenylene-Based Structures via DFT Analysis

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In 1941, W. C. Lothrop proposed a novel organic compound, the biphenylene molecule, composed of two six-membered aromatic rings separated by a four-membered ring [1]. Connecting two of these molecules with one another causes the formation of carbon octagons between them, resulting in a Biphenylene Network (BPN). Recent advancements in materials research have highlighted the BPN as a promising allotrope of sp^2-hybridized carbon atoms, distinct from graphene sheets, due to its unique electronic properties [2]. Synthesis of BPN was recently achieved through an on-surface interpolymer dehydrofluorination (HF-zipping) reaction, opening avenues for diverse applications in materials science. This study delves into the investigation of the impact of strain on the BPN's electronic properties, encompassing its density of states (DOS), band structure, and energy gap. Our primary objective is to assess the BPN's electronic tunability under strain and its transition from a semi-metallic into a semi-conducting state. Additionally, mechanical properties such as Young's modulus were obtained, revealing BPN's brittle nature as it loses integrity under strain. Utilizing the DFT method implemented in the Quantum Espresso software for simulations, our findings unveil a semi-metallic behavior in BPN, with the application of strain resulting in the uniaxial transition into a semi-conducting state.

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Exploring the Potential of Rose Bengal as a Photosensitizer in Photodynamic Therapy for Colorectal Cancer

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The colorectal cancer currently ranks as the third most common form of cancer globally and is accountable for the second-highest number of cancer-related fatalities.[1] To tackle this challenge, innovative treatments are under investigation, aiming to effectively combat cancer while minimizing adverse effects. Photodynamic therapy (PDT) stands out as a non-invasive treatment approach employing a photosensitizer (PS) to trigger cancer cell death through light-induced mechanisms.[2] Rose Bengal (RB), an amphiphilic PS belonging to the xanthene family, demonstrates significant efficiency in generating singlet oxygen ($^1O_2$), a reactive agent capable of oxidizing biological components. This research evaluated RB's impact on the cell membrane of colorectal carcinoma (Caco-2) using Langmuir and Langmuir Blodgett films with concentrations ranging from 1 to 25 × 10^{-6} mol/L. Additionally, the study investigated RB's photodynamic effectiveness at various concentrations (ranging from 0.5 to 25 × 10^{-6} mol/L) and incubation periods (0.5, 3, and 24 hours) in Caco-2 in vitro cultures. Cell viability was assessed using MTT assays 24 hours following 1-hour irradiation at 525 nm (32.3 mW/cm^2) in in vitro experiments. The incorporation of RB onto the membrane models was confirmed by a roughly 140% relative area shift at the highest concentration, alterations in domain heights assessed via AFM images, and changes in bands in PM-IRRAS indicating RB's increased affinity with polar groups, particularly affected by PS photoactivation. In vitro tests demonstrated that concentrations above 5 × 10^{-6} mol/L reduced cell viability by approximately 80%, regardless of the incubation period, resulting in morphological changes indicative of apoptotic-necrotic processes. In summary, RB exhibits promising potential as a photosensitizer in the photodynamic therapy of colorectal cancer.

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Gas sensor based on highly effective slot-die printed PEDOT:PSS@ZnO hybrid nanocomposite for methanol and CO2 detection

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This study presents the development of gas sensors based on PEDOT:PSS@ZnO hybrid active layer slot-die printing aqueous ink. Two different ZnOs were studied to form the nanocomposites, as well as the use of glass and PET substrates to manufacture the devices. Despite the influence of the morphology of the active layer, all device variations studied here exhibited high response values for methanol gas at low working temperatures, in addition to presenting good repeatability, reversibility, and the possibility of technology transfer to flexible substrates. The best devices showed responses greater than 700% in detecting 500 ppb methanol at room temperature, the highest reported to date [1]. For the CO_2 response at 206 ppm, the devices showed a smooth curve in ≈20%. This study can contribute to the future development of sensors for the detection of this gases, thus expanding the applicability of the composites used [2].

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Hole transport in low-donor content organic solar cells

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Organic solar cells present numerous advantages over traditional photovoltaic systems, including flexibility, affordability, and the availability of abundant materials, making them a promising option for energy generation [1,2]. A notable scenario involves diluted configurations, where a limited quantity of electron-donating molecules is dispersed within an acceptor matrix, limiting hole transport due to the absence of continuous pathways. Despite this, diluted systems exhibit reasonable performance [3], prompting discussions on the underlying mechanisms facilitating this efficiency [4]. In this study, we explore hole transport by assessing hole mobility across various donor:acceptor systems with differing donor concentrations. Surprisingly, we discovered a correlation between hole mobility and the energy difference between the donor's Highest Occupied Molecular Orbital (HOMO) and the acceptor's Lowest Unoccupied Molecular Orbital (LUMO), rather than the acceptor's HOMO, as previously suggested. This correlation indicates that as the energy offset decreases, the mobility increases. Molecular modeling supports this correlation, proposing a contribution from the acceptor's LUMO-mediated superexchange mechanism. These findings validate our experimental observations and indicate a previously overlooked transport mechanism, dependent on the interaction between the donor's HOMO and the acceptor's LUMO [5].

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Inducing Crystallization of Er/Yb:BaTiO3 Perovskite with fs-Laser Pulses

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Perovskite films have garnered significant interest for their potential applications in photonics and optoelectronics, such as light-emitting diodes, photodetectors, and energy-harvesting devices [1]. These applications are susceptible to variations in the crystallization, , and distribution of grains within the perovskite films [2]. Consequently, extensive research has been conducted to enhance the quality of thin films and explore the impact of sintering on the crystalline phase of the material. Despite the development of various sintering techniques [3], fs-laser sintering has emerged as a versatile and efficient option, delivering precise and localized energy distribution to the sample. This method enables the production of highly crystalline devices with intricate structures, albeit its effectiveness relies on specific processing parameters.

This study illustrates the crystallization process of amorphous $Er^{3+}/Yb^{3+}:BaTiO_3$ (BTEY) thin film using fs-laser processing at 1030 nm. The threshold fluence required for laser processing was determined as 1.1 J/cm^2 at a repetition rate of 1 kHz, along with the optimal irradiation conditions for crystallization. Raman spectroscopy confirmed the crystallization occurring at a 1 kHz repetition rate. Additionally, an enhancement in sample emission was observed in the crystallized regions, along with changes in surface potential. These findings shed light on the potential of utilizing fs-laser pulses for BTEY crystallization, which holds significance for device applications.

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Island formation in growth of thin film organic materials: C60 and picene

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Organic semiconductor thin films grown on amorphous silica substrates are essential for applications in photovoltaics and electronics. Some materials like C60 and picene show strong island growth which in the course of the growth process revert back to desirable flat layer-by-layer growth. Such an unusual non-monotonic behavior of the film roughness was deemed anomalous in the literature [1]. On the basis of kinetic Monte Carlo simulations of simple lattice models we argue that such a growth mode is quite normal [2,3]. Further we discuss a new scaling regime for island-forming heteroepitactic thin film system where a variable substrate energy triggers the appearance of islands. Finally, we discuss and rationalize the rougness evolution of C60 and picene films obtained by organic molecular beam deposition using the simple lattice models.

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Laser engineering of MXenes towards their environmental and mechanical stability

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This century has introduced several new and innovative materials to be used as building blocks for advanced electronics. MXenes are among these materials, highly valued for their applications in optoelectronics, sensors, and energy storage devices. These applications are possible due to the material's high metallic electrical conductivity, transparency in thin films, and significant surface area. However, MXenes face significant challenges, including rapid oxidation and poor mechanical stability, particularly in multilayer configurations. Building upon our previous insights into fabricating flexible nanomaterial-based sensors using laser processing [1], we anticipate that this approach will greatly help to overcome these challenges, maintaining excellent MXenes properties. In this study, we demonstrate how laser transfer enables the integration of MXenes onto glass and polymer substrates using a simple, room-temperature experimental setup. Raman spectra confirm the retention of MXenes original peaks, along with the emergence of graphene peaks, likely due to carbonization from localized high temperatures at the laser spot. Our findings show that the samples exhibit minimized degradation after one week in an environmental chamber (relative humidity 95%, temperature 40°C), making them suitable for long-term use in electronics, particularly in electrothermal heaters and memristors.

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Mapping the electric field distribution within polymeric transistors by sum-frequency generation microscopy

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Organic transistors have the potential to enable novel devices and applications that were previously impossible with traditional inorganic materials. To fully exploit the potential of these devices, it is crucial to investigate the physical and chemical events within them. In this context, understanding the electric field distribution across the dielectric layer of an organic field-effect transistor (OFET) could provide valuable insights, given its close relationship with the charge density in the channel. In our work, we applied sum-frequency generation (SFG) vibrational spectroscopy and microscopy to probe the electric field distribution within OFETs fabricated with P3HT and PMMA as the organic semiconductor and dielectric, respectively. SFG is a non-linear optical effect sensitive to breaking inversion symmetry, such as the molecular alignment induced by an intense electric field. In this contribution, we obtained SFG spectra and SFG images of the C=O stretch from the polar methyl methacrylate groups in the PMMA dielectric layer. Our results demonstrate the expected quadratic dependence of the SFG signal on gate voltage. Moreover, the SFG images indicate that the electric field within the PMMA layer is non-homogeneous along the channel. Additionally, the distributions of SFG signal intensities observed along the channel during output curve measurements are consistent with the gradual channel approximation [1]. Furthermore, we will show that it is possible to perform point-by-point SFG spectroscopy at any location within the channel. With this study, we hope to contribute for a better understanding of the physics of OFETs, with important implications for improving their performance.

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Mixed Conduction Properties in PEDOT:PSS Films: The effects of Modulating PSS Molecular Weight

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Poly(3,4-ethylenedioxythiophene): Poly(styrene sulfonate) (PEDOT) has gained significant popularity in both academic and industrial fields, especially due to its vast applications in several devices. However, despite its popularity and prominence in organic electronics, there is still a lack of scientific references regarding the synthesis and production of PEDOT inks. In the study presented here, we explore the mixed conduction properties of PEDOT films through variations in the molecular weight (Mw) of PSS. The synthesis of PSS was conducted via free radical polymerization, with adjustments made to the reaction time and temperature. Mw values were determined using Static Light Scattering (SLS). We employed transconductance and volumetric capacitance measurements to assess the performance of the PEDOT films. Our findings confirms a notable correlation between the molecular weight of PSS and the mixed conduction behavior of PEDOT.[1] Increases in PSS molecular weight led to enhancements in ionic conductivity, while electronic conductivity exhibited an inverse trend. This suggests an interplay between the molecular structure of PSS and the conduction properties of PEDOT films. These insights underscore the significance of molecular engineering for optimizing the performance of conductive polymer materials in various electronic and electrochemical applications.

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Nanostraw Injection: Mitigating Lysosomal Entrapment of Photothermal Nanoagents and Modulating Cell Death Mechanisms in Triple Negative Breast Carcinomas

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With 2.3 million cases annually, breast cancer is the leading malignancy affecting women globally. The rise of triple negative breast tumors presents a formidable challenge in patient care. These aggressive tumors, lacking estrogen, progesterone, and human epidermal growth factor 2 receptors, are notoriously difficult to treat. In the quest for more efficient and less invasive therapies, photothermal therapy (PTT) has emerged. PTT utilizes nanoagents to convert light into heat, inducing cell death via hyperthermia and oxidative stress.[1] Herein, nanostraw-assisted injection[2] were used for delivering the nanoagents gold-shell isolated nanoparticles (AuSHINs) into MDA-MB-231 cells, a triple-negative breast cancer line. This method ensures precise AuSHINs delivery, circumventing endosomal entrapment and enhancing phototherapeutic efficacy. Although cellular uptake of AuSHINs was higher for 2.0 h incubation compared to injection, the signal intensity from injected cells was notably stronger. Confocal microscopies revealed distinct localization patterns: incubation led to colocalization with lysosomes, while injection facilitated localization within the endoplasmic reticulum. This localization shift potentially enhances PTT efficiency by circumventing lysosomal entrapment. Upon irradiation of AuSHINs injected into MDA-MB-231 cells, viability decreased to 34.8% compared to 70.3% for 2.0 h incubation. The delivery method also influenced the cell death pathways and the generation of ROS, correlating PTT efficiency with the treatment strategy. These findings underscore the superior PTT efficiency of AuSHINs delivered via nanostraw injection compared to incubation, suggesting potential therapeutic strategies for breast cancer treatment leveraging PTT technology.

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Nanostructured Energy Storage Systems: Using Metallic Oxides and Graphene Oxide for Supercapacitors

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Nanostructured films have garnered significant attention in energy storage applications, particularly within the domain of supercapacitors. A promising approach involves integrating various metallic oxides into graphene oxide matrices. Carbon and metal oxide-based materials have attracted considerable interest due to their potential across a wide array of technological applications in energy storage [1-3]. In this context, our research focuses on the fabrication of Layer-by-Layer (LbL) and Langmuir-Blodgett (LB) films comprising graphene oxide and metal oxide nanoparticles embedded within electrodes. These films serve as customized interfaces with the capability to function effectively in supercapacitor devices. Thus, we explored the incorporation of different metal oxide nanostructures, including MnO_2, ZnO, NbO_2, and WO_3, into graphene sheets. These were combined with polyelectrolytes for LbL film formation or phospholipids for LB film formation. Here, we present insights into the fabrication techniques and characterization methods employed to develop strategies for modifying conductive electrodes. Additionally, we discuss the advantages of arranging graphene oxide and metallic oxides in LbL or LB fashion films, highlighting their potential properties for exploitation in supercapacitor devices.

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Natural Dielectrics for Bio-Organic Electronics

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Organic electronics has an immense potential for the development of products that are both sustainable and environmentally friendly. In this presentation, a large list of natural origin dielectric materials is introduced and demonstrated in the fabrication of organic field effect transistors, e.g. resins, gums, waxes, alkaloids, nucleobases, lignins and celluloses, natural clays, etc. Apart for their outstanding dielectric and film forming properties, most of the above-mentioned natural dielectrics are inherently, biocompatible (even edible) and have well known medical properties. Thus, this class of dielectrics may find suitable applications in the branches of science where dielectric materials are part of bio-integrated electronics.

Non-symmetrical fluorenyl-benzothiadiazole derivatives with AIEE and TADF: photophysical properties and applications in OLEDs

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Organic electronics, particularly organic light-emitting diodes (OLEDs), is an expanding field with enormous potential for flexible and efficient electronic devices. One of the key phenomena for 3rd-generation OLEDs is thermally activated delayed fluorescence (TADF). TADF enables the harvesting of singlet and triplet excitons for light emission, which significantly increases OLED efficiency [1]. Another important photophysical phenomena is Aggregation Induced Enhanced Emission (AIEE), present when rotations and vibrations are restricted in non-planar molecules, preventing energy dissipation, favoring radiative decay of excited species, and increasing the luminescence of aggregated states [2]. In this research, three new fluorenyl-benzothiadiazole derivatives were synthed: FL-BTD-Ar, FL-BTD-OAr, and FL-BTD-IDB. The synthesis was performed by Suzuki-Miyaura and Buchwald-Hartwig reactions. The compounds exhibited absorption in the violet and blue regions and showed emissions in the green region for FL-BTD-Ar and FL-BTD-OAr, and in the orange region for FL-BTD-IDB, with fluorescence quantum yields in THF of 0.67, 0.65, and 0.07, respectively. All compounds presented AIEE and compound FL-BTD-IDB presented both AIEE and TADF. The performance of the materials as emitter layers for OLEDs were then evaluated. The OLEDs with the non-TADF emitters showed significant improvements in luminance, 6450 cd/m2 (FL-BTD-OAr) and 3246 cd/m2 (FL-BTD-Ar), compared to a previously described BTD-based TADF (2980 cd/m2) [3]. In addition, the OLED fabricated with the material displaying both AIEE and TADF (FL-BTD-IDB) exhibited max. luminance of 10210 cd/m2.

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Optimization and Characterization of Organic Thin Film Transistors for Gas Sensing Applications

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The fabrication and characterization of organic thin film transistors (OTFTs) for gas sensing applications for detecting Geosmin and Isoborneol in water, are being explored using high-mobility organic semiconductors such as 2,7-Dioctyl[1]benzothieno[3,2-b][1]benzothiophene (C8-BTBT), Poly(3,3‴-didodecyl[2,2′:5′,2″:5″,2‴-quaterthiophene]-5,5‴-diyl) (PQT-12), and Poly{[N,N'-bis(2-octyldodecyl)naphthalene-1,4,5,8-bis(dicarboximide)-2,6-diyl]-alt-5,5'-(2,2'-bithiophene)} (PNDI(2OD)2T) [1]. Organic dielectrics like Poly(4-vinylphenol) (PVP) and Poly(methyl methacrylate) (PMMA) [2] cross-linked with Poly-melamine-formaldehyde (PMF) are also being studied. Electronic devices are fabricated through processes like metallization, photolithography, and corrosion [3]. The analysis of the effect of oxygen and solvents on OTFTs I-V curves on thin dielectric films are carried out with techniques such as Atomic Force Microscopy (AFM), Raman and Fourier Transform Infrared spectroscopy. Spectral characterization includes UV-vis spectroscopy and X-ray diffraction spectroscopy. Optimized proportions of PVP:PMF were found to improve the insulating/semiconductor interface and performance [2]. Challenges in forming C8-BTBT semiconductor films, the impact of solvent choice on film thickness, and the morphology and roughness of PQT-12 and PNDI(2OD)2T films, all impact transistor conductivity. Therefore, the next steps are refining semiconductor film fabrication methodologies, using different solvents and deepening the understanding of necessary surface treatments to improve performance in OTFTs [3].

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Organic Semiconductors in Flexible Field-Effect Transistors

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In this presentation, methods to determine the flexibility of organic field-effect transistors (FETs) and strategies to improve the mechanical robustness are discussed [1]. Free-standing and flexible FETs based on molecular semiconductor/polystyrene bilayers were obtained by well-controlled phase separation of both components [2]. The crystallinity and blend morphology strongly depended on the molecular weight of polystyrene, and under optimized conditions, distinct phase separation with a well-defined and trap-free interface between both fractions was achieved. Due to the distinct bilayer morphology, the resulting flexible FETs revealed high charge carrier mobilities and pronounced environmental and bias stress stabilities. The fatigue behavior of flexible FETs based on conjugated polymers was also studied [3]. An especial bending setup allowed to perform precise multiple deformation cycles of the transistor channel area while monitoring the device behavior. The transistors showed high operational stability upon 100 bending cycles at a radius of 500 µm. Thinner polymer films were more sensitive to the deformation-induced defects leading to a larger decrease in device performance. In thicker polymer films, the crack propagation less affects the semiconductor/dielectric interface resulting in a more stable device operation.

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PVC films coated with graphene nanoplatelets ink for applications in photovoltaic devices

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Nanostructured polymers have been consolidated as a promising possibility in order to develop more sustainable materials with lower cost of production and environmental impacts. In this context, polyvinyl chloride (PVC) has been object of intense research since its characteristics are in accordance with these requirements. Furthermore, PVC presents some interesting characteristics for electrical applications such as high stability under environmental conditions, acting as an efficient barrier against oxygen and water [1, 2]. At the same time, the search for new synthesis routes for graphene and its derivatives has also consolidated itself as one of the most prominent fields of research. In this work, these two branches of research are addressed through the development of new flexible substrates based on PVC coated by graphene nanoplatelets produced from lignin. The lignin nanocarbon was produced from pyrolysis of biomass according the method devolved by Rocha et al. [3] while the PVC films are produced by the "Blade Coating" technique. Characterization techniques such as infrared spectroscopy, Raman spectroscopy, mechanical and electrical measurements were performed and the results showed an acquisition of a conductive, flexible and transparent PVC-lignin nanocarbon film, suitable for application as a substrate for organic photovoltaic devices.

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Refractive index changes in solid-state laser materials

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Pump-induced wavefront aberrations in laser resonators are a crucial problem of solid-state lasers design, particularly the power scaling of these lasers [1]. These aberrations can be caused by spatially inhomogeneous refractive index changes (RICs) due to the nonlinear refractive index of the host material, thermal lens (TL) and population lens (PL), which is an athermal effect. The host n_2 contribution is a fast host nonlinearity (sub-picoseconds) while TL and PL are slow, with response time typically longer than ~10-4 sec. The TL effect appears due to the temperature distribution associated with the heat generated due to pumping of the active media. PL is caused by light-induced population of the excited metastable state, due to difference between the polarizabilities of excited and ground state, $\Delta p = p_{ex} - p_g$.

Several methods have been used to characterize laser materials as well as practical lasers. In this paper, we explored the dual beam (excitation and probe) mode-mismatched TL configuration to characterize thermal and electronic RICs in Cr3+ and Yb3+ doped crystals. Electronic and thermal contributions can be discriminated using time-resolved experiments and by their spatial profile. We remind here that the TL typical response time is determined by transverse heat diffusion ($tc = \omega^2/4D$) while in PL it depends only on the excited state lifetime (tf). In order to improve the discrimination of PL and TL effects, we increased the TL response time using a probe beam diameter much greater than the excitation one, since the larger the probe beam the longer takes the TL signal to reach steady state. Therefore, we obtained a relatively fast PL effect followed by slow TL with response time, typically two orders of magnitude longer.

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Simultaneous electrodeposition of thin poly-methylene blue films and gold nanoparticles for sensing platform

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The supramolecular arrangement of the thin films can be molded from different deposition techniques, giving the new materials specific properties that can be controlled [1]. The possibility of tunning the materials properties shows advantages for the development of sensing platforms [2]. This work uses the technique of potentiodynamic electrodeposition for the formation of thin films of methylene blue and gold nanoparticles (AuNPs) simultaneously. The electrodeposition was performed using twenty potential cycles in an aqueous solution containing the methylene blue monomer and gold (III) chloride, with the screen-printed carbon electrode (SPCE) as the substrate. The electrochemical behavior of the modified SPCE in a redox probe ([Fe(CN)6]3−/[Fe(CN)6]4−) indicates changes in charge transfer, which affect the effective surface area. The poly(methylene) blue (poly-MB) showed no changes in charge transfer with an increase in the number of potential cycles applied but showed an increase in coverage, reaching 0.0066 cm2 after twenty potential cycles. Additionally, the coverage surface showed more influence on the amount of AuNPs deposited than the amount of poly-MB formed. The presence of AuNPs also promotes an increase in charge transfer at high coverage (0.0087 cm2). The hybrid film of poly-MB+AuNPs showed promising properties as a spectroelectrochemical platform, with the fluorescence of methylene blue influenced by the applied potential. In this case, Raman spectroscopy was used as the spectroscopic technique, and the presence of AuNPs enhanced the poly-MB signal.

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Single-Response Duplexing of Electrochemical Label-Free Biosensor from the Same Tag

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Multiplexing is a valuable strategy to boost throughput and improve clinical accuracy [1]. Exploiting the vertical, meshed design of reproducible and low-cost ultra-dense electrochemical chips, the unprecedented single-response multiplexing of typical label-free biosensors is reported. Using a cheap, handheld one-channel workstation and a single redox probe, that is, ferro/ferricyanide, the recognition events taking place on two spatially resolved locations of the same working electrode can be tracked along a single voltammetry scan by collecting the electrochemical signatures of the probe in relation to different quasi-reference electrodes, Au (0 V) and Ag/AgCl ink (+0.2 V). This spatial isolation prevents crosstalk between the redox tags and interferences over functionalization and binding steps, representing an advantage over the existing non-spatially resolved single-response multiplex strategies [2]. As proof of concept, peptide-tethered immunosensors are demonstrated to provide the duplex detection of COVID-19 antibodies, thereby doubling the throughput while achieving 100% accuracy in serum samples. The approach is envisioned to enable broad applications in high-throughput and multi-analyte platforms, as it can be tailored to other biosensing devices and formats.

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Stretch Evolution of Electronic Coupling of the Thiophenyl Anchoring Group with Gold in Mechanically Controllable Break Junctions

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Mechanically controllable break junctions (MCBJs) are devices, in which the electrical properties of single molecules can be investigated with extreme precision using atomically fine shaped metal tips. The current-voltage (IV) characteristics in such junctions are considerably affected by the binding positions of the anchoring groups on the tip and the configuration of the molecule.[1] Hence, characterizing the electronic transport properties during a single tip-tip opening provides interesting insights into the tip-molecule interaction. In this work, we present a novel, high-throughput approach to simulate the time evolution of the electronic transport characteristics. For this, we performed transport calculations using the self-consistent charge scheme of the density-functional-based tight binding (SCC-DFTB) [2] approach and the Green’s function formalism. We evaluated the energy level and the coupling of the dominating transport channel using the single level model.[3] In contrast to standard approaches, we consider not just one molecule orientation but many thermodynamically relevant configurations. The obtained parameters were averaged using statistical weights obtained from Metropolis simulation considering up to 80 000 different configurations for 19 selected tip-tip distances. The evolution of the averaged quantities with respect to the tip-tip separation reveals characteristic features also observed in experiments for similar molecular systems. Our approach allows us to relate these features to binding-site and molecule-curvature effects and therefore provides a better interpretation of the experimental results.

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Substituting small molecule by polymeric macromolecules in Light Harvesting Capacitor: improving coherency of photogenerated dipoles

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Light Harvesting Capacitor (LHC) is a nanoscaled photovoltaic device that consists of donor-acceptor Active Layers (AL) separated from electrodes by Transparent Insulating (TI) layers. The photogenerated opposite charges drift in random directions, not being extracted at the electrodes due to the TIs, yielding an internal polarization of the active layer. Nanodipole (ND) generation is coherent when they align normal to the electrodes. Change in density of coherent NDs causes Transient Current (TC) through external circuit. Building an LHC by piling up insulated ALs between pair of electrodes improve its performance, since each ND add up stronger TC. [1] Therefore, Layer-by-Layer (LbL) dip coating is well suited to build multistacked LHCs. [2] We use continuous wave Photoinduced Absorption and Transient Absorption spectroscopies, as well as TC measurements to compare photogeneration of charges and of ND in different LHCs: (1) made of Polymeric Donor (PD)/Molecular Acceptor (MA) materials, and (2) PD/Polymeric Acceptor (PA). We show that charge photogeneration is stronger in the first type, but with more randomly oriented NDs, suggesting that MAs tend to interpenetrate the PD chains. Conversely, in the second type, the opposite: photogeneration of charges is lower, but with stronger coherently oriented NDs, suggesting that LbL of these materials lead to less interpenetration of layers. This is an advance on nanoscale fabrication of LHCs, showing that it is open to further improvements.

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Synaptic Ion-Gating Vertical Transistors for Advanced Neuromorphic Systems

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Bioinspired devices have emerged as pivotal components in the realm of artificial intelligence and neuromorphic electronics, offering promises of low energy consumption,[1] multi-modal sensing,[2] and multifunctional integration.[3] Among these, the ion-gating vertical transistor (IGVT) architecture has recently garnered significant attention for its capability to emulate brain-like perception, encompassing artificial vision, touch, taste, and hearing. Here the latest advancements in IGVT technology are introduced and reviewed, highlighting its superior data processing speeds and memory capabilities over conventional neuromorphic devices.[1] Fundamental concepts including signal processing, transduction, plasticity, and multi-stimulus perception are comprehensively discussed. Furthermore, special emphasis is placed on the development and optimization of multi-modal flexible sensor technologies, propelling IGVTs as the forefront solution for future high-end theoretical and experimental advancements in neuromorphic research.

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Synthesis And Chemosensory Action Of Tetrahydropyridine Derivatives

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Chemosensors are substances that exhibit the ability to detect and signal physical or chemical changes upon interaction with forms of matter or energy [1]. This signaling mechanism primarily involves the formation of chemical bonds or intermolecular interactions between the sensor molecule and the analyte [2]. Among the range of chemosensors available, colorimetric and fluorescence sensors stand out due to their advantageous features such as high sensitivity, cost-effectiveness, and versatility in applications [3]. The primary objective of this research was to synthesize a tetrahydropyridine derivatives through a multicomponent reaction involving *p*-tolualdehyde, methyl-4-aminobenzoate, and methyl acetoacetate, resulting in the formation of a tri-ester-tetrahydropyridine **1**, followed by a hydrolysis reaction to produce a tri-acid-tetrahydropyridine **2**. Subsequently, the synthesized compounds were subjected to testing to assess their potential as chemical sensors for solvents, salts, and variations in pH. Structural characterization of the synthesized molecules was conducted using NMR, and their sensor capabilities were further evaluated through the spectroscopic technique UV-vis. Both derivatives (**1** and **2**) exhibited notable selectivity towards solvents such as methanol, ethanol, and N-butanol. Furthermore, the addition of $NaNO_3$ to compound 1 and $Fe(NO_3)_3$ to compound **2** resulted in significant hyperchromic shifts. Lastly derivative **2** was selective towards NaOH with a detection capacity as low as **1** uL.

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Ultrafast microfluidic solvent extraction and sensors 4.0 to determine multiple scaling ions from a single impedance scan.

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Flow assurance plays an important role in designing safe and efficient operation techniques along oil and gas explorations. In this way, approaches able to provide fast and field-deployable monitoring of scaling ions in crude oils may benefit the petrochemical industry in its long-standing mission to devise ideal flow conditions by aiding the adoption of optimum dosages of off-the-shelf products. We here describe a scalable platform toward rapid (~10 min) determination of multiple scaling ions in crude oils. Our platform is based on turbulence-mediated ultrafast and efficient microfluidic solvent extraction (µSE) combined with impedimetric sensors and machine learning to determine different ions from a single impedance plot [1]. 3D-printed µSE devices were able to afford ultra-fast (residence time of ~1.0 s) extractions. Nanocellulose-based foams allowed us to rapidly separate the water-oil phases, with the aqueous phase being sampled for posterior detection. Using scalable drop-casting or microfluidic electrochemical sensors to generate impedance data, multi-output machine-learning algorithms could be continuously trained on diverse real water samples to gradually refine and improve the accuracy of predictions. This learning capability provided robust performance under non-ideal conditions (i.e., complex samples), yielding the multidetermination of ions in 50 produced water samples (Mg^{2+}, Ca^{2+}, Sr^{2+}, and Cl^{-}) and 49 crude oils (Ca^{2+} and Cl^{-}). The accuracies ranged from ~96 to 100%. Importantly, ML models trained on standard solutions delivered poor accuracy, showing the relevance of learning supervised algorithms with real samples to deliver accurate capacitive analyses [2].

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UNDERSTANDING STABILITY IN ORGANIC SOLAR CELLS: EXPLORING THE INFLUENCE OF SMALL MOLECULE BR-2PACz ADDITION ON HTLs

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Organic solar cells (OSCs) have achieved notable power conversion efficiencies (PCEs) exceeding 18% [1], yet research on their degradation in continuous use and ambient conditions remains limited. Adherence to Intentional Summer on Organic Photovoltaic Stability (ISOS) protocols [2] is incomplete, hindering data comparison and replication. This study aims to develop and characterize organic photovoltaic devices while adhering to ISOS protocols to investigate stability and degradation phenomena. Hence, this study aims to develop and characterize organic photovoltaic devices while adhering to ISOS protocols to investigate stability and degradation phenomena. For this purpose, the influence of BR-2PACz in the PEDOT:PSS hole transport layers (HTL's) within the ITO/PEDOT:PSS/BR-2PACz/PBDB-T-2F:BTP-4F/PDINN/Ag structure will be evaluated. Characterization involved a ThermoOriel class AAA solar simulator and a Keithley source and meter 2400 for J-V measurements under illumination (100 mW/cm2). Preliminary results show significant improvements in Jsc, FF, and PCE. Three degradation protocols (ISOS-D1, ISOS-L1, and ISOS-O2) will measure degradation during continuous operation, exposing the device to atmospheric air without encapsulation. This study aims to elucidate HTLs influence on device stability and propose innovative approaches for fabricating solar cell materials with enhanced efficiency and stability, potentially advancing next-generation solar cells significantly.

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Unravelling the Optical Excitations of Perfluorinated Acenes: Insights from Crystal Polymorphs

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Perfluorinated acenes hold significant promise in the realm of organic optoelectronics [1]. As the packing arrangement of molecules in the solid state significantly impacts the electronic and optical properties, it is crucial to explicitly simulate crystalline phases to understand electronic correlations and excitations in these materials. In this study, we show a roadmap to describe excitons in organic materials appropriately, in general. We investigate from first principles, using density functional theory and many-body perturbation theory, the electronic structure, and the optical excitations of two crystal polymorphs of perfluorotetracene, considering for comparison tetracene and the corresponding isolated molecules. This way, we can assess the effects of fluorination as well as the crystal periodicity. While the absorption spectra are only mildly influenced by the packing motif, our analysis gives insight into the binding energies and the spatial distribution of the excitons. By extending our analysis to the entire UV-visible spectral range, we provide a complete understanding of the optical excitations in these materials [2].

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Analysis of the influence of different peripheral groups on multiphoton absorption in sulfonated imidazopyridines

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Significant importance has been attributed to organic compounds in photonics research, from monitoring biological processes using fluorescent probes to bioimaging through two-photon absorption fluorescence microscopy. Particularly noteworthy are molecules derived from imidazopyridines, which have emerged as excellent candidates for applications in biology and medicine due to the broad range of optical properties resulting from high electron delocalization and tautomer formation in excited states. [1,2] Within the scope of this study, the objective is to evaluate the linear and nonlinear absorption characteristics of a series of sulfonated imidazopyridines, alongside investigating the dynamics of their excited states. This assessment employs various experimental methods, including UV-Vis spectroscopy, fluorimetry, z-scan, and pump-probe experiments, supplemented by theoretical simulations utilizing Density Functional Theory (DFT). The findings thus far unveil a reasonable concurrence between simulated and experimental absorption spectra, fluorescence across the molecule array, and two-photon cross-sections nearing 40 GM. These outcomes imply the potential efficacy of these compounds in imaging procedures.

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Application of Advanced Oxidation Processes (AOPs) in the Synthesis of Highly-Conductive PEDOT:PSS Inks

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Poly(3,4-ethylenedioxythiophene): Poly(styrenesulfonate), PEDOT:PSS, is one of the most prominent materials in the organic electronic area. However, its production and intellectual property are concentrated in a few companies, leading to obstacles in the development of understanding of the synthesis. Here, we aimed to apply concepts of pollutant decontamination by advanced oxidation processes (AOP) in the synthesis of PEDOT:PSS inks. While AOPs are commonly used in several areas, their application in the synthesis of PEDOT:PSS has not been explored. We conducted synthesis of PEDOT:PSS, varying only the transition metal catalyst salt. The inks were made using 1 mole equivalent of oxidant (Na2S2O8) and EDOT, 1.6 mole equivalent of PSS, and 0.01 mole equivalent of metallic cation catalyst. The resulting inks were drop-casted, and the electrical conductivities were obtained using the 4-point method [1]. The results indicated that the inks obtained using iron cations had the highest conductivity, observed at approximately 109 S/cm. In contrast, inks obtained with the other cations presented significantly lower conductivities, with silver cations presenting only 2.0 S/cm. An analysis of the redox potential of the catalysts and the reagents indicated that the closer the redox potential of the metallic cations was to half the potential of EDOT/sulfate radical (formed during the breakdown of the persulfate anion), the higher the resulting electrical conductivity. In other words, if the reduction potential of a cation is intermediary relative to the potential of the reaction, the catalytic power is higher.

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Biomimetic Approach to Filtration Membrane Enhancement: The Role of Nanovesicles in Dye Filtration

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Dyes are toxic to the environment and human health and present difficult degradation. The use of filters, specifically in nanofiltration and reverse osmosis, is a good example of the use of membranes in water treatment [1]. The modification of membranes using biomimetic models, such as the incorporation of aquaporin, has shown promising results. However, the high cost and difficulty of large scale production led to the investigation of alternative materials to improve membrane technology. Herein, we present a modification to a commercial PTFE membrane using DOPC-Cholesterol-Amphotericin B vesicles to improve the membrane performance for dye filtration. AmB, in contact with DOPC and Chol vesicles, presents a structuration that creates ionic channels on the membrane surface, which has the potential to be used for filtration. In this work, we present the method for ionic channel production using DOPC-Chol-AmB vesicles, the membrane modification, and its characterization. By measuring the water contact angle, it was observed that the membrane became less hydrophobic after the modification. Water permeability tests also showed successful membrane modification, where the modified membrane showed greater permeability than the unmodified one. The modification was also analyzed using AFM and SEM microscopy techniques, in which agglomerates were observed. It was possible to prove the existence of ionic channels through impedance tests, as the modified membranes showed conductivity, unlike unmodified ones. The following steps of this work include filtration tests.

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Characterization of conjugated polymer/zinc oxide nanocomposite

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The optical and electrical properties of conducting polymers, arising from their highly delocalized and electron-dense π-bonds along their backbone, are of significant interest for applications in electronic devices and have potential in several fields. [1,2] However, to enhance these properties, inorganic nanoparticles like metal oxides can be integrated into the polymeric matrix. Zinc oxide (ZnO), for example, owing to its wide bandgap, is a material commonly employed in conjugated polymer composites.[3] In this context, the aim of this work was to prepare and characterize the composite formed by the conjugated copolymer poly(9,9-dioctylfluorene)-co-trans-stilbene (PFSTB) and ZnO nanoparticles. The characterizations involve absorption, emission, electric and structural properties using UV-Vis, fluorescence, I-V curve and infrared spectroscopy, respectively. Composite samples were prepared by adding ZnO to the solution composed of the PFSTB copolymer and organic solvent. For better homogenization, the dispersion was subjected to ultrasonication. Then, the material was spin-coated onto the substrate to form a thin film, and to analyze the impact of thickness, the number of layers deposited on the quartz substrate was varied. The results obtained contributed to a better understanding of the PFSTB/ZnO composite properties and its potential application in electronic devices.

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Characterization of self-assembled films incorporating DPPE liposomes immobilized on various deposition matrices for biosensor applications

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Self-assembled films offer a precise method for creating nanometer-thin layers through molecular self-assembly, exploiting electrostatic interactions. They are crucial in developing highly sensitive and selective biosensors for precise molecular recognition in medical diagnostics, environmental monitoring, and bioanalytical applications. One promising avenue to enhance biosensor performance is by incorporating them into liposomes, spherical lipid vesicles capable of encapsulating a wide array of substances, including biomolecules. This study focuses on immobilizing DPPE (dipalmitoylphosphatidylethanolamine) liposomes onto different deposition matrices to identify the optimal immobilization matrix for use as a biomarker. The matrices under scrutiny include Silk Fibroin (SF) and Polyvinyl Chloride (PVC). SF's fibrous nature and polarity affect its interaction with liposomes, potentially impacting encapsulation efficiency and controlled release in biosensors. In contrast, PVC's porous structure promotes efficient liposome encapsulation. Using the Layer-by-Layer (LbL) technique, polymeric matrices are absorbed onto Mica plates, followed by DPPE-containing PBS solution application. AFM evaluates layer efficacy. Results indicate PVC as the superior deposition matrix due to sample uniformity and sphere diameter averaging 200 nm, aligning with typical DPPE liposome diameters. This finding suggests PVC holds promise for developing more sensitive and specific biosensors, vital for early and accurate clinical condition detection, thus advancing diagnostics and treatment efficacy.

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Chemical and morphological characterization of plasticlasts, an emerging plastic material from marine pollution (Trindade Island, Brazil)

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Improper plastic disposal represents a concern for the scientific community due to its notable resistance to degradation and the damage it causes to marine life. In 2022, a novel type of marine pollution resembling rocks, termed plastistones, was reported on Trindade Island, Brazil, which, when eroded by natural agents, fragments into smaller particles called plastisclasts [1]. The aim of this study was to characterize plasticlasts collected on Trindade Island and determine their chemical composition and physical properties. To achieve this goal, a diverse methodological approach was adopted, incorporating conventional methods such as the Archimedes principle for density measurement, and specific techniques such as Raman scattering spectroscopy. The analyses were conducted individually on a set of 24 samples with distinct characteristics. This allowed for detailed characterization and both macroscopic and microscopic separation, including classifications by polymer type, color, grain roundness, and density. Raman spectroscopy identified that the samples consist predominantly of high-density polyethylene, a material often improperly discarded in nature. The plasticlasts exhibited low sphericity, with particles generally ranging from angular to subangular. The samples with types of green, varied between 0.2g and 2.7g, with densities ranging from 0.6 g/cm³ to 0.9 g/cm³ and diameters from 1 to 2.5 cm. Characterization of plasticlasts is crucial for understanding their formation and consequences in nature, as well as establishing connections with human actions in Anthropocene context.

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Combining thermodynamic principles of (de-)doping with drift-diffusion concepts of ions to simulate electronic responses of organic electrochemical transistors

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Organic electrochemical transistors (OECTs) are viable options as potential transducers between ionic fluxes and electrical signals. Although OECTs have been heavily investigated experimentally, the fundamental processes, that govern the functioning of this type of device, are still debated in the literature [1-3]. While first approaches to model OECTs relayed on a capacitive description of the ion uptake of the semiconducting layer[1], more recent ones attempt to describe the ionic flux on more fundamental drift-diffusion concepts [2]. Other works approach the functioning of OECTs solely by the thermodynamic principles of the (de-)doping reaction involved [3]. All of these models can reproduce the response of experimental devices to some extend but are incapable to include all parameters that evidently influence the functioning of real OECTs, especially when describing the transient-response regime. Our work aims at combining the drift-diffusion approach, which is appropriate to model the ion concentration distribution within the OECT, with the thermodynamic approach, that describes the conversion of ion concentration and electrical potential to electronic charge carrier density. In this conference contribution, we will present our strategy to merge the aspects of these methods together with first results of our implementation of the drift-diffusion description of the ion concentration profile in a simplified 1D picture.

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Comparing the two-photon absorption cross-section in the first and second therapeutic windows for chalcone-ligand tetraphenylporphyrins

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Organic compounds having nonlinear properties are critical for increasing light penetration into tissues by allowing absorption within biological spectrum windows. Porphyrins, a unique class of molecules, possess a remarkable property: a high triplet quantum yield facilitating singlet oxygen generation, crucial for photodynamic therapy (PDT) applications. When coupled with a significant third-order nonlinearity, termed two-photon absorption (TPA), these molecules become even more effective photosensitizers for PDT as they enhance tissue depth penetration [1].

This study aims to ascertain the two-photon absorption cross-sections of different chalcone-ligand tetraphenylporphyrins, each demonstrating triplet quantum yields in the order of 30%. To characterize this property, we utilized a femtosecond pulsed laser, and an Optical Parametric Amplifier, allowing for a wide excitation wavelength range. This setup facilitates the measurement of the fluorescence response of the molecules following the simultaneous absorption of two degenerate photons. Additionally, a well-characterized molecule, free-based tetraphenylporphyrin (TPP), serves as a reference for each measurement [2]. We anticipate that the cross-sections of the chalcone-ligand tetraphenylporphyrins will exceed those of TPP due to their increased molecular asymmetry, thus enhancing their potential as effective PDT photosensitizers.

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Developing Nanostructured Films for Enhanced Environmental Sensing

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With the advancement of industrialization, there was an increase in human negligence, with several compounds being discarded directly into the environment, causing their degradation. Among these compounds, a class in abundance is heavy metals[1]. Among them, the most dangerous is mercury, which is widespread in air, water, and soil and can induce damage to the central nervous system[2], gastrointestinal, and respiratory[1]. Although mercury sensors exist, there is an urgent need for more accessible, more sensitive, and simple sensors. Therefore, this work aims to study the structuring of nanostructured films for application in sensors to detect mercury. For this, a perylene derivative was studied, which are macrocycles of excellent stability[2], processed in evaporated and Langmuir form, deposited on glass substrates using PVD and Langmuir-Schaefer techniques. The growth of the films was monitored by UV-Vis absorption spectroscopy, and their morphology and structuring were characterized by micro-Raman (optical microscopy coupled to Raman spectrograph). The partial results showed excellent deposition of the films, with homogeneous morphology and possible presence of molecular organization, inferred by UV-Vis and fluorescence analyses. The following steps include film analysis by FTIR, AFM, and the application of film-based sensors to detect mercury.

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Development and Characterization of Metal Phthalocyanine Nanostructured Thin Films for Electrochemical Lead Detection

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The presence of heavy metals in water and soil, originating from industrial activities, poses a serious threat to both the environment and human health. Lead (Pb), which has been widely used in electronic materials, can accumulate in organisms, causing problems in child [1]. The monitoring of lead in water is essential for the effective management and mitigation of these environmental hazards. This work aims at the fabrication and characterization of nanostructured thin films of metal phthalocyanines in electrochemical sensors for lead detection. Phthalocyanines are highly conjugated macrocycles, which give them excellent electroactivity and photoconductivity [2]. Hence, a study was conducted with gallium and copper phthalocyanines, processed through the Langmuir-Scheafer technique, and deposited onto glass. The growth of the films was monitored by UV-Vis absorption spectroscopy, and their structure were characterized by micro-Raman. The UV-vis spectra indicated the linear growth of the films as the layers increased, evidenced by the increase in intensity of the absorption bands with each deposition (CuPc, λmax = 734 nm and GaPc, λmax = 707nm)) suggesting uniform structure and potential molecular organization. The Raman spectra showed characteristic peaks related to isoindole strech (1529 cm-1), benzene strech (and 1590 cm-1) pyrolle strech (1340 cm-1) and pyrolle breath (1140 cm-1). The initial results indicated a high-quality deposition of the films. Subsequent steps will include FTIR and AFM analyses, as well as the utilization of the film for lead detection, aiming to enhance the sensor performance.

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Development of a biosensor using gold-silica nanocomposites and NS5A-1 peptide onto screen printed electrodes for anti-HCV detection.

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The Si-Au nanocomposite holds significant promise across various fields,especially in biosensors,where its properties such as conductivity,increased surface area,and structure can enhance sensitivity,selectivity,and stability.This study explores the use of the Si-Au nanocomposite combined with the NS5A-1 antigenic peptide to develop a biosensor for detecting anti-HCV antibodies,aiding in Hepatitis C diagnosis.These components were applied onto printed,and disposable electrodes using Tyvek□ as a substrate,and graphite with organic solvent for printing.They were prepared with pre-cut molds,separated into counter/reference and working electrodes,with graphite + base deposited.For Si-Au nanocomposite and peptide preparation,the peptide in methanol was added to dispersed Si-Au solution and subjected to an ultrasonic bath.Dynamic light scattering(DLS) confirmed peptide incorporation,with the average diameter increasing from 406 nm to 928 nm post-NS5A-1 peptide addition,indicating enhanced Si-Au interaction.Biosensor assembly involved silk fibroin(SF) adsorption onto printed electrodes,followed by nanocomposite addition.Cyclic voltammetry(CV) monitored biosensor assembly,revealing nanocomposite adsorption through increased voltammogram area by 2.7 µA.V.Atomic force microscopy(AFM) confirmed the presence of clusters observed in DLS.Once the biosensor was completed,electrodes were exposed to varying concentrations of anti-HCV antibodies.CV measurements were conducted using a phosphate-buffered saline(PBS) electrolyte to monitor changes in system capacitance with increasing antibody concentration.These results showed that the combination of disposable,flexible,and low-cost screen-printed electrodes with gold-silica nanocomposites and the NS5A-1 peptide resulted in more sensitive biosensor applications.

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Development of an electrical impedance-based immunosensor for fetal red blood cell detection as a potential diagnosis of fetomaternal hemorrhage

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Fetomaternal hemorrhage (FMH) involves the transfer of fetal blood into the maternal bloodstream, often resulting from disruptions in the placental barrier. This process underlies conditions like perinatal hemolytic disease, which can lead to severe fetal complications, even death. The detection and quantification of fetal red blood cells in the maternal circulation is crucial to mitigate these consequences for both the mother and the fetus. Considering the importance of diagnosis, in this work an immunosensor was developed to detect fetal cells. This device was assembled using a commercial anti-CD71 monoclonal antibody associated with silk fibroin (SF) as an immobilization matrix, employing the Layer-by-Layer technique, on an interdigitated gold electrode. Electrical impedance spectroscopy (IS) measurements were performed for the detection process. As a proof of concept, human umbilical cord blood (UCB) and adult peripheral blood (PBA) samples were analyzed by flow cytometry (FC). Confirmation of anti-CD71 immobilization on the electrode-SF structure was achieved through PM-IRRAS measurements with an increase in the band near 1500 cm-1. The samples were added on immunosensor and the patterns were evident in the readings considering the capacitance values. IS measurements of the immunosensor subjected to the UCB sample were close to 0.30 nF at 10Hz, while for the PBA samples they were lower than 0.10 nF at 10Hz. These results show its potential as a technology at the point of care, the immunosensor developed here can help in the diagnosis of FMH, thereby facilitating timely intervention and improved maternal and fetal outcomes.

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Development of a sensor using Molecularly Imprinted Membrane (MIM) for the detection of Methylene blue

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Molecularly Imprinted Membranes (MIM) are part of Molecular Imprinting Technology (MIT), which creates selective sites in a matrix to memorize a target molecule's template.[1] Initially developed for separation membranes, MIMs are also applicable in sensor developments. This work focuses on Methylene Blue (MB) as a target molecule once MB is a dye widely used and known for its potential environmental and health risks. Detecting MB is thus necessary, and the work's goal is to develop an electrochemical sensor for MB detection using MIM. Initially, π-A isotherms of DPPC with and without MB were studied, showing an increase in the mean molecular area and fluidity for DPPC monolayer in the dye's presence, indicating interactions between DPPC-MB. The sensor was fabricated using the Langmuir-Schaefer (LS) deposition method, employing DPPC phospholipid and PAH polyelectrolyte. Deposition involved DPPC with PAH in the aqueous subphase, and similarly for the system with MB, using ITO glass as the substrate. MIM formation involved removing the dye from the electrode via cyclic voltammetry in KCl (0.1 mol/L). Both DPPC+PAH films and those containing MB were analyzed using cyclic voltammetry and UV-Vis spectroscopy, confirming dye presence and its removal. Atomic Force Microscopy (AFM) revealed greater roughness in films with MB, validating the successful dye removal for MIM formation. Subsequently, electrodes with MIM were immersed in MB solutions, effectively absorbing the dye into the film's cavities, and enabling MB detection.

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Development of chemical sensors based on polyaniline/poly (lactic acid) nanofibers

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The exploration of nanoscale materials has become a crucial domain in the pursuit of novel materials with diverse applications, emphasizing the production of polymeric nanofibers and nanoblends using various techniques across scientific research fields [1-3]. Among the most prominent techniques for obtaining nanofibers from polymeric materials, Solution Blow Spinning (SBS) stands out [1,3]. The materials obtained through this technique have a wide range of applications, including filters, optical and chemical sensors, tissue engineering, controlled drug release, medicinal dressings, among others [1-3]. This research explored the obtaining nanofibers of polyaniline (PANI) and of polylactic acid (PLA) for use as electrical chemical sensors. PLA is a thermoplastic aliphatic polyester, biodegradable, and derived from renewable sources, known for its excellent mechanical properties and transparency, and its applications include fields such as medicine and food packaging, among others [3]. PANI is a semiconducting polymer with the potential for high electrical conductivity, a property easily controlled by the concentration of dopants during its synthesis [3]. This polymer has been extensively studied for applications in solar cells, electronic devices, and other areas, being considered an extremely versatile conductor. The combination of PANI/PLA composites obtained by SBS presents itself as a highly promising approach for sensor applications. The characterization of these materials will be carried out through morphological, structural, and electrical techniques.

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Developments of nanofibers of polyaniline/polylactic acid/titanium dioxide for applications as biosensors.

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Driven by unique properties distinct from larger-scale counterparts, nanoscale materials have become a crucial domain in the pursuit of novel materials with diverse applications, emphasizing the production of polymeric nanofibers and nanoblends using various techniques across scientific research fields [1-5]. This study focuses on obtaining nanofibers of polyaniline (PANI), a semiconducting polymer, and polylactic acid (PLA), a biodegradable thermoplastic aliphatic polyester derived from renewable sources, doped with titanium dioxide ($TiO2$) for use as biosensors. The method used for its synthesis was the Solution Blow Spinning (SBS), an outstanding among the most prominent techniques for obtaining nanofibers of polymeric materials [1,5]. The results obtained, so far, showed that the SBS technique was highly effective for the production of nanofibers. Furthermore, impedance tests were carried out and presented satisfactory results, indicating the possibility of using the nanofibers as capacitive sensors. The evaluation and characterization of the electrical properties of the material are still in progress, focusing on its later application as a biosensor.

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Does agreement with experimental data prove a theoretical model?A novel drift-diffusion approach for steady-state responses of organic electrochemical transistors and comparison to existing model

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Among the notable advantages of organic semiconductors over traditional inorganic materials, the ability to possess mixed ionic and electronic conductivity stands out as particularly interesting. For example, it enabled the development of the organic electrochemical transistor (OECT), a transducers of ion fluxes into electronic current [1]. Most advances and performance improvements of OECTs, however, were accomplished based on more controlled device fabrication and the use of novel synthed materials. A targeted material design suggested by a profound theory of the working mechanisms of OECTs, is in fact still missing. For the rational optimization of OECTs and OECT-based applications, however, it is essential to have theoretical models capable to predict and analyze the experimental data. In this conference contribution, we will first extend the commonly used capazitive model [1]. Second, we present a drift-diffusion approach based on which we determine the ion uptake by the mixed conductor, which enables an alternative expression for the source-drain current. By comparing to experimental data, we will show that both models, as well as a thermodynamic model recently proposed [3], can describe the I-V characteristics of OECTs with same margins of error, although the individual model parameters arise from different physical and chemical fundamentals. By correlating, the individual expressions, we discuss interconversions which allows to analyze literature data from the past century from the viewpoint of each model. Based on the conclusions drawn we will conclude guidelines for a good experimental practice to benchmark OECT devices.

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EC-SERS detection of diquat using screen-printed gold electrodes

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In recent decades, a new class of compounds capable of significantly damaging water quality has been identified and classified as emerging pollutants. This class includes surfactants, personal hygiene products, pharmaceutical products, plasticizers, pesticides, and their degradation products, among others. Diquat (DQ) herbicides have high toxicity to humans and are harmful to the environment [1]. Furthermore, there is no legislation in Brazil that requires water supply companies to carry out DQ detection tests. Therefore, for environmental and public health reasons, it is essential, in addition to implementing public policies and specific legislation, to develop techniques and methods for detecting, monitoring, and controlling this compound in the environment. In this work, we exploited the electrochemical surface-enhanced Raman spectroscopy (EC-SERS) detection of diquat in ultrapure water using screen-printed gold electrodes (DRP-220BT, Metrohm Drop-Sens). The analysis of SERS spectra at various redox potentials (-0.1 V to -1.1 V) revealed different DQ species on the electrode surface. These spectra were obtained for 10-4 mol/L DQ using a laser line at 633 nm.

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Effects of Plasma Cleaning on ITO Substrates and Polymer/ITO Interface in Organic Electronic Devices: Morphological, Optical, and Electrical Insights

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The technological advance in organic electronic devices necessitates studying substrate influence on their optical, electrical, and morphological properties. Many works empha the benefits of ITO plasma treatment on device parameters. However, scientific results on quantitative morphological aspects, turn-on voltage, and ITO/active layers barrier after plasma cleaning are limited. We studied argon, oxygen, and nitrogen plasma cleaning effects on ITO and subsequent consequences on active layers and final device. Contact angle behavior after plasma treatment indicates increased wettability on ITO with longer plasma time, providing greater homogeneity. First and second-order statistical functions evaluated surface fractal behavior. Statistical analysis revealed oxygen plasma resulted in more uniform surfaces post-cleaning, with greater correlation length. Here, we go beyond, showing that the MEH-PPV overlay's topography is affected; manifesting polymer/substrate interaction and polymer organization modification. Using the Fowler-Nordheim model, we estimated ITO/active layer barrier height, showing significant correlation with injection threshold voltage. Ideality factor decreased from 11.08 for untreated ITO devices to 7.56 for oxygen plasma-treated ones. With PEDOT:PSS introduction, ideality factor reduced to 3.75. Surface relief images and current-voltage curves suggest different surface treatment affects polymer/ITO interface.

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Electrical and optical properties of polyaniline/oxides films producing by surface polymerization.

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Semiconductive polymer composites have gained significant attention in the past decade [1-2]. Polyaniline (PANI) has been extensively researched, yet surface polymerization methodology has received limited attention [1-2]. This research aims to produce composite films incorporating titanium dioxide (TiO_2), tin dioxide (SnO_2), and zinc oxide (ZnO) into PANI. These oxides exhibit versatility in multiple applications, and their integration into PANI aims to enhance overall functionality and performance.

TiO_2, known for its wide energy gap (approximately 3.2 eV), is commonly utilized in polymer composites. The present study utilized commercial anatase-phase [3-4]. SnO_2, a semiconductor with diverse technological applications, is used in solar cells, liquid crystal displays, and gas sensors [5]. ZnO, a versatile semiconductor applied in gas sensors, ultrasonic oscillators, and transparent electrodes in solar cells, was obtained based on modifications from the work of K.G.B. Alves et al. [6]. The films were produced using surface polymerization techniques, drawing from modifications of the methodology outlined by Park C. H. et al. [7]. The films underwent electrical and optical characterization, demonstrating significant potential for applications in various fields.

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Electrical characterization of liquid-gated transistors based on reduced graphene oxide towards neuromorphic behavior

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The area of machine learning (ML) evolved at an unprecedented pace at the beginning of the 21st century. Algorithms overcame the performance of humans in a myriad of tasks; playing chess, and the recognition of patterns in images and sounds, to mention a few. Following this success, the concern about the consumption of energy to train the ML models has also increased. However, the digital computer is not particularly efficient for this task. In comparison, the human brain has highly parallelized processing ability with an amount of 10^{15} operations being realized simultaneously, which results in an efficiency of 20fJ per operation [1]. Interested in the unparallel capacities, researchers started the development of devices that could mimic the behavior of the neural system together with the possibilities to work in an artificial neural network. Such devices are called neuromorphic devices. Here, we investigated the potential ability of electrolyte-gated transistors (EGTs) based on few-flake reduced graphene oxide (rGO) to perform neuromorphic functions. Particularly, we evaluated the time-dependent current response of rGO EGTs when a train of squared pulsed voltage was applied to the gate. The channel current after the stimulus was measured for a different number of pulses (1 – 50 pulses) varying the period (10ms – 45s) and the time interval between the pulses (10ms – 60s). Short low voltage pulses (< 1V) induced in rGO EGTs excitatory postsynaptic current of the order of few seconds. Conversely, long-term memory (t > 10 min) was achieved when a threshold voltage and a minimum pulse width were employed. Synaptic devices have a range of applications beyond computation, such as (bio)sensing [2] and bioelectronics [3], which makes rGO EGTs versatile electronic devices.

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Electrochemical Reduction of Cysteamine/Graphene Oxide Film on Screen-Printed Gold Electrodes aiming Electrochemical Immunosensor Development

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Recent advances in medicine, agriculture and food engineering have continually encouraged the development of new techniques, methods and analytical devices. One of the main demands is the creation of devices for diagnosing and monitoring diseases, such as biosensors that present high selectivity and sensitivity, cost-effectiveness, speed, portability, and user-friendliness. The use of graphene oxide (GO) to modify the working electrode of an electrochemical immunosensor is interesting, either for its semiconductor characteristics after partial reduction or its ability to bind to proteins in their oxygen portions. In this work, screen-printed gold electrodes (SPGE) were modified with a self-assembled monolayer of Cysteamine Hydrochloride (Cys) followed by a GO layer. Through cyclic voltammetry and electrochemical impedance spectroscopy we investigated experimental parameters to optimize the growth of the Cys/GO film: the adsorption time, concentration of the GO suspension, and the number of electrochemical reduction cycles. The ideal concentration and adsorption time were defined as 10 mmol/L and 30 min for Cys, and 0.5 mg/mL and 3 min for GO. Raman spectroscopy analysis (633 nm) allowed to investigate structural changes following the electrochemical reduction cycles. The characteristic carbon materials bands appeared at 1350 (D band) and 1580 cm-1 (G band) and relative intensity (ID/IG) increased from the as-prepared GO film to the reduced films, indicating augmented structural defects and suggesting a decrease in the of sp2 domains. Also, a shift in the G band position towards lower wavenumbers was noted (about 9 cm-1), indicating the reduction of GO (similar behavior is observed for chemical reduction). In conclusion, we have fabricated and characterized self-assembled Cys/GO films on commercial SPGE aiming for future applications as support to antibody loading towards an immunosensor for Dengue diagnosis. Acknowledgments: SBPMat, INEO, Capes, and FAPESP.

Electrochemical sensor with PANI thin films for ascorbic acid detection

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This study developed an electrochemical sensor to detect ascorbic acid (AA) using polyaniline (PANI) drop-casted thin films. PANI is chosen for its ability to alter physical properties when exposed to chemicals. The PANI synthesized used in this study showed higher solubility in polar solvents, in addition to being substantially less dense. Two sensor designs were applied using PANI thin films. Two sensors were fabricated by drop-casting PANI on FTO and screen-printed electrodes (SPE). The methods used for the electrochemical transduction were cyclic voltammetry (CV) and linear sweep voltammetry (LSV) to measure different concentrations of AA. The CV method showed a sensitivity of 13 ± 2 μA/decade, while LSV showed 9 ± 1 μA/decade, indicating potential for sensor development. Employing disposable SPEs aims for broader applications due to their miniaturization , simplicity and cost-effectiveness. This study demonstrates the feasibility of developing electrochemical sensors based on PANI to detect antioxidant agents, with potential applications in different areas.

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Electrolyte-gated transistor applied as a dosimeter

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A dosimeter is a device that measures the captured dose of external ionizing radiation incident on it. There are several types of dosimeters, whose response is based on changes that the incident radiation promote in the physical and/or chemical properties of the active layer of the device. In this work, it was developed a dosimeter based on an ion gel electrolyte-gated transistors (EGTs). To quantify the sensing response, a sequence of typical electrical measurements in transistors is carried out, whose sensing can be detected e.g., through changes in the electrical properties formed at the electrolyte/semiconductor interface. The EGT structure is based on Indium-tin-oxide (ITO) interdigitated electrodes to form the source and drain; poly(3-hexylthiophene-2,5diyl) (P3HT) as the channel; the electrolyte film is an ion gel composed by poly(vinylidenefluoride-co-hexafluoropropylene) (P(VDF-HFP) and (1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide [EMIM][TFSI]) [1]. The gate is an ITO/PET film. The ion gel film alone receives the X-ray dose, before to being transferred to EGT, which changes its molecular conformation structure when compared to one who did not receive radiation. Dosimeter quantification was based on the typical transistor parameters extraction, comparing performance of EGTs using ion gel without irradiation and those who received doses of 10Gy and 20Gy. More significant results were obtained when the ionic doping of the channel has already occurred in the EGT, making it operates as an organic electrochemical transistor (OECT). The hysteresis profile of the transfer curve shows considerable changes, and distinctions can be measured through the threshold voltage shift value. The EGT structure studied shows promise for use as a dosimeter, e.g. for radiation in radiotherapy treatment.

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Electronic Structure of Natural L-Amino Acids by Density Functional Theory

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Amino acids are the building blocks of life as building blocks of nucleic acids and also show a fluorescence emission in the UV region of the electromagnetic spectra, making them as good candidates for biosensor devices. In this work, we show our results for the electronic structure of some amino acids, such as glycine, alanine, arginine, cysteine, glutamate, asparagine and tyrosine, by means of Density Functional Theory calculations [1] within the B3LYP exchange correlation functional. We have used both the 6-31G and 6-311G atomic basis set as well to describe the molecular wavefunctions. [2] Physical quantities such as dipole moment, total energy, band gap, electrostatic potential and infrared and Raman spectra were also evaluated. From the obtained results, it is interesting to remark that the different amino acid side chains produce significant variations in these physical quantities. In terms of dipole moment, there is a large difference from the other amino acids in arginine, which has a dipole of 15.5 Debye, while the rest remain in the range of around 4.0 Debye. Most of the obtained values for their band gaps (HOMO-LUMO energy difference) were around 5 eV and also show interesting fluorescence spectra. We are now extending our study to the formation of the peptide bond in order to check its influence on the fluorescence emitted by these systems. [3]

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ENHANCING ORGANIC SOLAR CELLS WITH SELF-ASSEMBLED MONOLAYERS: A SURFACE AND INTERFACIAL INVESTIGATION

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For optimizing organic solar cells (OSCs), the engineering of hole transport layers (HTL) plays a pivotal role in achieving higher efficiency and stability. This study investigates the effectiveness of the Br-2PACz molecule as a novel self-assembled monolayer (SAM) on indium tin oxide (ITO)-coated substrates, focusing on both rigid and flexible substrates. Br-2PACz SAMs have promising electronic properties and compatibility with oxides such as ITO, shifting its work function and acting as a substitute for the commonly used PEDOT:PSS HTL. Various deposition techniques were explored to identify optimal conditions for forming uniform and organized SAMs on different Glass/ITO and PET/ITO substrates. We employed atomic force microscopy (AFM) for topographical information and Kelvin probe technique to obtain work function values. The latter revealed significant differences in work function of ITO coated by Br-2PACz, indicating the influence of ITO morphology and deposition method on the film properties. Furthermore, SFG vibrational spectroscopy [1], provided insights into the molecular orientation and organization of Br-2PACz on these substrates, shedding light on the molecular packing and alignment relative to the substrate surface. Such molecular-level organization is critical for the efficient transport of holes and the reduction of recombination losses at the HTL/anode interface. The combined AFM and SFG spectroscopy approach not only validates the promising application of Br-2PACz in enhancing OSC performance but also provides a framework for future studies on buffer layer materials and their interaction with various substrates.

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Evaluation of absorption in minimum inhibitory concentration bioassay for conjugated polymer and silver nanocomposite

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Aiming to study the influence of bioactivity on optical properties, samples of silver nanoparticles (AgNP) and conjugated polymer nanoparticles (CPN) derived from fluorene and thiophene were tested, along with the nanocomposite, against E. coli (MO). UV spectra were obtained before and after incubation for the minimum inhibitory concentration (MIC). Two groups of curves were compared: MIC curves before and after complete inhibition; and curves with complete and partial inhibition of MO. In general, some curves exhibited behavior with negative absorbance and a change in baseline due to MO in the medium. When analyzing the first group of curves for AgNP, the band at 400 nm, attributed to silver, was perceived. However, in the 24h curve, this material was consumed to inhibit the MO, resulting in a change in the curve pattern. This could be attributed to the silver nanoparticles returning to their cationic form (as Ag+), which would promote the displacement of maximum absorption to smaller wavelengths than expected [1,2]. The second group of curves provided information that, as the AgNP interacted and inactivated the MO, the band appeared more negative, proportional to its inhibition capacity. At concentrations following the MIC, this occurred more subtly, since not all MO were inactivated. In the case of the nanocomposite, regardless of the proportion, they exhibited a very similar behavior. The stability of the CPN stands out, which avoids drastic disturbances in the profile, intensity, and displacement of the curves. Finally, it is concluded that UV detection of MIC is possible, as a pattern in the behavior of all the analyzed samples was observed, demonstrating the possibility of applying these materials in optoelectronic devices.

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Expansion of the Electrochemical Model in Organic Electrochemical Transistors (e-OECT): Considerations regarding the channel's conductivity

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Organic Electrochemical Transistors (OECTs) have attracted significant interest in recent years due to their ability to transduce ionic flux into electronic signals with high gain. These devices' operations are based on ion migration from the electrolyte to the bulk of the channel, promoting its oxidation/reduction. Thereby resulting in substantial current densities at low operating voltages. OECTs devices are successfully applied in neuromorphic computing, biosensors, and logic computing [1]. Despite the successful implementation of OECTs, the fundamental processes that regulate their operations and sensing capabilities, remain unclear. Recently, a model based on the electrochemical and thermodynamics principles has been developed and applied to OECT architecture [2]. It was shown to be capable of describing the steady-state OECT behavior, which was associated with the electrochemical characteristics of channel-electrolyte interaction and device operation. Now we propose a model expansion, considering the residual undoped channel's conductivity (σ_0). The model was compared to its original version, and the effects of the modification over the steady-state and transconductance curves were evaluated. In addition, the expansion was applied to experimental data of OECTs and OECT-based inverters. σ_0 conductivity parameter addition promoted a better adjustment between theoretical and experimental curves when compared to the original model, especially for depletion-mode OECTs, and improved the results interpretations and device's understanding.

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Exploring imidazopyridine ligands in tetraphenylporphyrins: possible application for photodynamic and photothermal therapy

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Molecules with light-absorbing capabilities exhibit diverse post-absorption energy liberation properties, including heat dissipation or emission of different light wavelengths. Porphyrin molecules have emerged as promising candidates for photodynamic therapy (PDT) or photothermal therapy (PTT) due to their unique attributes. Effective photosensitizers in PDT must possess key characteristics, such as high triplet quantum yield and singlet oxygen generation. The former facilitates the transition from a singlet excited state to a longer-lived triplet state, prolonging interaction time. Engaging with triplet oxygen molecules induces their conversion to reactive singlet oxygen species, triggering cytotoxic effects and leading to cell death [1]. Conversely, for PTT, a molecule with a high internal conversion rate is required, dissipating absorbed energy predominantly as heat.

In this study, we investigated neutral and cationic tetraphenylporphyrins with imidazopyridine ligands to elucidate their electronic states and determine their radiative and non-radiative rates, including the intersystem crossing rate, influenced by the triplet quantum yield. Our objective was to understand distinct ligand features. Additionally, these molecules demonstrate promising singlet oxygen generation and cytotoxic effects against *E. coli* [2], demonstrating the importance of elucidating their photophysical properties. Measuring the triplet quantum yield entails meticulous techniques; thus, we employed a double pulse excitation method with a femtosecond pulsed laser, centered at 515 nm. Analysis of the resulting two-fluorescence decay curves allows accurate determination of triplet quantum yield [3], informing potential applications.

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Exploring PVK Functionalization with a Small Condensed Molecule for Improved Emissive Efficiency in OLED

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Organic Light-Emitting Diode (OLED) has emerged as the premier material for cutting-edge technology manufacturing, owing to its related advantages that align with the demands of today's society. However, its manufacturing process remains tied to complex methods. Polymers stand out as an alternative to overcome this issue due to their ease of processing, enabling serial manufacturing processes. Polyvinylcarbazole (PVK) was one of the pioneering polymers employed as an emissive layer in OLEDs. While PVK is easy to synthe and offers high color purity, its emissive efficiency in OLED devices is lacking [1]. Therefore, this project aims to investigate PVK functionalization with a small condensed molecule to enhance emissive efficiency [2]. Initially, PVK was synthed via cationic reaction ($\eta = 80.3\%$). To activate PVK ends for the subsequent functionalization step, the carbazole units underwent bromination using N-bromosuccinimide (NBS) ($\eta = 34.8\%$). Finally, the anthracene unit was incorporated into the PVK backbone through a Suzuki-Miayura cross-coupling reaction ($\eta = 90\%$). Comprehensive characterization of all samples was conducted using NMR-1H/13C, TGA, GPC, UV-vis spectroscopy, optical microscopy, profilometry, cyclic voltammetry, and spectrofluorimetry. The NMR results showed the characteristic and broad peaks corresponding to the proposed structures. The optic bandgap, aligns with the expected blue emission, around 3 eV, supported by cyclic voltammetry indicating high oxidation potential values ≈ 1 eV. Thus, the proposed polymers were successfully synthed and the primary results exhibited the expected emission in the blue region, indicating that the anthracene unit maintained PVK's blue emission.

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Fabrication and characterization of Organic Electrochemical Transistors: Towards a Comprehensive Evaluation of Existing Models

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The Organic Electrochemical Transistor (OECT) is based on the property of some organic films to possess both ionic and electronic conductivity. These systems, also known as organic mixed ionic electronic conductors (OMIEC), enable the conversion of ionic flows into electrical signals[1]. Although many experimental data have been published over the last years and several comparisons with theoretical expressions have been discussed, the underlaying models are still highly debated. This is because they arise from different physical and chemical fundamentals such that different works consider certain parameters but ignore the influence of others. Our work therefore aims at obtaining a more comprehensive view by scanning systematically as much experimental conditions as possible and evaluate the applicability of the different models. This includes the choice of the electrolyte (solvent, salt, and concentration), the OMIEC (material, additives, post-fabrication treatments), the architecture of the device (geometry, contact and substrate material). In doing so, better indication can be given where and to what extend each model fails in describing the responses of real OECT devices and, thus, enables the formulation of an improved model that combines the different approaches. In this conference contribution, first measurement will be presented in which the PEDOT:PSS based depletion-mode OECTs are analyzed focusing on the properties of the electrolyte. In particular, NaCl, KCl, and LiCl solutions in water are studied considering concentration from 0.01 M to 1 M. Furthermore, we compare the obtained results to a capacitive model [2], a thermodynamic model [3] as well as a recently developed drift-diffusion model.

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Fabrication of microfluidic channels using direct laser writing

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Laser fabrication techniques [1] allow the production of several miniaturized devices, which are often required in technological application. In these techniques, due to the precise control of the laser beam, it is possible induce changes in the surface or inside the sample, achieving structures with high resolution and without shape limitation. Laser fabrication techniques also ensure great reproducibility of the manufactured devices, an essential feature for many high-tech areas. For instance, microfluidic channels are important structures employee in miniaturized platforms, and can be easily produced using laser fabrication systems [2]. In this work, we evaluate the fabrication of microchannels in borosilicate glasses or acrylate bulks, using CW (405 nm) or pulsed lasers (Q-switched EOM, 532 nm, 100 mJ – single pulse). We developed a dedicated mechanical-computational system to move the sample. Using motorized stages, we are able to move the sample in xy plan, while to change the sample in the z-axis, we use a manual micrometer. The laser beam is focused into the sample using microscope objectives. We evaluate different parameters for the laser fabrication process, such as, the sample translation speed and intensity of the laser beam employed during the manufacturing procedure. We also use distinct microscope objective (with different numerical aperture – NA and work distances – wd), to evaluate the resolution achieving in our fabricated channels. The resulting structures were analyzed by transmission optical microscopy. Our preliminary results indicate that we are able to produced microchannels with resolution about of hundreds of micrometers.

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Impact of crystal violet concentration on silver colloid aggregation and, consequently, on SERS signal

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The surface-enhanced Raman scattering (SERS) technique favors the detection of target molecules at low concentrations. In this study, SERS spectra of crystal violet (CV) were obtained using colloidal silver nanoparticles (AgNPs) substrate. The objective was to study the effect of CV concentration on the aggregation of AgNPs. Typically, the SERS signal increases with analyte concentration up to a maximum value. This behavior is related not only with the analyte concentration increase but also (in many cases) with the aggregation of nanoparticles, resulting in a greater number of hot spots. After that, the analyte tends either to stay in excess in the colloid or to form a thicker layer on the surface of the nanoparticle aggregates, preventing SERS spectra of increasing in intensity continuously. In the case of CV, the results showed that at low CV concentrations, a weak SERS signal was obtained and negligible changes in the and zeta potential of AgNPs were observed, suggesting minimal AgNPs aggregation. The most CV intense SERS signal occurred at 3.6×10^{-7} mol/L, which was attributed to the highest level of AgNPs aggregation, confirmed by e zeta potential (+3 mV) results. However, for higher CV concentrations, the SERS signal dropped significantly, contrary to expectations. The latter could be associated with colloid degradation (precipitation due to excess of aggregation). However, and zeta potential values obtained for CV at 9.1×10^{-7} mol/L were 110 nm (average) and +14 mV, respectively, revealing indeed a decrease of AgNPs aggregation. The current hypothesis is that the positive charge of CV favors CV-AgNPs interactions to the detriment of AgNPs-AgNPs interactions.

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Impact of Temperature on the Aggregation of L-Cysteine-Modified AuNPs in the Presence of Acephate

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Pesticides are chemicals used in crops in order to control pests on the plantations. However, their irregular use can lead to negative effects on environment and human health. Among these agrochemicals, we can highlight acephate[1] (ACE), an insecticide of the organophosphorus family with the highest degree of irregular use in Brazil between 2017 and 2018. Then, there is a need to develop an effective approach to control its presence in the environment. In this work, we used gold nanoparticles stabilized with citrate (AuNPs) and functionalized with L-cysteine (CYS). The kinetics ruling the interaction between CYS and AuNP were studied and the effect of ACE onto the formation of AuNP-CYS complex was monitored. For this purpose, UV-Vis extinction spectroscopy was used for monitoring the AuNP plasmon band in the absence and presence of CYS, ACE or their mixture (CYS/ACE) at different temperatures: 24, 37 and 50 °C. Fourier-transform infrared absorption (FT-IR) and Raman scattering spectroscopies were employed to investigate the adsorption of CYS on AuNPs and the system's potential to detect ACE was evaluated monitoring the UV-Vis spectral changes by the presence of the pesticide. The FT-IR and Raman analysis showed that CYS was adsorbed on the AuNP surface. The UV-Vis extinction spectra revealed a shift of the plasmon band from 520 to ~630 nm in the presence of CYS ($1x10^{-5}$ M), confirming its aggregation for all the temperatures, being faster at 50 °C. In the presence of ACE, the aggregation of the AuNP+CYS was weaker than observed in its absence, mainly at lower temperatures (24 and 30 °C). In summary, the results show that ACE inhibits AuNP-CYS aggregation, mainly at lower temperatures, revealing the potential of the system as a colorimetric sensor.

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Imparting Graphene Oxide and Laccase into Lipid Langmuir-Blodgett Films: Potential Biosensing Platforms for Phenolic Compounds in Bioelectronics

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This research endeavor focused on immobilizing graphene oxide and laccase within lipid Langmuir-Blodgett films, a promising avenue for bioelectronics applications. Specifically, we aimed to explore the feasibility of these integrated films as biosensors for detecting phenolic compounds. In this study, we employed the Langmuir monolayer technique to integrate the Lacase enzyme and graphene oxide into lipid films composed of 1,2-dimyristoyl-sn-glycero-3-phosphate acid (DMPA). These lipid films were subsequently transferred onto solid support as Langmuir-Blodgett (LB) films to assess their enzymatic activity. Lacases are known for their exceptional ability to oxidize various phenolic substrates. We utilized the "salt out" strategy in the aqueous subphase to ensure optimal enzyme adsorption at the air-water interface and sequential transfer to the solid support. Characterization of the floating monolayer involved Surface Pressure-Area isotherms, Surface Potential-Area Isotherms, Surface Rheology using oscillating barriers, Brewster angle microscopy, and polarization-modulated infrared reflection absorption spectroscopy. The adsorption of the enzyme and graphene oxide at the air-water interface led to monolayer condensation, resulting in higher surface pressures for smaller molecular areas. The enzyme's catalytic activity was evaluated using UV-vis spectroscopy, revealing activity levels not previously observed using pure water as an aqueous subphase. Further characterization of the immobilized film was conducted using quartz crystal microbalance and fluorescence spectroscopy. Remarkably, catalytic activity was observed in the films of laccase immobilized with graphene oxide, and further characterization using electrochemistry to evaluate the bioelectronic device for energy storage. We hypothec that graphene oxide may contribute to preserving this activity for extended periods during storage.

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Improving the performance of Organic Field-Effect Transistors through Interface Functionalization with Self-Assembled Monolayers

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Organic Field-Effect Transistors (OFETs) have attracted significant interest as essential components of flexible organic electronics. They offer several advantages, such as cost-effective processability, flexibility, and stretchability, making them ideal for innovative applications. OFETs are three-terminal devices with the drain and source terminals separated from the gate by a dielectric. When voltage is applied to the gate, charges accumulate at the dielectric/semiconductor interface, so that the drain-source current can be modulated by the gate voltage. The dielectric/semiconductor interface plays a critical role in this process as its chemistry influences the structure of the organic semiconductor at the interface, thereby affecting the mobility of charge carriers. In this study, we will employ Sum Frequency Generation (SFG) vibrational spectroscopy to probe the conformational organization of insulating self-assembled monolayers (SAMs) at the dielectric/semiconductor interface. Additionally, the SAMs will be characterized by their wettability and Atomic Force Microscopy (AFM). The impact of SAMs on OFETs performance will be assessed by observing changes in their electrical characteristics. We will explore the interface effects on bottom-gate, top-contact transistors that use P3HT and Al2O3/SAMs as a semiconductor and dielectric, respectively. These OFETs are an excellent system for our objective because they can operate at low voltage and provide a high on/off ratio [1]. Through this study, we aim to understand how to control the performance of OFETs by modifying the device interfaces.

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Influence of chloride oxidation state on electrochemical doping of polythiophenes

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The optoelectronic characteristics of polythiophenes undergo significant alterations upon exposure to electrolytes and the application of an electric potential, a phenomenon known as electrochemical doping. This process has garnered recent attention in the development of organic electrochemical transistors for biosensing and neuromorphic computing applications [1]. However, a comprehensive understanding of anion migration into the polymeric matrix, crucial for effective doping, is still not well understood. In this study, we explore the impact of chloride anion oxidation state on the electrochemical doping of a commonly used semiconducting polymer, poly(3-hexylthiophene) (P3HT). Aqueous electrolytes comprising 0.1M NaCl or NaClOx ($1 \leq x \leq 4$) were employed, providing varying oxidation states from -1 to +7. Doping levels were assessed using two-terminal DC and AC conductivity measurements in conjunction with spectroelectrochemical analysis. Additionally, output and transfer characteristics of an electrolyte-gated organic transistor were examined to establish correlations between chloride oxidation state and device performance. Our findings contribute to a deeper understanding of anion migration within the polymer matrix, pivotal for achieving efficient electrochemical doping, with implications for biosensing applications targeting diverse ion species.

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Influence of the acceptor unit in the electrochemical and optical properties of terpolymers based on benzothiadiazole and diketopyrrolopyrrole

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The donor-acceptor (D-A) approach with alternating electron-rich (D) and electron-deficient (A) units along the conjugated polymer backbone, is an effective method to control the optical and electrochemical properties of conjugated copolymers [1]. In this work, two conventional D-A copolymers and random terpolymers D-A1-D-A2 composed of fluorene (D), benzothiadiazole (A1), and thiophene-diketopyrrolopyrrole-thiophene (A2) as building blocks were designed, synthesized, and analyzed in terms of optical and electrochemical properties. The D-A1, D-A2, and D-A1-D-A2 systems (with the D:A1:A2 molar ratio equal to 1.0:0.75:0.25) were synthesized using a Suzuki cross-coupling reaction. The chemical structure of the copolymers was determined by NMR. The electronic spectra of binary D-A copolymers showed an intermolecular charge transfer band (ICT) at 445 and 650 nm for D-A1 and D-A2, respectively. By incorporating 25% of the electron-withdrawing diketopyrrolopyrrole derivative (A2) into the D-A1 structure, the random terpolymer D-A1-D-A2 showed a small blue shift in the ICT bands, suggesting that the absorption spectral ranges of the terpolymers could be adjusted by controlling the molar ratio of A1 and A2 units, which act as moderate and strong accepting units, respectively. Regarding luminescence, green charge transfer emission (535 nm) from the D-A1 unit and red charge transfer emission (658 nm) from the D-A2 segments were observed. Initial findings indicate that the redox potentials of the D-A1-D-A2 structures can be effectively adjusted by incorporating varying proportions of the A2 unit into the polymer chain, demonstrating that terpolymer synthesis is a simple and effective strategy for tuning the optical and electrochemical properties of conjugated polymers.

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Interactions of Baicalein with DPPC and A375 Derived Cell Membrane Models

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Baicalein, a natural antioxidant with antiviral properties,[1] interacts with plasma membranes, yet the precise mechanisms remain elusive. Understanding these interactions at a molecular level is crucial for elucidating its therapeutic effects. In this study, lipid membranes derived from 1,2-dipalmitoyl-sn-glycero-3-phosphocholine (DPPC) and skin primary melanoma lipid extract (A375) were utilized to assess the molecular interactions of baicalein. Langmuir monolayers[2] of DPPC and A375 were characterized using surface pressure versus occupied molecular area (π-A) isotherms. Langmuir films were formulated with DPPC or A375 and baicalein at various concentrations (5:1, 2:1, 1:1, and 1:2 lipidic extract to baicalein ratios).The isotherms revealed a displacement of curves containing baicalein above those of pure DPPC and A375, indicating the insertion of baicalein molecules into the DPPC and A375 monolayers. Additionally, data from DPPC and A375 and baicalein monolayers were used to calculate the compressibility modulus. Baicalein insertion into DPPC monolayers decreased the maximum compression value from 145 mN/m to values between 140 mN/m and 108 mN/m. Similarly, interaction with A375 monolayers reduced the maximum compression value from 63 mN/m to values between 57 mN/m and 49 mN/m. These findings provide insights into the molecular mechanisms underlying baicalein's therapeutic properties.

Investigating of outdoor real-world lifetime in PTB7-Th:PC71BM organic solar cells: Insights from stability studies and characterization techniques

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One of the main obstacles limiting the application of organic photovoltaic (OPV) devices is performance degradation. Advancements in donor and acceptor materials and interfacial materials for improved charge carrier collection and phase separation morphology have contributed to high power conversion efficiency (PCE). However, commercialization requires extending device stability for at least 10 years to make these devices financially competitive. To understand how OPVs would work in real-world conditions, it's necessary to study the device in contact with the external environment, including changes in day and night and possible climate instability. This helps gain a better understanding of the processes of generation and recombination of photo-generated charge carriers, from their generation to their collection by the electrodes. In this study, we investigated the outdoor real-world lifetime of PTB7-Th:PC71BM organic solar cells. Outdoor lifetime studies followed ISOS-O2, with J-V measurements periodically acquired under natural sunlight and without encapsulation. We focused on factors that can form traps or barriers to charge carriers. Additionally, changes in the parameters Voc, Jsc, FF, PCE, and resistances were observed with exposure, and the T80 of the devices was calculated. Through photovoltaic measurements combined with other experimental techniques, it is possible to confirm chemical degradation and changes in materials due to outdoor exposure at the nanoscale.

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Investigating the entrapped water within a self-healing Layer-by-Layer (LbL) structure and its associated properties.

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Nanosystems play a crucial role in advancing technology, particularly in fields like organic electronics, soft robotics, sensing, and biosensing, where tailored properties are essential for progress to enable the realization of multiple functionalities and refined features. A notable attribute is the self-healing property seen in the LbL thin film of PEI/PAA (poly(ethyleneimine) (PEI) and poly(acrylic acid) (PAA)) [1], affected by entrapped water altering material properties [2]. Hence, for applications in organic electronics, it's crucial to investigate the mechanisms for altering the amount of entrapped water and their impact on the electrical properties in each scenario. A study on the growth of (PEI/PAA) films under various relative humidity (RH) conditions was conducted, the change in the amount of entrapped water is expected. Impedance tests are conducted for each layer during the LbL assembly, with careful control of the RH at four different values. I vs V characterizations are performed after deposition. Those characterizations allow a qualitative analysis, in contrast, time-resolved TeraHertz spectroscopy was conducted due its well-known dependence on water in this spectral range and may enable quantitative water analysis [3]. Impedance measurements and I vs V characterizations demonstrate increased capacitive components and a negative differential resistance (NDR) effect in films grown at higher RH levels. Previous measurements using THz spectroscopy show a delay in the pulse from the wettest film to the driest film. Our findings indicate an increase in entrapped water with changing growth conditions and the potential for quantification.

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Investigating Weak Localization and Weak Antilocalization in Multilayered Reduced Graphene Oxide Flakes

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Since the isolation of graphene in 2004 and the experimental observation of its unique electronic properties, the research field of two-dimensional materials (2DMs) has received enormous scientific interest [1]. Among the large variety of existing 2DMs graphene oxide (GO) has emerged as a crucial material for scalable manufacturing of diverse applications. However, GO is an insulating material and to improve its conductivity, one can rely on diverse reduction methods (e.g. thermal, chemical, electrochemical, etc.) to obtain reduced graphene oxide (rGO). In this study, we aim to compare the influence of the reduction process on the electrical transport properties of multilayered rGO thin films which were prepared by different methods such as electrochemical and thermal reduction. From magnetotransport measurements, we observed weak localization (WL) and weak antilocalization (WAL) phenomena in such films. These anomalous transport properties are typical of disordered systems, being essentially caused by quantum-interference of the charge carriers [2]. In our discussion, we will analyze the WL and WAL effects in rGO films, considering the underlying physics and possible implications on the performance of rGO-based electronic devices.

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Investigation of PDOF-co-PEDOT copolymer/silver nanoparticles nanostructured films synergy for chlorpyrifos SERS sensing

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Sensors composed of nanocomposite materials have been widely explored as they exhibit enhanced properties resulting from the compounds of which they are composed. Thus, the combination of conjugated polymers (CP) and metallic nanoparticles can bring several advantages, such as structural stability, increase in surface area and improved thermal, optical and conductive properties [1]. In this work, the synergy between the copolymer poly (9,9-dioctylfluorene-co-3,4-ethylenedioxythiophene) (PDOF-co-PEDOT) and silver nanoparticles (AgNP) and their effect as a surface-enhanced Raman scattering (SERS) sensor for the detection of the pesticide chlorpyrifos (CLP) will be investigated. PDOF-co-PEDOT in macro- and nanoform (NCP) was used to produce the films in order to analyze the influence of this factor on the morphology of the films and the SERS effect. The TEM images show that the AgNP are adsorbed on the NCP surface and form a nanostructure with an average diameter of 90 nm (value according to DLS) and a negative zeta potential (-49.60 eV). These structures could be transferred to a solid substrate and formed films in which the morphology and RMS values (by AFM images) were influenced by the macro- and nanoform of PDOF-co-PEDOT. Pesticide adsorption tests were performed on the SERS substrates. This showed that a minimum adsorption time of 6 hours is required for efficient detection of the pollutant. Furthermore, low concentrations of the analyte could be detected, with a detection limit of 10-7 M and 10-8 M CLP for NCP/AgNP and PDOF-co-PEDOT/AgNP film, respectively, demonstrating the influence of the macro- and nano-status of the CP on the SERS effect.

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Layer-by-Layer films consisting of reduced graphene oxide combined with manganese oxide and niobium oxide for supercapacitor applications

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The integration of novel nanostructured materials has emerged as a growing focus in energy storage research [1]. Carbon-based materials such as nanotubes and graphene, when paired with metallic oxides, have emerged as prominent contenders in this domain [2]. In this investigation, we focused on enhancing an indium tin oxide substrate through the application of films containing a combination of polyelectrolyte polyethyleneimine and graphene oxide, alongside metallic oxides like manganese oxide and niobium oxide, employing the Layer-by-Layer deposition technique. Following the fabrication of the films, graphene oxide underwent electrochemical reduction to yield reduced graphene oxide (rGO). Cyclic voltammetry analysis revealed that the PEI/rGO system exhibited a capacitance per unit area of 20.42 mF cm-2, while the PEI/rGO-MnO2 system demonstrated 36.57 mF cm-2, and the PEI/rGO-NbO2 system showed 30.14 mF cm-2 when utilizing a 1 M potassium chloride electrolyte at a scan rate of 1 mV s-1. Through galvanostatic charge and discharge measurements, specific capacitance values of 144.85 F g-1 and 183.77 F g-1 were attained for systems containing manganese and niobium, respectively, compared to 29 F g-1 for the PEI-rGO system, under a fixed current of 20 microamperes. Remarkably, by combining both manganese oxide and niobium oxide, the capacitance per unit area surged to 119 mF cm-2, while the specific capacitance soared to 353 F g-1. In terms of long-term stability, all films exhibited negligible capacitance loss, with none exceeding 2.57% after 10,000 cycles. These findings underscore the feasibility of integrating these materials via the LbL technique, elucidating the synergistic interplay between manganese oxide and niobium oxide for as a potential energy storage system.

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Luminescent properties of quinoline lactones

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Quinolines are organic compounds with interesting luminescent properties that vary according to the nature and position of the groups attached to the heterocyclic ring [1]. This work describes the synthesis and luminescent properties of new quinoline lactones. The compounds were synthed from an assisted microwave multicomponent reaction between tetronic acid, anilines, and aromatic aldehydes. The quinolines obtained content indole and triazole group attached in the heterocyclic ring. The compounds were subjected to UV-Vis absorption and fluorescence analysis when diluted in different solvents [2]. The results show that the quinolines have two absorption bands, with higher intensity at 345-360 nm. The emission bands were observed between 415-520 nm, and quantum yield varied at 4-9% relative to standard 9,10-diphenyl anthracene. The compounds showed solvatochromism as a function of the analyzed solvent (DMSO, chloroform, ethanol, and H_2O). Analysis carried out in DMSO with different concentrations of TFA (Trifluoroacetic acid) showed that the quinolines with the triazole group have a decrease in the intensity of the emission band proportional to the increase in the acid concentration. Although preliminary, the studies indicate a possible use of these quinolines as pH sensors

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Magnetic-plasmonic nanoparticles with dual electrochemical and SERS function

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Magnetic nanoparticles (MNP) are widely investigated in biomedical field for applications as hyperthermia and drug targeting systems. The control by an external magnetic force has also included MNP in sensing applications for the enrichment and separation of targets from the complex matrix. Here, we have synthesized gold nanoparticles conjugated to MNPs (AuMNP) focusing on electrochemical and SERS (surface-enhanced Raman scattering) sensing applications. First, magnetite nanoparticles were obtained by the coprecipitation method using phytic acid as a soft-template [1]. Subsequently, the gold salt was adsorbed and reduced by sodium citrate. The average of gold nanoparticles was 10.2 nm and the MNPs presented diameters of 17-23 nm. The UV-vis absorption spectra confirmed the extinction bands of MNP and the plasmonic band of gold. When applied to SERS detection of dopamine (DA), the magnetic concentration of AuMNP suspension allowed increased reproducibility and repeatability. For instance, the repeatability test indicated a standard deviation of 19.4 a.u. and 800 a.u. for the magnetically concentrated and suspension (without magnet) measurements [1]. Analyzing the effect in the SERS detection of methyl parathion (MP), the magnetic concentration promoted an improved sensitivity (SERS intensity of 1827 a.u. and 998 a.u for the magnetic concentrated and suspension, respectively). In the electrochemical study, AuMNP with different concentrations of MP were magnetically concentrated before the electrochemical analysis, and promoted enhanced peak current. In summary, the magnetic concentration of the AuMNP demonstrated the capacity to increase reproducibility and repeatability in SERS detection as well as provide enhanced sensitivity for both SERS and electrochemical detection.

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Maximizing electrochemical efficiency of laser-induced graphene electrodes

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Laser-induced graphene (LIG) is a three-dimensional porous material formed through the laser irradiation of a polymeric precursor (in most cases, polyimide, commonly known as Kapton). Its versatility lies in its ability to adopt tailored properties based on manufacturing parameters, making it both cost-effective and industrially compatible. Since the discovery of LIG in 2014 [1], this material has been used in electrochemistry and electronics for the most diverse applications, including sensors and biosensors [2]. Here, we study the influence of the number of laser scan repetitions on the electrical and electrochemical properties of LIG electrodes. Electrochemical sensors were fabricated in a three-electrode configuration onto commercial polyimide using a 5 W diode laser operating at 445 nm, with a focus diameter of 0.3 mm. The laser scan speed was kept constant, and the number of scans was varied from 1 to 3, in order to vary the electrode LIG tchickness. The electrodes went under cyclic voltammetry analysis using the Randles-Sevcik equation to estimate their effective area. The effective electrode areas ranged from 16 mm² to 28 mm² under laser conditions of 50% of power and scan speed of 100 mm/s. These electrodes were then subjected to an electrochemical treatment using constant potential (-1.5 V) in a phosphate-buffered saline solution (PBS). After treatment, a considerable increase in the electroactive area was achieved, reaching values close to 100 mm2. These results suggest that the produced LIG electrodes hold potential as a feasible option for the development of cost-effective yet high-performance electrodes for applications in sensors, biosensors, micro-capacitors, and transistors. Acknowledgement:

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Mechanisms of synergistic effects of phototherapies to enhance tumor cells death gold nanorods conjugated with toluidine blue-O

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Phototherapeutic approaches hold significant promise for the non-invasive treatment of aggressive tumors, particularly through the combined application of heat induction and oxidative pathways. Herein, the phototoxicity of gold shell-isolated nanorods conjugated with toluidine blue-O (AuSHINRs@TBO) against human colorectal tumor cells (Caco-2) was explored, utilizing the synergistic effects of photodynamic (PDT) and photothermal therapies (PTT). The incorporation of AuSHINRs@TBO expanded the isotherms, indicating strong attractive forces that hindered the insertion of these positively charged particles into the lipid films. PM-IRRAS highlights attractive electrostatic interactions with negatively charged groups of the Caco-2 lipid extract. Mechanistic insights into these effects were gained through studies employing bioinspired tumor membranes, utilizing Langmuir monolayers of Caco-2 lipid extract. Upon irradiation, these monolayers exhibited an approximately 1.0% increase in surface area, suggestive of reactive oxygen species (ROS) generation and subsequent interaction with lipid extracts, leading to hydroperoxide formation. The oxidative effects were facilitated by the penetration of AuSHINRs@TBO into polar groups of the extract, enabling oxidative reactions with alkyl chain unsaturations. Evaluation of mitochondrial metabolic activity (MTT) in Caco-2 cell cultures revealed a photothermal effect attributable to AuSHINRs, facilitated by enhanced light absorption via localized surface plasmon resonance (LSPR). Furthermore, the introduction of AuSHINRs@TBO resulted in phototoxicity against Caco-2 cells, with oxidative processes, such as hydroperoxidation, contributing to a reduction in cell viability from 85.5% to 39.0%[1]. These findings were further supported by confocal fluorescence microscopy, which highlighted the Caco-2 plasma membrane as the primary site of cell death induction.

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Melanin as a signal amplifier in biosensor construction for detecting anti-HCV antibodies

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Melanin is a semiconductor biopolymer characterized by its natural electronic delocalization, which promotes electron transport, making it promising for application in electronic devices. In this context, the association of melanin with the antigenic peptide NS5A-1 was explored in the construction of biosensors for detecting anti-HCV antibodies, as an alternative in the diagnosis of hepatitis C. This study aims to investigate the efficacy of melanin coupled with NS5A-1 in biosensor construction for anti-HCV detection with higher efficiency than those reported in the literature. Initially, melanin and NS5A-1 were prepared in methanol, for a final dispersion with 0.5 mg/mL of peptide and 0.1 mg/mL of melanin. This mixture was immobilized in Layer-by-Layer (LbL) films on screen printed carbon electrodes, using silk fibroin (SF) as the immobilization matrix, and cyclic voltammetry (CV) measurements were performed following the deposition of each layer at a potential of -0.6 V to 0.6 V. The adsorption of these materials was confirmed by two methods: increasing capacitance and atomic force microscopy (AFM). The SF/melanin+NS5A-1 film was also subjected to concentrations of anti-HCV to verify its detection from the voltammogram areas. Compared to SF/NS5A-1 biosensors reported in the literature, it was observed that the results presented a similar current difference at low potentials (7 µA), however, there was a significant increase in the voltammogram areas. The SF/melanin+NS5A-1 system expressed a higher value, indicating it to be more capacitive, meaning with greater electron passage, leading to enhanced biosensor sensitivity. Thus, melanin proves to be efficient in amplifying the electrode signal and promising for the construction of the biosensors in question.

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Nanostructured films incorporating WO_3 microflowers and reduced graphene oxide as electroactive interfaces in supercapacitor devices

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The study dedicated to new nanostructures is crucial in the development of innovative energy storage devices such as adaptive displays, artificial skin, and wearable technologies [1–3]. In this context, our study focused on fabricating layer-by-layer (LbL) films comprising 1 to 20 bilayers, incorporating tungsten oxide microflowers (MF) dispersed in polyethylenimine (PEI) and graphene oxide (GO). These films were evaluated for their electrochemical properties to assess their suitability as supercapacitors. The MF were characterized using microscopic techniques and spectroscopic analyses. These analyses provided insights into the morphology, crystallinity, and orthorhombic phase of the MF. Initially, electrochemical measurements were conducted to reduce GO (rGO), followed by cyclic voltammetry measurements from 0.0 V to 0.7 V at 1 $mV.s^{-1}$ to 100 $mV.s^{-1}$, and charge-discharge cycling. Our findings revealed an improvement in specific capacitance with an increasing number of bilayers, with a capacitance retention rate of 83% over 1,000 cycles. The LbL films reached a maximum specific capacitance of 2,9 mF/cm^2 at a current of 140 $\mu A/cm^2$. Additionally, atomic force microscopy (AFM) measurements demonstrated an elevation in film roughness proportional to the number of bilayers, which correlated directly with the observed specific capacitance enhancement. Thus, the LbL films comprising MF and rGO exhibited favorable characteristics and demonstrated promising potential for supercapacitor applications.

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Nanostructured ZnO Semiconductor Films for Applications in Electronic Devices

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Abstract: Currently, the use of environmentally harmful materials in the production of devices is considered a major challenge in the development of electronic devices. Consequently, the search for semiconductor active layers, in general, has intensified. Among the available materials, zinc oxide (ZnO) stands out as one of the most studied due to its environmentally friendly nature and its ability to be diluted in water [1]. Additionally, with the advancement of material technology, there is a growing demand for the study of nanostructured films with various compositions and distinct morphological, electrical, and optical characteristics. This study aims to manufacture and characterize films based on ZnO. To achieve this, the spin coating technique was employed, involving depositions of solutions containing zinc oxide and polymers. Optical measurements were conducted using UV-vis, revealing the films' transmittance, which exhibited values above 60% for longer wavelengths and experienced a decay to zero in the ultraviolet range. Furthermore, scanning electron microscopy (SEM) and a wettability measure were employed to examine their surface energy. At the same time, electrical properties were characterized at room temperature and low temperatures using a cold finger and a two-point technique. These results contribute to the understanding of the performance of these films, highlighting potential technological applications. This, in turn, opens avenues for future innovations in nanostructured electronic devices, such as sensors for the detection and monitoring of marine pollution, for instance.

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non-symmetric tristriazolotriazines with room temperature mesomorphism

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molecular non-symmetry is a feature of interest in the liquid crystals (LCs) research due to the observed decrease in the transition temperatures, enhanced mesophase stability, and the prevention of crystallization through glass transitions, when compared to the symmetric compounds.[1,2] This behaviour is of great interest for technological applications. However, for the tristriazolotriazines (TTTs) based LCs research, to date, there has been no description of non-symmetric molecules, i.e., those with unequal arms. Therefore, this work aims to fill this gap by reporting two non-symmetric compounds derived from the TTT core (311 and 331). The non-symmetric 311, presented a waxy appearance at room temperature, no mesomorphic behavior was identified, as well as no crystallization during the cooling processes, remaining in super cooled amorphous state. On the other hand, 331 presented room temperature Colh phase with impressive stability, ranging from -13 to 201 °C, significantly better than the 9-chain symmetric TTT, which presented Colh between 133 and 177 °C.[3] The Colh mesophase was confirmed by XRD, which showed a typical diffraction pattern in addition to the π-stacking broad peak. Compound 311 and 331 presented intense fluorescence in the blue region with quantum yields of 52 and 35% in solution (37 and 67% in thin film), respectively, higher than the 6% reported for the 9-chain symmetric TTT. The findings show that non-symmetry is promising for the TTT derivatives, this being the first case reported, and whose behaviour may favour future applications attempts.

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Optical properties of MEH-PPV thin films produced by different methods

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Charge transport in thin films is a complicated phenomenon that depends on the degree of ordering, resulting in the formation of traps or charge centers [1]. The study of anisotropy in polymeric thin films plays an important role when the polymer is used as the active layer, helping to understand how inter and intrachain charge transport occurs [2]. MEH-PVV is a conjugated polymer with semiconductor properties, with side structures that modify its solubility and emission properties, rendering it an excellent semiconductor for electronic devices [3]. In this study, the effects of, optical response, and anisotropy of MEH-PPV thin films produced by drop-casting (DpC), spin-casting (SC), and Langmuir-Blodgett (LB) techniques were investigated. The results indicate a preferential planar ordering at the interface of LB thin films. DpC films exhibit a certain degree of ordering of transition dipoles induced by the solvent. SC films shows shorter conjugation length induced by the technique. DpC films exhibit absorption maxima similar to LB films, the conjugation lengths are greater in the latter. DpC films also show lower anisotropy values due to the predominance of volume effects, while LB films show higher values due to preferential orderings. Absorption spectra suggest that conjugation lengths in SC films are shorter compared to LB films. In conclusion, the LB technique demonstrates potential in the linear growth and ordering of multilayered films.

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Optimizing impedance response stability in microfluidic electronic tongues through flow control

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In the developing area of artificial taste technology, microfluidic electronic tongues (me-tongues) mark notable progress in automated taste evaluation [1,2]. Previous research has not extensively explored the influence of measurement conditions, particularly fluid dynamics, on the performance and accuracy of these devices. This study investigates the performance of a me-tongue equipped with four sensing units: one bare interdigitated electrode (IDE) and three IDEs coated with ten bilayers of layer-by-layer (LbL) films, each possessing unique electrical characteristics derived from an organic macromolecule, montmorillonite clay, and a conducting polymer. The study assesses the impedance of solutions that mimic basic human tastes within a microfluidic channel under both static and flow conditions. Our results indicate a quicker stabilization of impedance responses under flow conditions across all tested units compared to static conditions. Solutions including distilled water, saccharose, caffeine, NaCl, glutamic acid, and HCl (1 mM concentration) were tested over 60 minutes at a frequency of 1 kHz. Additionally, the enhanced clustering performance of the me-tongue under flow conditions demonstrates its superior discrimination capabilities. The rapid response stabilization under flow conditions suggests that dynamic measurements can significantly enhance the operational efficiency and reliability of me-tongue systems in applications requiring real-time analysis. These findings underscore the potential of me-tongues to transform taste assessment methods crucial for quality control in the food and beverage industries.

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OPTIMIZING NON-FULLERENE ORGANIC SOLAR CELLS THROUGH SIMULATION: INSIGHTS ON PM6:Y6 BLENDS AND BUFFER LAYER ENGINEERING

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Organic Solar Cells (OSCs) are a promising alternative in photovoltaic technology, noted for their flexibility, light weight, and cost efficiency compared to other technologies. This study focuses on the optimization of non-fullerene OSCs, specifically PM6:Y6 blends, with modifications to buffer layers such as electron transport layers (ETL) and hole transport layers (HTL) to identify ideal fabrication parameters. Using OghmaNano software for simulations, we employed the Transfer Matrix Method (TMM) for optical simulations [1] and transient models including Photo-CELIV (Charge Extraction by Linearly Increasing Voltage) [2], Transient Photocurrent (TPC), and Transient Photovoltage (TPV). These methods enabled us to understand the relationship between physical parameters of optimization like layer thickness, donor:acceptor ratio, and material type, providing insights into exciton generation rate, charge mobility, recombination rate, and trap effects in both simulated and experimental OSCs. These adjustments aim to optimize interfacial properties, reduce charge recombination, and enhance device performance through changes in the active layer parameters, different types of PEDOT:PSS as HTL and ETLs such as PFN-Br and PDINN. Our findings offer a deeper understanding of OSCs and underscore the impact of non-fullerene acceptors and buffer layer engineering on final device performance, with data from our simulations helping to achieve higher accuracy, reduce experimental errors, and minimize material waste.

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Optoelectronic p-n junction of organic-inorganic heterostructure of titanium dioxide and quinoline derivatives

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The combination of inorganic and organic semiconductors is becoming increasingly attractive due to several application possibilities in the field of optoelectronics. Within this context, the present work aims to build devices based on thin film heterojunction of titanium dioxide (TiO_2), an n-type semiconductor [1], with quinoline derivatives, which presents acceptor-like centers (p-type organic material) and has luminescence in the blue range [2], an interesting optical property. The quinoline derivative used here is the molecule 4-(6-(diethylamine)-4-phenylquinolin-2-yl)benzoicacid, which is solubilized in organic solvents (acetone and tetrahydrofuran) for deposition via spin-coating. In the other hand, TiO 2 films have been obtained from a sol-gel solution via dip and spin coating techniques. Electrical measurements carried out with parallel FTO contacts (on the film surface) for both materials separately led to a conduction in the order of nanoAmps at ambient temperature and pressure. In vacuum, TiO_2 film has a fall in electrical conduction, showing a potential for applications in the sensing of gases with reducing characteristics. Morphology images obtained by SEM show more homogeneous surfaces when using spin-coating deposition, which may be facilitating the electrical conduction process. Photoluminescence measurements show that the quinoline derivative emits at 485 nm when excited at 205 nm. From the obtained results, it is noted that the combination of quinoline luminescence with the transparent inorganic matrix of TiO 2 has great potential to generate a p-n junction, which can act as a photodiode or transparent transistor of high electronic mobility, since this phenomenon is observed at the junction interface.

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Performance evaluation of PEDOT:PSS and CuNPs coatings in corrosion protection of carbon steel

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Current research into corrosion protection for metals has predominantly centered on polymeric coatings. These coatings may consist of either a single polymeric element or multiple layers that enhance adhesion to the metal surface[1]. Conversely, the deposition of nanoparticles onto the surface of metal alloys has garnered significant attention due to their properties and potential applications across various technological fields, such as catalysis and conductive paints[2]. This study evaluates the efficacy of PEDOT:PSS and copper metallic nanoparticle (CuNPs) coatings in preventing corrosion in CA50 carbon steel. Four epoxy coatings modified with PEDOT:PSS and CuNPs were prepared and subsequently characterized through potentiodynamic polarization measurements in a solution representative of the pore water found in concrete. Additionally, they were analyzed by scanning electron and optical microscopies before and after corrosion tests. The coatings exhibited satisfactory application, demonstrating that greater addition of polymer resulted in thinner layers without negatively impacting corrosion protection. Linear polarization curves of the coated CA50 steel revealed that the composite with a higher polymer addition displayed greater corrosion resistance (57.4x10-12 µAcm-2), indicating an inhibitory efficiency exceeding 10 times compared to coatings with epoxy alone (2.24x10-10 µA cm-2).

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Photodynamic effects on melanoma cell membrane models using methylene violet photosensitizer

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Skin cancer comprises one in every three cancer diagnoses worldwide[1]. Photodynamic therapy (PDT) holds particular significance in managing skin cancer. By utilizing a photosensitizing molecule (PS), PDT generates reactive oxygen species (ROS), including singlet oxygens ($^1O_2$), which can trigger cancer cell death via lipid hydroperoxidation in cell membranes[2]. This investigation unveils interactions between methylene violet 3RAX (VM), a photosensitizing molecule, and lipid membrane models created using monolayers of lipid extracts from A375 and SH-4 melanoma-derived cells on phosphate-buffered saline (PBS) as the subphase with varying VM concentrations. The surface pressure versus area (π-A) isotherms were used to characterize the membrane interaction process products by tracking displacements in surface area. Further analysis using Fourier Transform Infrared spectroscopy (FTIR) on Langmuir-Schaefer (LS) films demonstrated the incorporation of VM into the multilayers of the lipid extracts, offering insights into molecular interactions. The next steps will involve activating the PS to monitor physicochemical alterations within the lipid membranes, with a focus on variations in surface area relative to irradiation time. This approach aims to enhance our comprehension of the molecular mechanisms underlying PDT's efficacy against melanoma, potentially informing the development of more precise and minimally invasive therapeutic approaches.

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Photoinduced absorption spectroscopy: probing charge photogeneration in donor-acceptor systems

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Optical pump-probe experiments are versatile techniques that allow to characterize photophysical processes such as the photogeneration of charges in active materials of organic photovoltaic devices. [1] Continuous-wave Photoinduced Absorption (cw-PA) spectroscopy is a simple, yet efficient approach, in which the pump beam is a modulated continuous-wave laser and a light source of a broad-spectrum emission is the probe. Due to the modulation of the pump beam, measuring the probe transmission results in a small alternating signal, due to changes in the probe absorption at each wavelength induced by the pump laser. This change in transmission can be detected by a lock-in amplifier. Analysis of the resulting difference spectrum indicates photophysical processes such as charge transfer from donor to acceptor materials in active layers of organic photovoltaic devices. [2] In this conference contribution, we present details of our homemade setup and demonstrate the functionalities and fundamentals of the cw-PA technique. Furthermore, we present results obtained by applying the method to the characterization of material combinations used in emerging photovoltaic architectures. In particular, we utilize the method to investigate organic solar cells (OSCs), light harvesting capacitors and surface-mounted metal-organic frameworks.

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Polaron formation via doping process in an organic semiconductor polymer based on thiophene-phenylene

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The polymeric interaction with gamma radiation has been studied since the 1970s, and different effects have been observed depending on the polymer's chemical structure and the energy range used for the irradiation process. In this context, our research explores the doping of the conjugated polymer poly[5-(5-(10-chlorodecyloxy)-2-methoxy-4-(5-methylthiophen-2-yl)phenyl)-5'-(2-(2-ethylhexylo-xy)-5-methoxy-4-(5-methylthiophen-2-yl)phenyl)-2,2'bithiophene] (PTBT46). The study was developed by conducting its photophysical characterization using a range of techniques, including UV-Vis absorption, photoluminescence, photoluminescence excitation (PLE), and Fourier-transform infrared spectroscopy (FTIR). Our findings revealed a remarkable transformation in coloration, pH sensitivity, as well as alterations in its optical and electrical properties when PTBT46 was solubilized in halogenated solvents. Notably, while aromatic groups are known for their resilience to radiation, the role of the side chains becomes pivotal in their interaction with gamma radiation, primarily driven by steric effects. However, it is essential to recognize that ionizing radiation does exert an influence on the thiophene-based aromatic groups, as seen in the case of P3HT. Furthermore, the side chains also contribute significantly to the interaction dynamics with gamma radiation. This groundbreakingly discovery of extrinsic doping effects in organic semiconductors opens up a wealth of highly promising and advantageous applications, as the development of advanced radiation sensors.

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Potential Application of OECTs as biosensor

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Organic Electrochemical Transistors (OECTs) are a class of devices that can be applied as biosensors for the detection of diseases, hormones, etc [1]. To explore this potential in OECTs, devices in planar architecture were manufactured, using ITO as source and drain electrodes, poly-3(hexylthiophene) (P3HT) as semiconductor channel, phosphate-buffered saline (PBS) as electrolyte and platinum as gate electrode. This study analyzes the behavior of OECTs in which recombinant protein green fluorescent protein (GFP), produced by recombinant form in E. coli, was attached at the semiconductor's surface. A transistor containing only PBS as electrolyte was electrically characterized as a reference device, and compared to another one, containing GFP's antibody (anti-GFP), the monoclonal antibody of murine origin anti-GFP clone P66B3H of IgG1 k light chain isotype, dispersed in PBS as electrolyte. The comparison was carried out based on the extraction of the typical transistors parameters, like threshold voltage, on/off ratio, transconductance, among others. With the calculated parameters, it was possible to show their potential application for the detection of diseases using GFP and anti-GFP in the OECT architecture.

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Processing and optical characterization of new materials based on Moringa Oleifera and conjugated polymers for application in organic electronics devices.

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The field of new materials demonstrates its scientific importance in research, not only due to the understanding of various phenomena related to electronic conduction and recombination processes and mechanisms, but also because of its impact on the development of technological products. Within this field, we have electronic polymers, which have been widely applied in electronic and optoelectronic devices. There is also a growing interest in so-called green devices using organic materials. Recent research shows that Moringa oleifera can be a good candidate for the development of these new sustainable technologies. Thus, in this work, a comprehensive study of the production of new materials containing Moringa oleifera seeds and luminescent polymers was carried out, enabling the investigation of their optical and morphological properties to understand changes in the radiative process of the system and a possible application in devices such as biosensors, OLEDs, and JFET (Junction Field Effect Transistor).

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Raman Spectroscopy Analysis of Alizarin for pH-Sensitive Applications

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Alizarin is a red dye organic compound belonging to the anthraquinone class, mainly found in the root of *Rubia tinctorum*. It has historically been used in the textile industry for its pH-sensitive color-changing properties. Beyond its dyeing application, alizarin has emerged as a multifaceted compound with potential in biomedicine. Its unique photophysical properties and pH-dependent behavior make it an intriguing candidate for theranostic application [1]. Diseases often induce microenvironmental pH alterations, such as extracellular acidosis seen in cancer, and pH-sensitive probes are potential candidates for diagnosis in this case[2]. This study aims to characterize alizarin using Raman spectroscopy, focusing on its functional groups and their response to different pH environments. Herewith, two alizarin samples were studied: powdered alizarin and a solution in methanol applied to a glass slide to form a casting film. The Raman spectra obtained showed characteristic peaks corresponding to the anthraquinone ring C-C (centered at 1325 and 1450 cm^{-1}) and C=C bonds (1580 cm^{-1}), as well as the C=O bond (1610 cm^{-1}). These findings lay the groundwork for future investigations into alizarin's application in pH-sensitive theranostic approaches, using its Raman properties for targeted biomedical interventions.

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Reduced graphene oxide electrolyte-gated transistors for detection of microRNA-based stress biomarkers

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Reduced oxide graphene (rGO) is a conductive 2D material that exhibits ambipolar conduction when utilized in thin-film transistors. Particularly, rGO electrolyte-gated transistors (EGTs) enable the development of highly sensitive biosensors [1]. Due to the global impact of stress-related diseases that affect both humans and animals, this work aims to explore functionalization of rGO EGTs with single-stranded DNA (ssDNA) used as a capture probe (DNAcp) to detect miR-34a stress biomarker. The EGT interdigitated source and drain electrodes were coated using a poly(diallyldimethylammonium chloride, PDDA) to immobilize a graphene oxide. Thermal and electrochemical methods were employed to produce rGO. An ultra-high vacuum (10^(-10)mbar) at 350°C was used for thermal reduction, while the cyclic voltammetry technique for electrochemical reduction. Two methods were considered for ssDNA immobilization, 1-pyrenebutyric acid N-hydroxysuccinimide ester (PBASE) and 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride (EDC)/N-hydroxysuccinimide(NHS), using ethanolamine as blocking agents. Transfer curves were obtained by recording the source-drain current in the function of variation gate-source voltage from +0.5 to −0.5 V, with a constant source-drain voltage of 0.2 V. A ssDNA with a similar sequence of the biomarker complement to DNAcp was used in different incubation times and concentrations as negative control. Analytical curves were obtained from 0.01 to 500 fmol L−1 in phosphate-buffered saline (10 mmol L-1, pH 7.4). The best results were obtained for PBASE GO thermal reduction with a linear range from 0.01 to 500 fmol L−1, R2 = 0.996, and attomol-level sensitivity (limit of detection = 9.0 amol L−1). These results can contribute to the development of biosensors for the molecular diagnostics of stress.

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Reduced graphene oxide field-effect transistors gated by chitosan-based electrolytes

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Graphene and its derived materials present distinct physicochemical properties from conventional materials, enabling the development of various new electronic devices. In this study, reduced graphene oxide (rGO) field-effect transistors (FETs) were fabricated through electrochemical reduction of graphene oxide onto interdigitated electrodes and using chitosan as chitosan as gate electrolyte [1]. Initial electrical measurements in the resistor configuration showed good reproducibility of the devices with resistances between 400 and 600 Ohms. In the FET configuration, four chitosan solutions (5 mg/ml) at different concentrations of acetic acid were tested: 1.0, 2.5, 5.0, and 10%. Similar characteristics to graphene transistors were observed where conductivity is modulated by gate voltage around a specific point of minimum conductivity, around 0.66 – 0.70 V. These values did not change with the acid concentration. After drying the chitosan solutions, the devices did not exhibit the same conduction properties. To overcome this issue, a new chitosan-based electrolyte was prepared. In this case, different proportions of glycerol (which acts as a plasticizer) were added to the chitosan solutions [2]. The new electrolytes were deposited on the rGO transistors and dried at ambient temperature. It was observed that the properties of these solid electrolytes were adequate to control rGO FETs as a result of increased ionic mobility with the glycerol amount. Additional characterizations of electrolytes, as well as the rGO FETs, are in progress.

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Reduction of emission lifetime in copper(I) complexes

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Luminescent copper(I) complexes are an alternative to heavy metal-containing compounds such as iridium and platinum for optoelectronics applications. However, the emission lifetime reduction of these compounds is challenging due to the copper atom's relatively low spin-orbit coupling constant. Recently, we reported a [Cu(NN)(PP)]+ complex with 1,10-phenanthroline derivative containing the selenediazole moiety in which the addition of the heavier chalcogens contributed to reducing the photoluminescence lifetime to about 800 ns, the lowest lifetime reported for [Cu(NN)(PP)]+ materials [1]. Furthermore, this lower lifetime enhanced the performance of solution-processed OLEDs [2]. In this work, we explored the effects of the coper-iodide moiety (CuI) on photophysical properties, particularly the lifetime emission. Temperature-dependent photophysical studies and Density Functional Theory calculations revealed a combined thermally activated delayed fluorescence and phosphorescence emission mechanism, with a lifetime between 18.1 to 41 us and a phosphorescence decay rate in the order of 104 s-1, which is higher than usual for copper(I) complexes. Thus, CuI is a versatile moiety for speeding the phosphorescence decay pathway [3]. Blue emitters copper(I)-based complexes were also synthed, combining high emission efficiency, shorter lifetime, and easy synthesis.

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Self-organization of Silk Fibroin into self-assembled films associated with liposomes-melanin for application in biosensors

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Silk fibroin (SF) is a natural protein with unique properties and versatile applications. Consequently, the self-organization of SF has been explored in the manufacturing of various nanostructured materials and structures, such as thin films, hydrogels, nanofibers, and nanoparticles, with a wide range of applications[1]. In this work, the self-organization of SF into nanostructured films and the incorporation of melanin into liposomes were investigated, expanding the spectrum of applications in venous thromboembolism (VTE) biosensors[2]. Initially, the structural self-organization of SF into nanostructured films was investigated using different deposition methods: the molding method, continuous vertical immersion for 2 hours, Layer-by-Layer (LbL) films by vertical immersion with and without drying, and horizontal drop deposition (drop LbL). The adsorption of SF onto the substrate and the formation of nanostructures were influenced by the adsorption method and the drying step, as shown by atomic force microscopy (AFM) images. The LbL technique with drying presented films with regular globular structures and β-sheet structures, as observed in AFM images and circular dichroism (CD) spectra. Dynamic light scattering (DLS), zeta potential, and fluorescence spectroscopy indicated the incorporation of melanin into liposomes. In biosensor construction, films containing melanin incorporated into liposomes showed higher affinity for adsorption. In the immobilization of anti-PDF antibodies and in the detection of different concentrations of fibrin degradation products (PDF), the film with liposomes exhibited the greatest increase in capacitance and conductance. Thus, the possibility of a new device for risk assessment and clinical diagnosis of the VTE spectrum was demonstrated, using liposomes and melanin in liposomes in immunosensors.

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Semi-Interpenetrating Networks of Polyaniline-Lignin for Enhanced Electrochemical Stability

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The increasing demand for renewable energy sources led researchers to investigate new materials for energy storage. Polyaniline (PANI) has been studied as a potential material for supercapacitor electrodes due to its pseudocapacitive behavior, low cost, high flexibility, and easy synthesis. However, the low electrochemical stability of PANI has hindered its performance in continuous operating devices. To address this challenge, an alternative approach involves incorporating a secondary material. Lignin (LIG) is the main constituent of lignocellulosic biomasses and presents a complex phenolic chemical structure. The phenolic groups, which give rise to faradaic reactions, could improve energy storage in supercapacitors based on conjugated polymers [1]. In this work, semi-interpenetrating networks of PANI–LIG were synthed and analyzed in terms of their electrochemical properties to improve the energy storage capacity and to offer a potential solution to overcome the stability issue. The results obtained from cyclic voltammetry showed that LIG improved the electrochemical stability of the PANI, probably due to the intermolecular interactions, such as hydrogen bonds and pi-stacking. Moreover, these interactions also act as a bridge to control the effect of counterions' entry/exit process, which leads to mechanical stress during the cycling process, which can lead to PANI degradation. Furthermore, the electrochemical activity of the LIG structure promotes an increase in the capacitance of the networks through the hydroquinone/quinone redox couple. These results pointed out that the PANI-LIG networks open new possibilities for employing Lignin in various other applications, thereby reducing waste generated by the paper industry and promoting a circular economy through green chemistry practices.

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Smart Sensing: Detecting SARS-CoV-2 with Supervised Machine Learning on a Simplified SERS Platform

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Surface-enhanced Raman scattering (SERS) offers rapid, specific detection of various substances, including the SARS-CoV-2 virus [1]. In this study, we developed a simple SERS biosensor based on a functionalized Au-nanoisland substrate for detecting the SARS-CoV-2 spike S1 antigen [2]. Integrating SERS with machine learning, we achieved precise antigen classification using logistic regression, linear discriminant analysis, and support vector machine. Our approach, utilizing the multidimensional calibration space concept, demonstrates the potential of machine learning in SERS biosensing for accurate antigen detection.

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Structural Properties of Alanine

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Alanine is one of the twenty amino acids composing proteins in our body, classified as non-essential. The interest in amino acids properties in the solid phase emerged at the beginning of this century when luminescence in the visible and ultraviolet range of alanine, doped or not with transition metals, was observed, making it attractive for potential applications in biosensors [1]. In this work, we will present preliminary results for the crystalline structure properties of solid alanine, employing the method of slow evaporation (SEM), obtained by X-ray diffraction of the samples. We also obtained, from theoretical calculations, their structural parameters by using the Density Functional Theory with van der Waals corrections, in order to guide the Rietveld analysis of the obtained X-ray spectra. Our preliminary results show that the alanine crystals formed during the crystallization process exhibit a combination of the β and L crystal forms. Moreover, our preliminary experimental data from thermogravimetry and differential thermal analysis are in good agreement with published experimental data [2], indicating an endothermic peak at 214.9°C (characteristic of the β phase). Further growth experiments via SEM are being conducted, controlling and adjusting the parameters involved in the evaporation method to improve the quality of alanine samples. We hope that our results provide guidelines for future experiments on this subject.

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Supramolecular profile of bilirubin in water

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It is well-known that high bilirubin (BR) levels in mammals' blood are toxic, especially in newborns [1]. BR also signals liver dysfunction, has antioxidant and anti-inflammatory activities, and has morphology switching by external stimulus [2]. Recent studies have shown several prospects for medical application, such as a pharmaceutical agent in bilirubin-based nanoparticle drug delivery or as a signaling molecule. BR's self-assembled structure in water is a determining factor for understanding its properties in water. In this work, we discuss the self-aggregation of BR from its dispersion in water using molecular dynamics (MD) simulations with the OPLS-AA forcefield, implemented in the GROMACS software suite. Cluster analysis as a function of time showed that the small aggregates merge to form a single spherical structure with hydrophobic characterized by radial distribution function (RDF). Accordingly, H-bonds are mostly intermolecular and responsible for becoming the aggregate water-insoluble. Furthermore, we found that central methylenes (C10) that bind portions of UCB dipyrrinones are distributed in the nanoaggregate as regular concentric layers with a radius of 0.42 nm [3].

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Sustainable Conductive Materials: Exploring Graphite Residue for Green Flexible Electronics

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In recent years, there has been growing interest in technologies and devices suitable for flexible and eco-friendly electronics. Consequently, the manufacturing of flexible, low-cost, and environmentally friendly integrated devices has received increased attention. Efforts have been focused on finding new materials to replace conductive metals, leading to the development of conducting polymers, which are now widely used in the market as alternatives to metals. [1,2] One promising approach involves incorporating graphite, which significantly enhances the electrical conductivity of polymers and other flexible materials suitable for sustainable electronics. The electrical conductivity and eco-friendly objectives have spurred research into graphite residues, transforming discarded materials into valuable resources for producing other conductive materials. In this study, we characterize graphite residues from agricultural seed processing using Raman spectroscopy and X-ray diffraction, targeting their future application in the production of green, flexible conducting electrodes. The results indicate that after chemical treatment, the graphite residue consists of pure graphite, showing potential for use in electrode manufacturing. Future steps will involve the electrical characterization of the residue both in its pristine form and within a polymer matrix.

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Synergistic Photothermal and Photodynamic Therapies: Advancements in Nanomedicine for Cancer Treatment

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Gold nanoparticles are valuable photothermal agents owing to their efficient photothermal conversion, photobleaching resistance, and potential surface functionalization.[1-2] Herein, we combined bioinspired membranes with in vitro assays to elicit the molecular mechanisms of gold shell-isolated nanoparticles (AuSHINs) on ductal mammary carcinoma cells (BT-474). Langmuir and Langmuir-Schaefer (LS) films were handled to build biomembranes from BT-474 lipid extract. AuSHINs incorporation led to surface pressure-area (π-A) isotherms expansion, increasing membrane flexibility. Fourier-transform infrared spectroscopy (FTIR) of LS multilayers revealed electrostatic AuSHINs interaction with head portions of BT-474 lipid extract, causing lipid chain disorganization. Limited AuSHINs insertion into monolayer contributed to hydroperoxidation of the unsaturated lipids upon irradiation, consistently with the surface area increments of ca. 2.0%. In fact, membrane disruption of irradiated BT-474 cells containing AuSHINs was confirmed by confocal microscopy and LDH leakage, with greater damage at 2.2 x 1013 AuSHINs/mL. Furthermore, the decrease in nuclei dimensions indicates cell death through photoinduced damage.

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Synthesis and characterization of PEDOT:PSS: Influence of PSS sulfonation on optical and electrical properties

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The polymer blend poly(3,4-ethylenedioxythiophene):polystyrene sulfonate (PEDOT:PSS) is a water-soluble organic compound, which has gained remarkable relevance in organic electronics due to its distinct properties, such as high ionic and electronic conductivities, stability when exposed to air, transparency in visible light and others. Although the oxidative polymerization reaction, [1] which is usually used to obtain PEDOT:PSS, is widely used, one can arise questions about the mechanism that is commonly believed to take place during the reaction. Our work therefore aims at analyzing whether an alternative mechanism occurs or not. To achieve this goal, several conditions need to be studied. In this conference contribution, we will focus on the sulfonation of the PSS and its impact on the final material properties. First, we performed titration of different commercially obtained PSS solutions where we found a discrepancy in the individual sulfonation degree. Second, we increased the concentration of sulfonated groups $(SO_3)^-$ versus non-sulfonated polystyrene units by common sulfonation techniques [2]. Third, we synthesized PEDOT:PSS via the oxidative polymerization reaction using these different PSS solutions. Finally, we performed characterizations during the individual synthetic steps as well as on the final ink. In particular we evaluated the influence of the sulfonation via optical spectroscopy methods, such as UV-vis and Raman, and electrical characterization such as the 4-point method. [3] The last one is the most important, as it will show how conductive the synthesized inks changes upon the different utilized synthetic conditions.

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Synthesis and evaluation of an Eu-BTD-Tb hybrid dyad as emitter for WOLEDs

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A multichromophoric hybrid structure containing the red emitter [Eu(hfaa)$_3$DPA]; the green emitter [Tb(hfaa)$_3$DPA], where hfaa = hexafluoroacetylacetonate and DPA = dipyridylamine; and the blue emitter 2,1,3-benzothiadiazole (BTD) was synthesized as a proof of concept for a single emitter white OLED. In the molecular architecture of the hybrid, the BTD nucleus acts as a covalent bridge between the two rare-earth complexes. The desired material was obtained by reacting the free-NH portions of the complexes with dibromobenzathiadiazole in a copper-catalyzed protocol. FTIR-ATR analyses confirmed the absence of N-H stretching, indicating the formation of the desired hybrid “Eu-BTD-Tb” structure. Multilayered OLEDs with structure ITO/MoO$_3$ mCP/SF$_3$PO: [Eu-BTD-Tb] (10%)/TPBi:[Eu-BTD-Tb] (10%)/TmPyPB/LiF/Al were fabricated based on our previous results [1]. The EL spectrum of the device showed the characteristic transitions of the Eu(III) ion, Tb(III) ion and BTD bridge, with emissions at 612, 543, and 490 nm, respectively. The device displayed reasonable brightness, with a current density (J) of 100 mA cm^{-2} at 13 V, showing limited electrical performance. However, the CIE coordinates (x = 0.32; y = 0.38), confirmed the white emission, suggesting promising results for the development of single-emitter white OLEDs.

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Synthesis of polylactic acid nanofibers incorporating carbon quantum

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In recent decades, scientific research has focused on developing optical sensors for detecting pollutants in water, undesirable chemical analytes in industry, and biosensors for medical and biological applications [1]. Two promising materials for these purposes are carbon quantum dots (QDCs) and polylactic acid (PLA). QDCs are unique fluorescent nanoparticles with easy excitability, a wide absorption spectrum, and a narrow emission spectrum covering the entire visible spectrum [2-4]. PLA is a biodegradable polymer derived from starch-rich plants like corn [5]. This research aims to synthe QDCs encapsulated in PLA nanofibers through the environmentally sustainable process of citric acid carbonization. The QDCs were produced using citric acid, sodium hydroxide, and chloroform [3,4]. The carbonization process involved heating citric acid until liquefaction, followed by pouring into chloroform. The resulting material was also poured into distilled water and an alkaline solution. Different pouring conditions influenced QDC formation, resulting in particles with diverse s and emission ranges. Nanofibers of PLA and PLA/QDCs were manufactured using the Solution Blow Spinning (SBS) technique [1, 6]. This process creates nanofibers through a blowing process, forming mats with varying QDC concentrations. Structural, morphological, and optical analyses were conducted on both QDCs and the produced mats. In conclusion, successful production of nanofibers incorporating QDCs has been achieved. It is anticipated that the PLA and PLA/QDCs nanofibers, as investigated in this study, demonstrate suitable properties for applications in sensor devices.
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$Tb_3Ga_5O_{12}$ single-crystals obtained from controlled crystallization of heavy metal oxide glasses

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One of the best-known compounds among $RE_3Ga_5O_{12}$ (RE = rare earths) is terbium gallium garnet (TGG), commonly used in the form of crystals for the construction of electromagnetic field detection devices, such as Faraday rotators[1,2]. Despite the array of synthesis methods available, production on a large scale faces some difficulties such as low quality of the crystal, significant time for crystal growth, and high cost to manufacture [3]. In this way, new methods of obtaining single crystals of TGG remain in focus. Glasses containing magnetic crystals have attracted attention for their potential in magneto-optical applications. However, achieving the growth of a TGG crystal within a glassy matrix without compromising optical properties poses a complex challenge[4]. In this work, we demonstrate that it is possible to obtain a transparent glass containing the TGG phase as well to isolate the crystal by dissolving the glassy phase. The crystals were observed by optical and scanning electron microscopies and presented cubic shapes with s between 50 to 70 micrometers. The Single-Crystal X-ray diffraction (XRD), EDS, mapping by electron dispersive X-ray spectroscopy, and Raman data confirmed the formation of the crystalline phase $Tb_3Ga_5O_{12}$ cubic space group Ia-3d in the samples.

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Triazine Host Alignment for Guest Perylene Tetraester Emitters in Thin Films

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The latest advances with organic semiconductors have provided competitive optoelectronic devices with new functionalities, as observed for OLEDs, OFETs, OPVs and sensors. The efficiency of these devices depends directly on the molecular ordering achieved by the active layer, since higher order improves charge transport, energy conversion and light outcoupling. In this sense, self-organizing molecules, such as liquid-crystalline materials, effectively play a role in this field. In a previous work, we demonstrated that the molecular alignment of a columnar liquid crystal (ColLC) in a diode structure improved the charge carrier mobility in five orders of magnitude and allowed electroluminescence emission [1]. Here, we investigate a triazine-based ColLC as aligning host for emissive molecules to be applied in the active layer of OLEDs, based on a work where we demonstrated the potential of the photophysical properties of liquid-crystalline triazine-based molecules for alignment-induced enhancement of light outcoupling [2]. As guest emissive molecule we investigated a thermally activated delayed fluorescent compound, which absorption band overlaps with the emission peak of the triazine-based host in order to optimize energy transfer [3]. The photophysical studies demonstrated that for 10.0 wt% concentration of the guest, the host emission is totally converted to the guest with increasing of the photoluminescence quantum yield, which is also influenced by the molecular organization of the medium. In this work we investigated the photophysical behavior of perylene derivatives in 1% wt drop casting films in a triazine (5A) host. The host's emission band coincides with good coupling with the emitters' absorption band, demonstrating good host/guest energy transfer.

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Tungsten oxide-reduced graphene oxide nanostrucutured films for energy storage applications

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The incorporation of new materials is a common practice in scientific research across various fields of knowledge [1,2]. This trend extends to supercapacitors, energy storage devices that have garnered increasing attention in recent decades. In this study, we proposed the incorporation of three distinct materials onto an indium tin oxide (ITO) substrate: Poly(amidoamine) (PAMAM), reduced graphene oxide (rGO), and tungsten oxide (WO3). The chosen method for material adsorption was the self-assembly Layer-by-Layer (LbL) technique. Films comprising 1, 5, 10, 15, and 20 bilayers were prepared and subsequently investigated via cyclic voltammetry and galvanostatic charge-discharge measurements. The findings revealed that in a 1 M KCl electrolyte, films consisting of PAMAM/rGO-WO3 with a higher number of bilayers exhibited the highest capacitances, reaching a maximum specific capacitance value of 73.58 F g-1 at a current of 3.0 µA, accompanied by an energy density of 5 Wh kg-1 and a power output of 60.61 W kg-1. Additionally, the same film demonstrated an area capacitance of 6.8 mF cm-2 at a scan rate of 1 mV s-1. Regarding stability, the films maintained their initial capacitances for up to 2,000 cycles under successive cycling conditions. These results highlight the effectiveness of the LbL technique in fabricating WO3 films with high capacitance values and excellent cycling stability, permitting their application as a supercapacitor electrode.

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Two-photon absorption in Bromo-Chalcone derivatives

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Chalcones are a family of organic compounds with promising nonlinear optical properties considering their small molecular , due to the presence of delocalized electrons. They have relatively simple synthesis, photoisomerization capability, and various interesting pharmacological properties. This study aims to characterize the linear and nonlinear properties of a series of bromo-chalcone derivatives. Initially, the samples were diluted in DMSO, and one-photon absorption (1PA) spectra were measured with the sample in darkness and subsequently under irradiation at 325 nm to investigate E/Z isomerization. The UV-Vis spectra of these samples exhibit, in general, two characteristic absorption bands and photo-irradiation with the 325 nm light systematically decreases the lower-energy band and increases the higher-energy one, with the presence of an isosbestic point. Next, the emission properties of the samples were measured, and only one of them (the one with the amine group as a substituent) showed significant fluorescence, with a quantum yield of about 14%. The mean two-photon absorption (2PA) cross-section of the blend was measured using the Z-Scan technique [1]. Nonlinear optics experiments were performed using 150-fs pulses from a Yb:KGW laser system, which, coupled with an optical parametric amplifier (OPA), allows tuning the excitation wavelength from UV to near-infrared. Almost all samples, except for the one with the amine group, exhibited a low 2PA cross-section, on the order of 30 GM. Conversely, the sample with the amine group exhibited a high 2PA cross-section, exceeding 80 GM for the lower-energy band. In support of the experimental results, computational simulations have been performed through Density Functional Theory (DFT) and using the sum-over-states (SOS) method.

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Underlying mechanism of incorporating carboxyl-functionalized nanodiamonds into cellular membrane models of *Escherichia coli* and *Staphylococcus aureus*

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Bacterial infections pose a global health challenge due to the increasing prevalence of antibiotic resistance. The bacterial envelope comprises the cell membrane and the cell wall, both serving as protective barriers. Variations in the composition and structure of cell membranes between Gram-negative and Gram-positive bacteria influence their responses to antimicrobial agents. Nanodiamonds, especially those functionalized with carboxyl groups (NDCOOHs), have demonstrated potential in combating bacterial infections, including resistant strains, by affecting the bacterial cell membranes and inducing cell death. Nevertheless, the underlying mechanisms of incorporating NDCOOHs into cell membranes of Gram-negative and Gram-positive bacteria remain incompletely understood, and in vitro and in vivo assays limit direct molecular investigations. This study utilizes Langmuir films of cell membrane models from *E. coli* and *S. aureus* to investigate the underlying mechanisms behind the incorporation of NDCOOHs into cell membranes of Gram-negative and Gram-positive bacteria. *E. coli* and *S. aureus* membrane models were examined with the NDCOOHs on PBS subphase, at volume ratios of 1:1, 1:2, and 1:4. The surface-pressure isotherms of E. coli monolayers revealed area shifts of 5.8% ± 1.6% (1:1), 7.1% ± 0.7% (1:2), and 5.7% ± 1.8% (1:4). Conversely, *S. aureus* monolayers exhibited area shifts of 3.5% ± 2.4% (1:1), 11.1% ± 2.5% (1:2), and 5.4% ± 3.8% (1:4). The compressibility modulus (C_s^{-1}) of the *E. coli* Langmuir film did not differ from that of the mixed films, while for *S. aureus*, it varied among the different volume ratios. Together, these results highlight the differences in incorporating NDCOOHs into Gram-negative and Gram-positive bacteria, for which the molecular mechanisms of interaction will be elucidated by in situ infrared spectroscopy (PM-IRRAS).

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Understanding the PEDOT:PSS-based HTL properties in Organic Photovoltaics

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The hole transport layer (HTL) in organic photovoltaics (OPVs) significantly influences both device stability and efficiency, by extracting holes from the active layer and conduction to the anode electrode. Despite its importance, the choice of HTL in technical literature often lacks a rational basis. Typically, OPVs make use of PEDOT:PSS inks as a HTL layer. However, commercial PEDOT:PSS are offered in several distinct products, mostly differing in its conductivity grades. Such changes in conductivity alter the material's Fermi Level, affecting the energy match with the donor's HOMO in the heterojunction (HJ) and the HTL's work function. Ideally, HTL layers must exhibit high-hole conduction, excellent adhesion to the active layer and energy level alignment that favors charge transfer from the HJ. We, therefore, decide to conduct a thorough investigation of the wished properties of PEDOT:PSS-based HTL in OPVs. To accomplish this, the HJ, electron transport layer (ETL) and cathode electrode were fixed, only varying the PEDOT:PSS HTL type. The device structure herein explored was ITO/PEDOT:PSS/PM6:Y6/PDINN/Ag, yielding devices with IPCE of around 10-14%. As for the PEDOT:PSS types, we have used a series of in-house synthed PEDOT:PSS inks, as already reported elsewhere[1]. Also, we have tested several commercially available PEDOT:PSS inks, for instance, the well-known high-conductive Heraeus PH1000, Clevios P and Clevios PVP 4083. For all the devices studied here, we characterized the organic films using UV-VIS, cyclic voltammetry, and photoemission spectroscopy (PES) to assess their energy levels and alignment. As for the OPVs, we have fully characterized them in terms of their electronic output and lifetime measurements. Based on all the results we were able to establish guidelines and rational choices of the correct physical-chemistry properties of PEDOT:PSS-based HTL for OPVs.

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Urbach energy in MEH-PPV thin films: Langmuir Blodgett films

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Both the injection of charges at the interfaces and the transport processes that occur in the semiconductor polymer are influenced by structural disorder and chemical impurities, causing the trapping of charges and the formation of electronic states in the band gap of the polymers that will hinder transport, preventing these materials from performing their intrinsic mobilities. Poly(2-methoxy-5-(2-ethylhexyloxy)-p-phenylenevinylene) (MEH-PPV) thin films were grown by the Langmuir-Blodgett (LB) method. The films obtained were characterized by UV-Vis spectrophotometry to evaluate the growth of the films and also polarized measurements to evaluate the existence of induced ordering through the difference in intensity of the absorption bands under different polarization conditions and was also used to explore the band-optical gap and study the behavior of states located in the gap. These localized states can be evaluated by studying the Urbach energy [1]. It was noted that the Urbach energy decreases with the increase in the number of layers (from 82 meV to 48 meV, under non polarized light) and presents different values in the different polarization directions (from 130 meV to 66 meV parallel and from 126 meV to 65 meV perpendicular to the dipper direction). By increasing the number of layers and moving from a polymer/substrate to a polymer/polymer interaction, the Urbach energy is affected due to the growth of the film microstructure. Preliminary results correlating the Urbach energy and the behavior of the I x V curves show variation in the linear coefficient found, making it possible to study the trap states using different methods.

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Zn:Sn Stoichiometric Ratio Influence on the Electrical Properties of Solution-processed Thin-film Transistors

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Field effect devices are components of interest in microelectronics applications. However, obtaining good devices involves the obtaining excellent field effect transistors. This work provides a systematic study on how the Zn:Sn atomic composition ratio affects the electrical properties of solution-processed zinc tin oxide (ZTO) thin-film transistors (TFTs). By the variation of the zinc acetate dihydrate and tin chloride dihydrate ratio on a 2-methoxyethanol solution and using the spin-coating deposition technique, followed by combustion at 650 K, onto SiO2 (thermally grown)/p-Si (boron) silicon substrates, we were able to fabricate high-performance bottom-gate, top contact thin-film transistors with field-effect mobilities superior to 1 $cm^2.V^{-1}.s^{-1}$. The TFT performance were analysed by the characterization of its electrical properties such as transfers and outputs curves, to obtain the saturation mobility (μ_{sat}), field-effect mobility (μ_{FE}), charge trap density (N_f) and subthreshold swing (SS) parameters. All the electrical characterization were made with the sample inside a cryostat, in dynamic vacuum below 10^{-3} mbar, with the temperature varying from 80 K up to 350 K. From the saturation mobility activation energy dependence on the Zn:Sn stoichiometric ratio, we could determine how the increase on the respective content of Sn in the samples shifts the depth of the gap states in the semiconductor, as well as the charge carrier concentration. The obtained device parameters were used to feed device characteristics simulations used to determine the carrier density profile in the transistor channel.

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EP07-Advanced photonic materials and nanostructures: synthesis, optical properties, and applications

An innovative approach to synthesize and process multifunctional nanomaterials: thin, flexible and transparent films for potential application in photonics

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This talk will demonstrate a novel and innovative route developed in our research group to synthe, stabilize and process complex and multicomponent nanomaterials as flexible, transparent and conductive thin films, to be applied in different technological systems and devices [1]. The so-called liquid-liquid interfacial route (LLIR) allows the preparation of thin and transparent films of different kind of nanomaterials through the controlled assembled of those materials at the liquid interface. Single-, bi-, tri- or multi-component material films can be prepared controlling the thickness, transparence and homogeneity and can be easily transferred to the surface of any solid substrates (including flexible ones) to target technological application. We will present here nanoarchitected materials (bi- or tri-components) obtained by the combination of 2-dimensional materials (MoS2, black phosphorous, graphene), carbon nanotubes, metal and metal oxide nanoparticles, Prussian blue analogues and conducting polymers, demonstrating specific applications as transparent electrodes, electrochromic materials, in photovoltaic devices and SERS substrates, among others. The huge potentiality to get unique materials for photonic devices and systems will be demonstrated and discussed.

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A novel synthetic approach for obtaining luminescent and magnetic single crystal garnets

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Luminescent single crystals are important from both scientific and commercial perspectives. They can be synthed using different techniques, and can find applications across various fields such as LED technology, infrared sensors, nano-thermometry, dosimetry, persistent luminescence, white light emission, magneto-optical current sensors, etc. In this work we will present the results of a new synthetic approach enabling the production of unique single crystals ($TR_3Ga_5O_{12}$, $TR_3Al_5O_{12}$ and $TR_3Al_{(5-x)}Ga_{(x)}O_{12}$, where TR=rare earths) utilizing glasses as reactional medium. In a first step, a desired composition in rare earths is mixture in a batch containing $97(40PbO\text{-}20GeO_2\text{-}15Ga_2O_3(Al_2O_3)25Bi_2O_3)\text{-}3TR_2O_3$ (in mol %). After melting the batch at 1200 °C a controlled cooling process is applied to allow the growth of the crystals. This method enables the synthesis of crystals ranging from one to up 200 µm in size. The resulting single crystals are then stabilized inside the glass matrix, and following a chemical treatment with nitric acid, can be extracted and selected. Characterization of the crystals involves various techniques including X-ray diffraction, micro-Raman spectroscopy, luminescence analysis, optical microscopy, and scanning electron microscopy. Additionally, the magnetic properties are examined using SQUID analysis.

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Combining ferroelectrics, plasmonic nanostructures and 2D materials for application in nanophotonics

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Layered transition metal dichalcogenides (TMDs) are a fascinating class of atomically thin materials in which d-electrons interactions result in unique physical phenomena, with significant implications across various domains including electronics, spintronics, and optoelectronics. Specifically, monolayer (1L) MoS2 is currently receiving considerable attention due to its electronic and optoelectronic characteristics as a direct bandgap semiconducting 2D material.

Different physical or chemical strategies can be used to tune the electronic and optical properties of monolayer TMD for diverse optoelectronic applications.

In this study, we present the integration of ferroelectrics, plasmonic nanostructures, and 2D materials into a single monolithic device and analyze their mutual interactions within the hybrid system. Specifically, three main investigations are undertaken: i) the combined impact of ferroelectricity and light on the optoelectronic properties of monolayer MoS2 deposited on domain-engineered ferroelectric crystals, ii) the optical behavior of MoS2 deposited on a metallic chain of silver nanoparticles, and iii) the extreme light-matter interaction phenomena enabling pulsed laser operation at the nanoscale [1].

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Comprehensive Measurement of Photothermal and Fluorescence Properties in Suspensions and Solutions: A Thermal Lens Z-Scan Approach

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Nanoparticle characterization and optimization for specific applications rely on properties like optical resonance wavelength and light interaction mechanisms. This study investigates spherical gold nanoparticles in aqueous solution using a multi-wavelength cw Z-scan thermal lens (TL) spectroscopic approach. Improvements in experimental setup using top-hat beams and theoretical calculations for moderate-high absorptions are detailed. Measurements yield photothermal efficiency across different nanoparticle s (5, 40, 60, and 80 nm) and wavelengths (blue, green, and red), validated against Mie theory. Advantages include minimal sample exposure to excitation light (1 mW) and modulation for equilibrium maintenance, ensuring a linear response range. Additionally, employing single-beam Z-scan thermal lens technique evaluates fluorescence quantum yield in solutions. Two scenarios are considered: solutions with substantial fluorescence and those with low fluorescence. Analytical calculations quantify uncertainties from random errors introduced by optical detectors. Solutions with low fluorescence contribute to significant errors, while higher fluorescence levels aid in reducing uncertainty. A review addresses the challenge of random errors in accurate fluorescence estimation across various situations. Integrating insights from both studies offers comprehensive understanding for nanoparticle selection and optimization, crucial for diverse applications.

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Single Particles, single molecules and single photons detection from plasmonic nanostructures

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Surface-enhanced Raman scattering (SERS) is a highly sensitive spectroscopy method. SERS is observed from molecules adsorbed on metallic nanostructures, such as noble metal nanoparticles (Au, Ag and Cu). The efficiency of the SERS processes rival that of fluorescence emissions, allowing the observation of events assigned to single molecules. Recently, our group have reported on strong fluctuations in SERS intensities from molecules adsorbed on single nanoparticles [1]. The super-localization of these emissions provide some insights into the nature of the nanoenvironment in a SERS system both in dry environments and solutions [2,3]. The results provide some insigths into the molecular adsorption dynamics at the single molecule level. Moreover, we have been studies the generation and detection of single photon pairs (Stokes and anti-Stokes) emitted from SERS systems. This type of measurements can be explored in quantum noise-limited spectroscopy and imaging systems.

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A novel quasi-1D material for THz guiding in the nanoscale

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Terahertz (THz) technology is transforming diverse fields such as medical imaging, security screening, and agriculture. However, the challenge of developing materials that can manipulate THz waves, particularly at the nanoscale, remains. Traditionally, the large wavelengths of THz waves pose barriers to confinement within nanometric structures. On the other hand, polaritons, which emerge from the interaction between photons and matter resonances, offer exceptional optical confinement with extended lifetimes. Therefore, the exploration of novel materials that can support THz polaritons is essential for progress in this area. In this context, our research introduces paratellurite (TeO2) nanowires as a novel platform for THz phonon polaritons (PhP). Despite its established applications in nonlinear and acousto-optics, the potential of paratellurite in THz nanophotonics has been unexplored. Leveraging advanced techniques such as terahertz scattering scanning near-field optical microscopy (s-SNOM) and large-scale light sources like synchrotron and free-electron lasers, we unveil the polaritonic properties of TeO2 nanowires. Our findings demonstrate that the nanowires can guide PhP in two bands (around 10 and 20 THz) and exhibit spectral signatures down to 5.5 THz. Thus, our research not only expands the limited repertoire of materials suitable for THz polaritonics but also provides profound insights into the polaritonic behaviors in low-dimensional systems.

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Assessing the loss of hollow-core optical fibers by analytically mimicking their fabrication process

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Microstructured hollow-core optical fibers stand nowadays as a key enabling technology to address a wide set of fundamental and application needs. Indeed, the recent endeavors by the hollow-core fiber scientific community entailed remarkable advances and allowed establishing these fibers as the current lowest-loss fiber optics working in the visible and ultraviolet ranges [1]. The fabrication process of hollow-core optical fibers, however, encompasses the utilization of expensive infrastructure. Besides, attaining ultralow-loss fibers experimentally presents itself as a challenging technical task, typically involving numerous fabrication campaigns before reaching optimized performances. Thus, the development of methods able to anticipate the fibers' performances prior to their experimental realization is highly desirable. Hence, in this work, we address this challenge by analytically mimicking the fabrication of tubular-lattice hollow-core optical fibers. By accounting for the variation of their microstructure's geometrical parameters during production, we assess their expected loss levels based on the scaling laws governing their light-guiding mechanism and determine the conditions for optimized light transmission through the fibers. Our research provides new insights into the fabrication of hollow-core fibers, offering a path to predict their performance before experimental realization. By determining optimum conditions considering geometry, fabrication limitations, and loss figures, our work significantly contributes to the ongoing efforts to further reduce the loss of hollow-core optical fibers.

Acknowledgments

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Boosting the Yb^{III} NIR Luminescence in 1D Coordination Polymers via Tb^{III}-Mediated Energy Transfer

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The recent pursuit of bright near-infrared (NIR) light sources has centered on novel luminescent materials for converting blue or near-UV radiation into NIR.[1] Such functionality holds promise for applications like NIR light-emitting diodes and luminescent solar concentrators. Yb^{III} complexes displaying high molar absorptivity and bright luminescence may offer a compelling solution. However, the mismatch between the ligand triplet state and the Yb^{III} $^2F_{5/2}$ emitting level reduces the energy transfer (ET) efficiency. To work around this issue, our aim is to use Tb^{III} to mediate the ligand-to-Yb^{III} ET process. For that, the 1D coordination polymer based on $[Ln(tfaa)_3(\mu\text{-dppeo})Ln(tfaa)_3]_n$ (tfaa− = trifluoroacetylacetonate, dppeo = [(diphenylphosphoryl)ethyl](diphenyl)phosphine oxide) is leveraged owing to its easy composition tunability. Their structure were investigated by single-crystal X-ray diffraction, powder X-ray diffraction, and FTIR. Upon ligand excitation, while the composition containing only Yb^{III} exhibits poor NIR luminescence, the inclusion of Tb^{III} significantly enhances the Yb^{III} luminescence, with emission quantum yields approaching 1%. This improvement suggests that Tb^{III} facilitates the ligand-to-Yb^{III} ET through the ligand-Tb^{III}-Yb^{III} ET channel. The Tb^{III}-to-Yb^{III} ET was further supported by the longer Yb^{III} $^2F_{5/2}$ level lifetime with increasing the Tb^{III} content. Additionally, the Yb^{III} emission intensity dependence on excitation power density hinted at a potential two-photon excitation mechanism contributing to the Yb^{III} emission. Overall, these findings provide valuable insights into improving the luminescence of Yb^{III} complexes, which is pivotal for advancing the development of brighter NIR light sources and furthering efforts in efficient energy conversion.

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CaF_2 OSL film for synchrotron X-ray dose measurements in tomographic imaging

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The Optically Stimulated Luminescence (OSL) is used for dose measurements, mostly in personal dosimetry and dating. OSL dosimetric materials present emission when excited by light after prior exposure to ionizing radiation. An emerging application is 2D dose measurements using OSL films. A challenge of 2D OSL dosimetry lies in dose delivery (>40 Gy/s) and small radiation fields, as in synchrotron radiation beamlines. Monitoring of procedures (drug delivery or growth) requires knowledge of the absorbed dose, due to deterministic effects or tissue reactions of ionizing radiation. This study estimates the doses in X-ray tomography from synchrotron light source using CaF_2 OSL film based on natural fluorite. The films are composed of CaF_2 crystals embedded in an elastomer matrix. For assessment of doses, a cross calibration of the films were performed, exposing them to ^{60}Co (1225 keV) and 22 keV X rays photons. The dose rate using OSL films was performed with samples irradiated at the Laboratório Nacional de Luz Síncrotron (LNLS) in Mogno line, during tomographic imaging sequences, subsequently evaluating the dose distribution on the OSL film. Calibration readout was carried using an automated Risø TL/OSL reader, estimating a dose rate of ~60 mGy/s at sample position during X-ray tomography. Validation of dose delivery involved comparing results from commercial OSL detector (BeO), simulated using Monte Carlo and obtained with OSL films. Dose distribution analysis employed a 1D homemade reader (spatial resolution of 1 mm). Results showed that during the imaging, doses ranging from 3 Gy to 12 Gy. Despite all the challenges in sample production and small field dosimetry, OSL films are feasible to estimate the dose rate as well as the 1D dose distribution in X-ray tomographic imaging using synchrotron radiation. In future research, the OSL film will be investigated for 2D dose measurements.

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Capturing and transducing photons at perovskite nanocrystal interfaces

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Harnessing sunlight to drive chemical transformations, or to store the sun’s energy in chemical bonds, begins with the development of materials capable of capturing visible light and converting that light into separated charge carriers. Our lab has been working towards developing and optimizing functionalized nanostructured wide bandgap semiconductor surfaces that act as the working electrode in sensitized photoelectrochemical cells. Charge separation processes within such nanohybrid architectures are analogous to the first steps of the electron transfer cascade observed in natural photosynthesis, where light absorption generates redox equivalents that are shuttled to catalytic sites. These processes rely on efficient light capture and conversion. To this end, our latest efforts to understand how perovskite nanocrystals behave in matrices with long-range order will be highlighted. Of focus will be the structural features that define superlattices composed of all-inorganic perovskites and the photonic effects that govern the photophysical properties of perovskite nanocrystal-photonic crystal hybrids.

Control of the photoluminescence quantum-yield of gold organometallic nanocomposites by pulsed laser driven CO2 reduction reaction

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In recent years, there has been a huge interest in the CO2 reduction reaction (CO2RR) for the production of value-added raw materials in gas or liquid form. However, CO2 fixation into nanoparticle systems has not yet been demonstrated. This research presents a novel approach to synthe functional nanomaterial in colloidal form by CO2 fixation through laser synthesis and processing of colloids (LSPC) in water [1]. These methods are historically considered as green-approaches, yielding ligand-free nanoparticles with no by-products. Our results show that carbon monoxide rich gold nanoparticles are observed after synthesis even in deionized water, while an alkaline water environment leads to C2 and C3 coupling, producing carboxylic acids as a typical fingerprint of the CO2RR. Selective C2 coupling is observed during laser processing of pre-existing gold colloids, while pulsed laser ablation of a gold target results in both C2 and C3 coupling to lactic acid. Remarkably, under certain conditions, photoluminescent organometallic nanocomposites are synthed in the blue spectral region with a quantum yield of about 20% [2]. These findings open new paths to be explored in energetics, photonics, catalysis, and synthesis of functional nanomaterials at the nanoscale.

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Design and Characterization of small molecular systems for photo-induced charge separation

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Dono-acceptor molecular systems with small acceptor species (non-fullerenes of the Y-family) have achieved impressive results in photovoltaic applications, as high efficiency and durability. In this talk I will show how theoretical predictions from quantum mechanical approaches can guide the design of such small molecular systems for photo-induced charge separation. We show some prominent candidates that mimic the Y6-PM6 system and as example we present the design of a naphthalene diimide with phenothiazine derivatives and, for the chosen system, we show that electrical properties under illumination are greatly improved. In particular, the dielectric constant of the system changes considerably with illumination, providing us important insights to understand the charge separation mechanism in donor-acceptor molecular systems.

Development of photonic nanostructures through thermal scanning probe lithography

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Thermal scanning probe lithography (t-SPL) has been a promising top-down nanofabrication method. It is based on heating a sharp nanometric scanning probe that locally and precisely evaporates the polymeric resist, creating the desired patterns. The t-SPL is a direct patterning technique, with sub-20nm resolution, and can be performed in standard ambient conditions [1]. To name a few strengths of t-SPL, it overcomes intrinsic issues to other lithography techniques, such as electron beam lithography (EBL), by not presenting proximity effects and being more affordable, as complex electron-optics setups are not necessary [2]. In this work, we investigate the t-SPL methodology and show its compatibility to post-patterning processes such as material deposition and liftoff. With the recent advances in silicon photonics, high resolution, in nanometric scales, is a crucial feature for the fabrication of photonic devices [3]. Here, we propose using and optimizing t-SPL to fabricate a variety of photonic nanostructures such as metasurfaces and lenses. We report patterning to 10nm resolution and evaluate the fabricated nanostructures with scanning electron microscopy (SEM) and atomic force microscopy (AFM).

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Earth-Abundant Talc 2D Layered Materials: Vibrational Properties, Nanophotonics, and Optoelectronic Applications

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pTalc emerges as a promising class of large bandgap lamellar insulators. Its applications have been explored from the fabrication of graphene-based devices to two-dimensional (2D) heterostructures based on transition metal dichalcogenides with enhanced optical properties, optoelectronics, and polaritonics [1–4]. Despite the extensive knowledge of the chemical composition of bulk talc, retrieved from standard techniques such as Raman and IR spectroscopies, very little is known about its optical properties at the sub-micron spatial scale. Here, we provide an overview of IR s-SNOM for studying nano-optics and local chemistry of 2D natural talc [2, 3, 5]. Additionally, we offer a brief update on applications that combine natural minerals, graphene, and talc layers into functional heterostructures. Moreover, we demonstrate that natural 2D talc supports hyperbolic phonon-polaritons (HPhP) similarly to the well-established 2D polaritonic hBN and α-MoO3 crystals in the far- and mid-IR range. Furthermore, we highlight recent advances in nano-optical modulation in graphene-talc devices driven by electrical control and twistronics.

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Effect of the amounts of Li^+ additive on the luminescence properties of phosphate-based phosphor

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Lithium orthophosphates $LiBaPO_4$ have attracted much interest for their use in the luminescent devices due of their excellent properties such a stable structure, thermal stability, flat voltage profile, moderate phonon and exceptional optical damage threshold [1,2]. In general, luminescent properties are observed when lithium orthophosphates are doped with rare earth ions [3]. Recently, Eu-doped $LiBaPO_4$ phosphates have received much attention for application as new white light emission diodes (W-LEDs) phosphors. In the literature, crystalline evolution, the effect of grain , the influence of dopant concentration on the structural and optical properties has been studied. In this work, Eu-doped $LiBaPO_4$ phosphors were synthed by sol–gel method using PVA as a chelating agent. The structures and photoluminescence (PL) properties of the as-prepared LiBaPO4 phosphors were investigated by X-ray diffraction (XRD), X-ray Absorption spectroscopy (XAS) and PL spectroscopy. The synthed samples were found to have single phase structure and the incorporation of dopant/ Li+ additive did not affect the crystal structure. The luminescence properties of the Eu-doped $LiBaPO_4$ phosphors strongly depended on the amounts of the Li^+ additive. All the spectra exhibit transitions that are assigned to the Eu^{3+} and Eu^{2+} activators. A dominate band from Eu^{2+} are observed for the sample with greater Li+ addiction. Therefore, we can conclude that Li^+ addiction contribute to the reduction $Eu^{3+} \rightarrow Eu^{2+}$.

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Excited-State Intramolecular Proton Transfer (ESIPT): A Versatile and Modular Process

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Excited-State Intramolecular Proton Transfer (ESIPT) is a photophysical process corresponding to a photoinduced proton transfer in the excited-state, occurring in heterocyclic systems that exhibit strong hydrogen bonding in their ground state (e.g. enol fragments). This very fast process (picosecond) leads to either the sole emission of the keto (K*) tautomer, a dual E*/K* emission when ESIPT process is partially frustrated. In selected cases, a competition with deprotonation is also possible, leading to highly emissive anionic species and paving the way to fluorescence molecular switches. Heterocyclic dyes displaying ESIPT fluorescence are characterized by enhanced photostability, solid-state fluorescence and environment-dependent emission profile. As such, applications of ESIPT emitters include optoelectronic devices, imaging, ratiometric sensing and security inks [1]. Molecular engineering studies in our group around different organic scaffolds led to the development of highly stimuli-responsive dyes, displaying multi-state fluorescence, which can be fine-tuned upon electronic substitution or environment (polarity, temperature, hydration). Additional properties such as aggregation-induced emission (AIE) [2]. or acid/base-mediated stabilization of supramolecular rotamers [3] can also be envisioned. Innovative applications of ESIPT luminescence for the ratiometric sensing of pH variations at the interface of electrodes or as linkers for supramolecular metallic assemblies switches will be also discussed in this presentation.

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Fluids and structured glass: design of a liquid-filled hollow-core fiber-based temperature sensor

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This study investigates a new configuration for attaining a temperature sensor based on liquid-filled hollow-core optical fibers. Previous research has demonstrated that assessing the spectral transmission characteristics of a water-filled microstructured hollow-core fiber allows for successfully monitoring temperature variations [1]. Although this approach is able to provide higher sensitivity compared to typical temperature fiber sensors, it displays suboptimal resolution performance as its operation is based on tracking the position of spectrally broad fiber transmission bands. To address this limitation and enhance the sensor's capabilities, we propose a novel configuration utilizing a partially liquid-filled hollow-core optical fiber. The hollow core's partial filling allows the fiber transmission bands to narrow in comparison with the fully-filled fiber case while maintaining its sensitivity to temperature variations thanks to the thermo-optic effect. Thus, we analytically examine the resulting transmission spectrum under varying temperature conditions to account for the essential sensor parameters such as sensitivity and resolution. Additionally, we explore the sensor optimization opportunities by investigating fibers with diverse geometrical characteristics and filling liquids. Our findings suggest a promising avenue for developing hollow-core fiber-based temperature sensors with improved resolution levels.

Acknowledgments

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In-situ growth of lanthanide metal-organic frameworks (Ln-MOFs) on oxide glass and optical fibers: a promising material for chemical sensing

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Owing to their intrinsic porosity and luminescent properties, lanthanide metal-organic frameworks (Ln-MOFs) have emerged as a promising material for chemical sensing. However, these applications usually demanded their deposition in a stable substrate with suitable chemical and physical properties. Thus, this work aims to present a simple, fast, and in situ synthesis and coating process of Ln-MOFs on oxide glass substrates. Pieces of tellurite glasses were coated by different Ln-MOFs containing carboxylate ligands complexed Eu(III) and Tb(III). The synthesis was performed by solvothermal method in microwave equipment, with glass samples inside the reactor to promote the in-situ growth of Ln-MOFs on the substrate's surface. Also, tellurite optical fibers were coated by Ln-MOFs using a hotplate and immersing only the end of the fiber (around 2–5 cm) in the Ln-MOFs precursors solution. The main results indicate the growth of different crystalline structures depending on the glass composition, with different amounts of fluoride ions, indicating the existence of chemical interactions between the glass surface and the Ln-MOF components. Moreover, the luminescent behavior shows thin and well-defined f-f electronic transitions of Eu(III) and Tb(III) ions and a significant energy transfer by the “antenna effect” mechanism. Finally, optical fibers coated with homogeneous, stable, and luminescent Ln-MOF films were obtained, representing a high-potential material for remote chemical sensing.

Laser-engraved porous silicon

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Porous silicon (PS) is a promising advanced material, which presents large surface area and photoluminescence properties. Its nanostructure and biocompatibility make it suitable for drug delivery and cosmetic applications. As its luminescence and electric properties are sensitive to the presence of gases and biomolecules, it can be employed as sensors. Although PS electroluminescence efficiency need to be be improved, PS seems to be the best material for development of an all-silicon optoelectronic transistor [1]. The conventional method of PS production is the electrochemical etching [2]. This method employs a solution of hydrofluoric acid (HF), which is quite toxic to environment. Here, it will be shown an environmentally friendly method to produce PS through infrared laser and its optical properties that is quite like obtained from conventional PS.

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Luminescent thermometry in the first biological window based on Nd-doped yttrium fluoride nanocrystals

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Here, we investigated the performance of yttrium fluoride (YF_3) nanocrystals doped with neodymium ions as luminescent temperature nanoprobes operating entirely in the first biological window (650-950 nm). Using the microwave hydrothermal method [1], particles of Nd:YF3 have been synthed and characterized by XRD, XPS and SEM. They presented a orthorhombic crystalline structure of YF3, with space group Pnma [D_{2h}^{16}] and a rod-like shape with average values of 633 ± 74 and 345 ± 27 nm for length and width, respectively. Using an 800 nm, CW laser as the excitation source, luminescence spectra of this material in the near infrared region, associated to the $^4F_{3/2} \rightarrow {}^4I_{9/2}$ of Nd^{3+}, were recorded at different environmental temperatures, in the range from 303 to 373 K. The performance of this material as a temperature sensor was evaluated for different strategies of optical temperature sensing, based on the luminescence intensity ratio (LIR) and peak-to-valley intensity ratio (PVIR) methods [2]. We observed that the sensor schemes using this material exhibited relatively good sensitivity, reproducibility, and repeatability. Moreover, the PVIR methodology presented higher relative sensitivity (0.69 $\%K^{-1}$) values in comparison with the LIR (0.22 $\%K^{-1}$). The results indicate that this is a promising material for the development of new luminescent thermometric strategies that operate within the first biological window.

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Materials for ultrafast UV pulse characterization using nonlinear ellipse rotation measurements in thick samples

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Technological advances make it possible to find several commercial ultrafast laser systems at UV range today. This brings new challenges and opportunities to study nonlinear materials in this important spectral range. As we know, to measure the material nonlinear optical properties, the laser pulse intensity or, indirectly, the pulse width, for instance, is crucial. However, it is not so simple to determine the pulse width at a wavelength below 400 nm since most pulse characterization systems use second-harmonic generation (SHG) crystals, which are opaque below 200 nm [1]. Recently, we developed a new method based on the nonlinear ellipse rotation (NER), a third-order nonlinear effect, measurement in thick nonlinear samples for both materials and ultrashort pulse characterization [2,3]. Our method works since a NER signal increases (decreases) as the pulse gets shorter (longer) with propagation along a thick dispersive sample. Due to the simplicity, single-beam configuration, no frequency conversion, absence of phase matching issues, and isotropic sample requirement, for instance, our method is promising to be used for ultrashort UV pulse characterization. Here, we have tested some thick and transparent samples at UV range to determine the pulse width using the NER measurements. For example, we are testing very thick fused silica and LLF1 glass (50 mm long) as possible good candidates to measure ultrafast laser pulses at 343 nm from the third-harmonic of a Yb:KGW laser. Silica (LLF1) has good transparency up to 200 nm (~330 nm) but has low (high) second-order dispersion.

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Microscaled design of the linear and non-linear optical properties of a Eu^{3+}-doped tantalum phosphate glass by thermal poling

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Sodium high tantalum phosphate glasses are relevant materials for photonic applications due to several properties such as high thermal, chemical and mechanical stability, wide optical window, low phonon energy and high quantum efficiency of luminescent ions. In addition, the development of materials whose properties can be controlled and modified at a micrometer scale is increasingly being sought. Thermal Micropoling can then be an instrument for controlling different properties, such as the refractive index, variation in the reactivity of the glasses, controlling the second harmonic response on a microscopic scale, etc. [1-3]. So, this work presents the study of thermal micropoling of a glass of composition $99.83[52.5NaPO_3\text{-}47.5Ta_2O_5]\text{-}0.17Eu_2O_3$ (with the europium used as a sensitive probe). The glass was thermally micropoled under nitrogen atmosphere using a microstructured electrode, 250°C and voltage of 900V. Microstructured electrode allowed the microprinting of patterns on the glass, according to optical micrographs and Atomic Force Microscopy measurements that indicates a spatial reliefs of 90 nm depth and the presence of edge effects between the poled and non-poled areas. The edge effect was also observed by SHG on the surface of the sample, in which SHG depends on the polarization state of the incident radiation, indicating that thermal micropoling induces both longitudinal and in-plane static electric fields. Also, a refractive index change was induced according to the imprinting structures. These results suggest a microscale control of the optical properties on the tantalum phosphate glass.

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Microvatity-mediated enhancement of optical gain in colloidal quantum dots

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Colloidal Quantum dots (CQDs) are nanoscale semiconductor crystals that exhibit wide excitation spectrum and stable, bright, narrow photoluminescence (PL). They also possess low optical-gain threshold and high-temperature stability for lasing [1]. These optical properties make CQDs highly versatile, finding applications in optical sensors, solar cells, and lasers. Moreover, they constitute a promising class of solution-processable gain media, with their properties directly controllable through quantum confinement effects, owing to their extremely small . Due to the expansion of nanotechnology, microlasers have been widely exploited, examples include microdisks, photonic crystals, and random lasers [1]. This study focused on understanding which parameters influence the optical gain properties in microcavities utilizing CQDs as gain media [1,2]. That is, we investigated how changes on concentration and of CQDs in microcavities influence ASE and lasing behavior. Specifically, we employed CdSe-based quantum dots solutions in SiO2 microcapillar. This process varies depending on the cavity, with a significant challenge being the integration of CQDs into capillary fibers. We have successfully developed a protocol for this integration. Furthermore, we aim to investigate how microcavity geometry affects these parameters through experiments involving microdisks, thin films, and microcapillar fibers [2,3]. To do so, we will conduct steady-state and time-resolved PL measurements to verify the achievement of ASE and also characterize the optical gain threshold.

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Persistent Phosphors for Luminescence Thermometry

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Optical thermometry based on luminescence (Luminescence Thermometry – LT) has been widely investigated due to the possibility to measure temperature in restrictive environments such as microdevices or biological systems, where access is challenging. However, one of the limitations of LT is the real time excitation that can cause local heating and generate inaccuracy of temperature measurement. One way to mitigate this limitation is to use persistent phosphors, materials that emit light even after the removal of the excitation source. In this presentation I intend to provide a review of the Persistent Luminescence Termometry (PeLT). I will define and explain the basics of persistent luminescence phenomenon, the studied systems for PeLT, advantages, disadvantages, and perspectives for the application of PeLT in real systems.

Plasmon-Enhanced Upconversion in circular and square nanostructures in Er3+/Yb3+ codoped GPG glasses

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Surface plasmons enable light confinement at the nanoscale, providing a versatile approach to modulate excitation and emission characteristics of quantum systems. Achieving electromagnetic field confinement within minute regions is crucial across various domains, including nanophotonics, biosensing, and beyond. The appeal of metallic nanostructures in plasmonics lies in their intriguing linear and nonlinear optical behaviors, intricately influenced by factors such as shape, depth, and periodicity. This study analyzes the influence of the shape and periodicity of Au-plasmonic nanostructures on the enhancement of upconversion emission from Er^{3+} (1.0 wt%) and Yb^{3+} (3.0 wt%) ions. The circular and square grating nanostructures were fabricated with varying periodicities ranging from 200 to 1000 nm on GeO2- PbO-Ga2O3 glasses (GPG: Er^{3+}/Yb^{3+}). Plasmon-enhanced upconversion was investigated by combining a confocal microscope with a typical motorized microscope setup. For all evaluated samples, upconversion emissions were observed in the green (~550 nm) and red (~655 nm) spectra under excitation with a continuous-wave laser in the near-infrared at 980 nm. Strong upconversion emission was observed, especially smaller periodicities nanostructures. The excitation of Er^{3+} ions causes the emission observed through the plasmonic nanostructures via extraordinary optical transmission from the periodic nanostructures. To explain this behavior, we propose an energy transfer mechanism $Yb^{3+} \rightarrow Er^{3+}$ followed by a resonant coupling between Er^{3+} and surface plasmon polariton. This coupling modifies the local field, improving the emission intensity of Er^{3+}. These findings can be very useful for nanophotonic device applications employing a transparent medium with optical gain.

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Recycling of electronic waste: Borogermanate glasses containing rare earth ions for magneto-optical applications.

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Magneto-optical (MO) glasses have attracted the attention of the scientific community in recent years due to the potential for developing MO sensors to detect magnetic fields and electrical currents from industrial equipment. Borogermanate glasses enable the solubilization of high concentrations of rare earth (RE) ions [1]. In this work, results of the synthesis and characterization of GeO_2-B_2O_3-Al_2O_3-Na_2O-BaO (BGeB) glasses containing different proportions (in %m/m) of residues obtained from fluorescent lamps, which include RE ions such as Eu^{3+} and Tb^{3+}. RE ions have a higher magnetic moment than transition metals [1]. Strongly paramagnetic ions, such as Tb^{3+}, enhance the magneto-optical effect in crystals, glasses, and optical fibers [1]. The preparation of borogermanate glasses containing x = 0.10, 20, 30 and 50 %m/m of electronic residue were obtained from the conventional melt quenching method at 1400°C, Subsequently, the molten liquids were cast in preheated steel molds below the glass transition temperature of the glasses (around 480°C). All BGeB-xRes glasses were characterized for Differential Scanning Calorimetry (DSC), X-ray Diffraction (XRD), Photoluminescence (PL) and UV-Vis-NIR absorption spectroscopies. The XRD patterns confirmed the non-crystalline nature of all samples, while from the DSC curves it was possible to attribute the typical temperatures of a glass. The BGeB-xRes glasses exhibit a glass transition temperature around 516°C. The transmission spectra of BGeB-xRes glasses show a wide optical transmission window (from 550 to 1.6 µm), the electronic transitions corresponding to Tb^{3+} and Eu^{3+} are observed with interesting intensity in the emission spectra of the materials. As conclusion, considering the importance of recycling electronic residue containing rare earth ions, highlighting the results of the use of these materials for the synthesis of glasses containing Eu^{3+} and Tb^{3+}.

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Relation between Particle Size and Structural Modification on the Optical Second Harmonic Generation at Perovskite Colloidal Systems

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Materials with micro and nanoscale dimensions have garnered significant attention due to their excellent nonlinear optical process conversion frequency capabilities [1,2]. This is crucial in photonics devices and applications in innovative sensing and imaging techniques across materials science and chemistry. In this context, the perovskite particles like BaTiO3 emerge as promising candidates for such applications [3]. Their non-centrosymmetric crystal structure at both micro and nanoscales is a crucial factor contributing to their distinctive second-order nonlinear (χ2) optical properties. Therefore, in this work, we aim to study the dispersion of Optical Second Harmonic Generation (SHG) at three different s (340,430 and 1040 nm) in BaTiO3 particles by using a tunable femtosecond laser (1064 to 1500 nm). Our outcomes indicate that larger particles have higher χ2 values when normalized by volume. So, through Raman spectroscopy and X-ray diffraction, we identified a systematic blueshift in Raman modes and pronounced lattice strain due to thermal treatment that promotes the enhancement of tetragonality at larger particles. Consequently, this led to a noticeable variation in the χ2 values when normalized by volume increased until two-fold. These findings reinforce the potential of BaTiO3 in revolutionizing optical and medical imaging applications and accentuate the significance of meticulously adjusting its structural parameters.

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Second-order nonlinear optical response of crystalline derivatives of bromochalcone

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We investigate theoretically and experimentally second harmonic generation (SHG) in four organic compounds, both being derivatives of bromochalcone ($C_{15}H_{11}BrO$) [1]. The compounds were synthetized by Claisen-Schmidt condensation and characterized using NMR, HR-MS, and UV-Vis. We calculated theoretically the first order hyperpolarizabilities of all molecules using program packages based on the time-dependent Hartree-Fock (TDHF) using MOPAC 2016 [2] and time-dependent density functional theory (TD-DFT), using Gaussian 16 program package [3]. Furthermore, SHG of crystalline powder of these compounds was characterized by Kurtz and Perry's powder method. We noticed that the SHG efficiencies increase by an order of magnitude by varying the position of Br, reaching up to 7 times larger than the KDP, and we assign these responses to their molecular structure and crystalline arrangements. The theoretical and experimental results evidence that the exchange of Br position influences the SHG efficiency of the investigated samples and that derivatives of bromochalcone are promising organic crystals aiming applications in devices based on second-order nonlinear responses.

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Solid state synthesis of Er-Yb co-doped $MgNb_2O_6$ ceramics and the exploration of their structural, up-conversion photoluminescence, photocatalysis, and adsorption properties

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Rare earth (RE) doped ceramic materials are now known to offer considerable promise as phosphors, providing avenues for a wide range of applications in the photon domain when synthed with appropriate compositions and crystal structures. Furthermore, because of the charge carriers (electron-hole pair) that these phosphors contain, they have the potential for both photoluminescence and photocatalysis. This research explores the solid-state synthesis of RE-doped $MgNb_2O_6$ and the characterization of their structural, optical, photocatalysis, and adsorption properties. Three different compositions of the columbite ($MgNb_2O_6$, $MgNb_2O_6$-Er, and $MgNb_2O_6$-Er-Yb) were synthed via solid state columbite route, and their crystal structures were confirmed to be orthorhombic for all three compositions with slight expansion in the bulk volume of the RE-doped compositions. The as-sintered RE-doped ceramic bodies' room temperature up-conversion photoluminescence spectra showed two emissions at roughly 553 nm and 669 nm, which corresponded to the transitions of Er^{3+} ions from $^2H_{11/2}$ to $^4I_{15/2}$ and $^4F_{9/2}$ to $^4I_{15/2}$, respectively. Then, as suggested by theoretical models present in the literature, it was confirmed that the emission intensity is proportional to the n^{th} power of the excitation intensity. This up-conversion photoluminescence was observed as an enhancement in the fluorescent intensity of the Er-Yb co-doped samples possibly due to the charge transfer process between Yb^{3+} and Er^{3+} ions. The photocatalysis under UV light and adsorption studies for the decolorization of Victoria blue dye were investigated and discussed based on the influence of up-conversion photoluminescence in the RE-doped $MgNb_2O_6$ Columbite.

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Spectroscopic Properties and potential luminescence thermometer based on Fe3+-Cr3+-Eu3+:LiAl5O8 phosphor

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The scientific interest in luminescent materials, commonly referred to as phosphors, has seen significant expansion in recent years, particularly driven by technological applications and sustainability concerns [1]. A primary focus of current research lies in energy conversion, responding to the escalating global demand for electricity. Among the various materials investigated, inorganic phosphors stand out as promising candidates, typically composed of a crystalline hosting optically active ions, such as lanthanides. Transition metal ions, when incorporated into a crystalline host, also hold potential for generating highly efficient phosphors. Our objective was obtaining optical properties of lithium aluminate (LiAl5O8) doped, in combinations, with Fe3+, Cr3+, and Eu3+ ions using photoluminescence spectroscopy [2]. The results clearly demonstrated the efficacy of the doping process, as evidenced by the characteristic optical transitions observed in all analyzed spectra. Notably, optimal excitation occurred at 285 nm, with Fe3+ presence enhancing Eu3+ and Cr3+ emissions, highlighting the influence of excitation energy on activating the luminescent properties of the system. The energy transfer processes in different directions were analyzed and explained. Furthermore, temperature measurements conducted on all samples revealed the material's sensitivity to thermal changes, even when doped individually, in combination, or tri-doped. Suggesting a potential application of Eu3+, Fe3+, and Cr3+ doped LiAl5O8 as a thermal sensor, leveraging its distinct optical properties for precise monitoring of temperature fluctuations. Such applications hold significance across a multitude of fields, ranging from industrial settings to scientific research, and contribute to driving advancements in luminescent thermometry.

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Study of synthesis parameters of $SrMoO_4$:Dy^{3+} and the role in the photodegradation system irradiated with commercial LED

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Strontium molybdate ($SrMoO_4$) have been the subject of intense research due to their promising technological importance in several scientific and technological fields [1-2]. Molybdate is considered a good host for several rare earth elements due to its efficient energy transfer from the tetragonal molybdate group to trivalent lanthanide activator and excellent chemical and thermal stabilities [3]. This work investigates the structural, morphological, optical, and photocatalytic properties of $Sr_{0.99}Dy_{0.01}MoO_4$ (SMO:0.1Dy) phosphors. In this work, SMO:0.1Dy were synthed using two different synthetic methods: the co-precipitation method and complex polymerization method. The samples obtained by co-precipitation method were heat treated with the microwave-assisted hydrothermal and convention furnace. The microstructural and optical characterizations were performed using X-ray diffraction (XRD), Raman, Fourier transformed infrared (FTIR), ultraviolet–visible (UV-Vis) spectroscopy, scanning electron microscope (SEM), and photoluminescence. The photocatalytic activity was investigated by monitoring the degradation of methylene blue (MB) using a commercial LED lamp in an optically isolated system. Spectroscopy measurements monitored the MB photodegradation reaction in the UV-Vis region. The results indicate that the MB degradation for the $Sr_{0.99}Dy_{0.01}MoO_4$ material obtained by co-precipitation and heat treated with microwave-assisted hydrothermal was more efficient for treatments performed using the white LED lamp and magnetic stirring.

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Thermal lens applied to the characterization of Nitrogen-Doped Graphene Quantum Dots

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This work aims to evaluate and compare the quantum efficiency (QY) of Nitrogen-doped Graphene Quantum Dots (N-GQDs) dispersed in different solvents through the thermal lens (TL) technique. The N-GQDs were obtained through the carbonization of sucrose in sulfuric acid and subsequent doping with nitric acid. The material was dispersed in dimethylformamide, dimethylsulfoxide, deionized water and isopropyl alcohol. The TL transient measurements were performed using the mode-mismatched dual-beam (pump and probe beams) configuration. A continuous wave diode laser operating at 532 nm was used as the pump beam, and a He-Ne laser (λ= 632.8 nm) was used as the probe beam, with TEM00 mode and power less than 1 mW. The QY values obtained were in the range of 30 – 45%. These values are higher than the QY of N-GQDS prepared with similar precursors [1,2] indicating that the synthesis method used in this work may be more suitable for biological applications and optoelectronic devices [1]. The results also showed that there is a small influence of the solvent on the QY of N-GQDs.

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Untangling the origin of supramolecular giant second harmonic generation by a structural and femtosecond polarized spectroscopy study

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The increasing demand for advanced materials with improved optical properties has sparked a surge of interest in molecular nonlinear optics. This field of study has facilitated the development of more efficient materials and contributed to the reduction in costs of emerging technologies. In special, the supramolecular structures have received significant attention due to the giant values of second-order optical susceptibility [1] as compared to molecular systems. The polybinaphthalenes derivatives have shown an ideal supramolecular structure to link different chromophores to optimize the nonlinear optical responses. In this context, we conducted the polarized spectral dependence of second harmonic generation (SHG) of four polybinaphthalenes functionalized with chromophores by using a tunable femtosecond laser. In addition, experimental measurements of DLS and AFM were carried out to uncover the effect of the structure in enhancing the second harmonic signal. Our outcomes reveal high χ2 values depending on the chromophore linked to the polymer backbone, which can reach values of up to 8 pm/V. Chirality was verified by the difference in χ2 values between the right and left-handed polarizations. An analysis of the spectral and structural measurements associated with the simulation, it was possible to conclude that quasi-phase matching generates the second harmonic signal and that the enhancement can be associated with resonance effects of the structure and the 2PA process. Therefore, the giant molecular SHG values associated with the chirality make this class of supramolecular structure an exceptional candidate for application in polarized SHG microscopy.

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Yttrium orthovanadates phosphors as up-conversion luminescent markers for gunshot residue identification

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In this work, yttrium orthovanadate phosphors doped with Er3+ and Yb3+ (YVO4: Er3+, Yb3+) were synthetized by the combustion method. After a post-synthesis heat treatment (1100 °C for 6 hours), samples were highly crystalline, with only the tetragonal zircon phase remaining. Additionally, all samples presented promising down and up conversion properties, exhibiting a strong green luminescence when excited by either UV or IR radiation. The up-conversion process involved the absorption of two-photons, with the intensity of the Er3+ transitions (2H11/2–4I15/2, 4S3/2–4I15/2 and 4F9/2–4I15/2) heightened with the Yb3+ content. The co-doped orthovanadate samples were introduced into 9mm non-toxic ammunition (NTA) for evaluation as luminescent markers for gunshot residues (GSR). After shots with marked ammunition were fired, these phosphors enabled the visual detection of luminescent GSR (LGSR) on the shooter, firearm and firing place, facilitating an analysis of the simulated crime scene. These residues also presented a chemical signature that enabled their identification as LGSR. Besides, the down and up conversion properties observed in the residues provide an additional security feature for the unequivocal characterization of the LGSR.

A Comparative Analysis of In2O3 Films Produced via Resistive Evaporation and Spin-Coating Techniques

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Indium oxide (In_2O_3) has gained prominence as multifunctional material due to its wide range of applications, spanning from electronic devices to solar cells [1] besides photocatalytic activities [2,3]. The ongoing work aims to analyze different In_2O_3 films produced by distinct deposition techniques, with variation in the precursor materials, number of layers, and types of substrate. By resistive evaporation, metallic indium is evaporated onto different substrates and thus oxidized in a furnace to 300ºC to form indium oxide films. X-ray diffractogram show peaks corresponding to cubic structure, where the main peak is related to the (101) crystallographic plane and has increasing intensity with the number of layers and with rougher substrates. Images obtained by confocal microscopy showed films very homogeneous, essential for electrical conduction on the material's surface. Optical transmittance reveals highly transparent films from visible to near infrared, and the transmittance reaches over 80% in the near infrared, exposing high potential to optoelectronic applications. These previous findings were motivation to deposition of films from indium oxide sol-gel solutions via spin coating. According to the literature [3], this sort of films is expected to exhibit good homogeneity and low roughness. However, an increase in surface defects is observed with increasing thickness, which can enhance photocatalytic efficiency. Both sort of films has been evaluated through structural, optical, and electrical measurements, providing valuable insights for the development of In_2O_3 films with optimized performance for various technological applications, considering not only the intrinsic properties of the material but also the deposition processes and substrate characteristics.

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Alkaline hydrothermal synthesis of titanium materials and their application in the photodegradation of pollutants

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Heterogeneous photocatalysis based on semiconductors is a technology that has been applied to solve environmental and energy problems. Different crystalline phases of titanium oxides (Ti) have been extensively studied in heterogeneous photocatalysis, but lamellar potassium titanates obtained by alkaline hydrothermal synthesis still deserve investigation, mainly in view of their high surface area. Thus, this work presents the synthesis of Ti materials by the hydrothermal method under different concentrations of KOH, resulting in four samples, namely as: Ti1 (obtained with the precursor of Ti in KOH 10^{-5} mol/L), Ti2 (10^{-2} mol/L), Ti3 (1 mol/L) and Ti4 (5 mol/L). The structural, morphological and electronic properties of the synthed materials were investigated using different characterization techniques, including X-ray diffraction (XRD), specific surface area (BET), Fourier transform infrared spectroscopy (FTIR), among others. According to the XRD analysis, the samples synthed at concentrations of 10^{-5} and 10^{-2} mol/L of KOH resulted in the formation of TiO_2 anatase crystalline phase and the samples obtained at concentrations of 1 and 5 mol/L resulted in formation of potassium titanates ($K_2Ti_8O_{17}$ and $K_3Ti_8O_{17}$). Surface analysis indicated the formation of materials with high surface areas, with emphasis on the Ti4 sample (2796 m^2g^{-1}). The photocatalytic activity of these materials was evaluated by the photodegradation of methylene blue (MB) and indigo carmine (IC) dyes, as well as the drug amiloride (AML). The best photocatalytic performances were observed for potassium titanates (Ti3 and Ti4) that showed removal efficiency of approximately 100% for all of tested molecules (MB, IC, AML). Therefore, the increase in the KOH concentration in the alkaline hydrothermal synthesis resulted in samples with improved properties in relation to the materials obtained in lower concentrations (Ti1 and Ti2).

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APPLICATIONS OF BISMUTH VANADATE (PHOTO) CATALYST IN ENVIRONMENTAL PROCESSES USING VISIBLE LIGHT

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The control of the synthesis of new materials, as well as the modification of already-known materials in order to improve their photocatalytic properties, is one of the aspects of greatest interest today. In this sense, the present study reports a simple hydrothermal synthesis method to form bismuth vanadate materials (BiVO4) for environmental applications using Visible light, such as: (photo) degradation of dyes (methylene blue and indigo carmine); and (photo) esterification of free fatty acids (FFA) present in waste cooking oil (WCO). The obtained materials were characterized by X-ray diffraction (XRD), UV–vis diffuse reflectance spectroscopy (DRS), scanning electron microscopy (SEM), and Fourier transform infrared spectrometry (FTIR). Due to the lower band gap value for the monoclinic phase, this is usually the desired phase when synthesizing BiVO4, as it is the phase with the highest photocatalytic efficiency. The results presented here demonstrate that BiVO4 can be a new possible photocatalyst to perform these environmental processes.

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Blue up-conversion emission of $Nd^{3+}/Tm^{3+}/Yb^{3+}$ triply doped aluminophosphate optical fibers

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Glasses containing rare-earth ions (RE^{3+}) for up-conversion luminescence have been widely explored in several photonic applications. Materials containing Tm^{3+} present intense blue emission when excited in the near-infrared range, allowing them to be used as solid-state lasers and other emitter devices. Tm^{3+} are generally combined with other rare-earth ions to improve the up-conversion efficiency; however, increasing the number of dopants can be an issue for their solubility in the glass matrix and fiber drawing. In this work, aluminum-phosphate glasses, a host matrix with high rare-earth solubility and fiber-drawing ability, were produced containing different amounts of Tm^{3+}, Nd^{3+}, and Yb^{3+}, as well as the respective triply-doped optical fibers. Glass samples containing RE^{3+} were excited at 808 nm and 980 nm to evaluate the mechanism involved in the luminescence process. In addition, tri-doped optical fibers were excited at 788 and 980 nm, and bright blue luminescence was observed at both wavelengths. Thus, due to the intense up-conversion emission measured on RE^{3+} triply doped optical fibers with low optical loss, the developed material presents great potential for fiber-based photonic applications.

Borogermanate glasses containing Dy^{3+} ions for magneto-optical applications

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In recent years, new magneto-optical (MO) materials have been applied as optical isolators, transducers, and sensors for magnetic fields and electric currents [1-2]. This work presents preliminary results from the synthesis and characterization of borogermanate glasses (BGB) containing high concentrations of dysprosium oxide (Dy_2O_3). The BGB-xDy glasses (x = 0, 8, 18, 22, 26, and 28 mol% of Dy_2O_3) were prepared from the conventional melt-quenching method. Mass stoichiometric ratios of the precursor reagents were weighed, ground, homogenized, and melted in a platinum crucible at temperatures between 1350 and 1500 °C, for 2 hours, and then cooled to room temperature. Characterization included Differential Scanning Calorimetry (DSC), X-ray Diffraction (XRD), UV-Visible, Raman, and Photoluminescence (PL) spectroscopies. All BGB-xDy glasses were transparent and colored, with XRD confirming their non-crystalline nature. The BBG-22Dy and BBG-28Dy glasses exhibited Tg values of 690 and 739 °C and Tx at 933 and 908 °C, respectively, with $\Delta T = Tx-Tg$ values of 243 and 169 °C for the respective samples. The emission spectra highlight the main electronic transition ($^4F_{9/2} \rightarrow {}^6H_{13/2}$) of Dy^{3+} ions at 574 nm. The UV-Vis spectra of BGB-Dy glasses show no absorption bands around 632 nm, indicating no absorption bands in this region. This will allow polarized light to pass through the glass samples for measurements of the faraday rotation angle at 632nm. In conclusion, the preliminary results indicate the development of new Faraday rotators, which may be applied for magnetic field and electric current sensors.

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$CaAl_{12}O_{19}$:Mn phosphor prepared by polymeric precursor method: synthesis, structural and photoluminescence properties

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Technological development and widely use of light-emitting devices have demanded the search for ecologically sustainable, inexpensive, accessible and efficient optoelectronic materials [1]. In this sense, the Mn-doped calcium aluminate compounds has received remarkable attention due to their fundamental properties, versatility and potential for varied technological applications [1]. $CaAl_{12}O_{19}$ (CA) is highly refractory and has a set of electronic and optical interesting properties, making this synthesis deeply studied [2]. As the formation of CA through the conventional solid state reaction method is difficult and requires high temperatures, an alternative is the use of the polymer precursor method, which allows the synthesis of oxides with controlled particle, high purity and chemical homogeneity, as well as a relatively low cost and not sophisticated equipment [2]. Thus, $CaAl_{12}O_{19}$:Mn samples were prepared by the polymer precursor method in the conventional and nitrogen atmosphere with high heating rate in the annealing. X-ray difractograms of samples prepared at 1300 °C in conventional atmosphere and heating rate show the presence of spurious phases such as Al_2O_3 and $CaAl_4O_7$. The formation of these spurious phases is associated with lower temperature crystallization of Al_2O_3. In order to avoid the precipitation of this phase, samples were prepared using N_2 atmosphere and high heating rate. This procedure decreased considerably the amount of the spurious phases even for the lower annealing temperature of 1200 °C, which is not achievable for conventional annealing. Photoluminescence of the sample with lower synthesis temperature was analyzed and the spectrum showed a strong red emission centered around 650 nm typical of ^2E - $^4A_2$ transition for Mn^{4+} ions.

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$CaAl_2O_4$-based phosphors prepared by polymeric precursor method: local structure and photoluminescence properties

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Calcium aluminate ($CaAl_2O_4$) is one of the most widely used alkaline earth aluminate compounds. Pure or doped calcium aluminate has received remarkable attention because of fundamental properties, versatility, and potential for several technological applications. $CaAl_2O_4$ doped with rare earths or transition metals has shown interesting luminescent properties and it has since been investigated as a possible host material for long-lasting persistent phosphors. In this context, this work shows the characterization of pure and doped (Mn, Pr and Zn) $CaAl_2O_4$ samples using electronic paramagnetic resonance (EPR), X-ray photoelectron and absorption spectroscopies (XPS and XAS) and the correlation with photoluminescent properties. These techniques can provide information about oxidation states, symmetry, and defects associated with the respective incorporations in the $CaAl_2O_4$ matrix, fundamental for a better understanding of the photoluminescent properties. Structural properties of the samples have also been characterized by conventional techniques such as scanning electron microscopy, X-ray diffraction, Raman spectroscopy and photoluminescence spectroscopy.

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Calix[4]arene functionalized with naphthylimide as achemosensor

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Optical chemosensors are devices capable of detecting analytes and transmitting measurable signals. This measurement can be obtained using UV-Vis, Raman, FTIR, and luminescence techniques. [1-3] In that research, a luminescent organic molecule functionalized in the supramolecule calix[4]arene has been used to verify its potential as a chemosensor.

The molecule 5, 11, 17, 23 - Tetra(tertbutyl)-25, 27 - (N(2-aminoethyl)-1,8-naphthylimide)-26, 28 - (dihydroxy)calix[4]arene is a chromophore ligand and was developed from n-(2-aminoethyl)-1,8-naphthylimide and calix[4]arene functionalized with dibromopropane. ^{1}HNMR (δ CDCl3, 300 MHz) 12.75ppm (s, NH) showed the NH of naphthylimide and the signals at 8.63 ppm (dd, CH), 8.25 ppm (dd, CH) and 7.82 ppm (dd, CH), refer to the hydrogens of the naphthylimide conjugated rings. The signals at 7.09 ppm, 7.00 ppm (s, mAr-H), and 1.23 ppm (s, tBu) refer to the calixarene moiety. FTIR shows stretching bands at 3408cm^{-1} assigned as ν(OH), 3049cm^{-1} assigned as v(CH-Ar), 1700cm^{-1} assigned as v(C=O), and 1361cm^{-1} assigned as v(CH_2-N), and 2960 and 2864 cm^{-1} assigned as ν(C-H Aliphatic).

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CeO_2, TiO_2 and Sepiolite for water treatment

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This work investigated a new catalyst based on the union of cerium dioxide (CeO_2), titanium dioxide (TiO_2), and Sepiolite (Sep) to evaluate the combination of the photocatalytic properties of CeO_2 and TiO_2 and the adsorption of Sep applied to the treatment of the pollutant drug ciprofloxacin hydrochloride (Cipro), with a view to application in aquatic treatments [1]. The main parameters studied were the effectiveness of preparing the composite of CeO_2 and TiO_2 with Sep, change in the optical absorption range and band gap structure due to doping, and change in pollutant concentration because of the action of adsorption and photocatalysis. The material was characterized using the following techniques: X-ray Fluorescence, X-ray Diffraction, Ultraviolet and Visible Spectrophotometry (UV-VIS) with Diffuse Reflectance (DRS) and Scanning Electron Microscopy (SEM) with X-rays (EDS). From XRF, after synthesis, 12.1% CeO_2, 24.5% TiO_2, 62.04% Sep were found. By XRD, the coexistence of phases corresponding to CeO_2, TiO_2 and sepiolite was identified, and these results indicated the formation of a new product from their union. Via UV-Vis measurements, an improved band gap of 2.5 eV was found, with Tauc graph; moreover after the adsorption and photocatalysis process, the Cipro removal efficiency was obtained (at a concentration of 30 ppm) which was more than 75%. The results are considered relevant, given that the material achieved combines low cost and a good pollutant removal rate, that is fundamental for aquatic depollution applications.

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Characterization of ZnO:Ho thin films grown by spray pyrolysis

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Zinc oxide (ZnO) is a semiconductor widely employed in the optoelectronics industry, due to aspects such as low cost and versatile manufacturing techniques and the possibility of producing transparent devices, the latter owing to its bandgap in the UV region. In this context, it is compelling to dope ZnO with rare earth (RE) ions, particularly trivalent holmium (Ho^{3+}), as it emits primary colors essential for the RGB system used in displays [1]. Motivated by the potential application of Ho-doped ZnO in display devices, the structural and optical properties of this material were investigated, exploring ZnO:Ho thin films with nominal doping concentrations in the range of 1-5% and aiming to determine an optimal condition for the RE's luminescence. The samples were characterized by X-Ray Diffraction, Scanning Electron Microscopy, UV-Vis Spectroscopy and Photoluminescence Spectroscopy (PL). Results revealed that the films are polycrystalline, with wurtzite hexagonal structure. The crystallite sizes calculated for the (002) and (101) ZnO orientations ranged from 6.9 nm to 18 nm, showing an increase with higher dopant concentration. UV-Vis spectroscopy showed Ho absorption peaks lying in the blue (450 nm), green (538 nm) and red (642 nm) regions. PL spectroscopy was performed using two excitation wavelengths, 450 nm and 325 nm. The spectra taken for low-temperatures exhibited Ho emissions in visible regions, with 5% being the Ho concentration presenting the most intense luminescence. Additionally, PL intensity was evaluated as a function of temperature, from 77 K to 216 K. Spectra comparison highlighted a decrease in intensity with increasing temperature, which was attributed to the increase in electron-phonon interactions. Splitting of Ho^{3+} levels $^5S_2$ and $^5F_2$ was also observed, attributed to the interaction between the ion and the crystalline field of ZnO.

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Construction and characterization of a wooden furnace for heat-treated materials studies

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Forgery of artworks often involves the use of artificial aging techniques, imitating the natural aging process of paintings. This can take decades to achieve naturally, especially with oil-based pigments. Following guidance obtained from interrogating a forger and receiving a tutorial on artificial aging, we constructed a wooden oven lined with aluminum foil to simulate the aging environment. The primary objective of this study was to develop and characterize an oven suitable for controlled experiments on the artificial aging of artworks. We utilized Raman scattering to analyze changes in canvases and materials subjected to heat treatment, and we plan to employ optical absorption spectroscopy and Verdet's constant measurements. Moreover, our research extends beyond the specific study of artworks to encompass a broader examination of the effects of heat treatment on various materials. By exploring how different materials react to controlled heating processes, we aim to deepen our understanding of their physical and chemical transformations. This comprehensive approach not only provides valuable insights for forensic sciences but also contributes significantly to the broader fields of material science and conservation.

Core-shell Ag@Au plasmonic nanostructures on graphene oxide: synthesis and optical properties

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The use of 2D materials as support for nanostructure growth offers several advantages, including reduced need of chemicals and stabilizers, and control over and morphology. Among 2D materials, graphene oxide (GO) stands out due to its functional groups, and optical and electronic properties. Plasmonic nanoparticles, such as gold and silver, present an increased absorption and scattering of the electromagnetic field at specific wavelengths, phenomena known as Localized Surface Plasmon Resonance (LSPR). When these plasmonic systems are combined in a multilayer configuration, novel effects can be observed such as plasmon hybridization and tunable optical properties. In this study, we have engineered core-shell Ag@Au core-shell nanoparticles on the surface of functionalized graphene oxide (GO). First, GO was functionalized with (3-mercaptopropyl)trimethoxysilane to introduce thiol groups, enhancing its affinity for metals. Silver nanoparticles were then grown on the GO surface and transmission electron microscopy images revealed structures with average diameters of 25 nm on the GO surface. To avoid galvanic replacement, high pH and concentrations of the reducing agent were used. The electron microscopy and energy-dispersive X-ray spectroscopy analysis proved the formation of a core-shell structure with an average diameter of 6 nm. This indicated partial galvanic replacement, which in this case, was beneficial for controlling the final shape and of the system. UV-visible spectroscopy revealed a plasmonic resonance band at ~520 nm. The study showcases 2D platforms' versatility on creating complex nanostructures like core-shell types without typical stabilizers, minimizing toxicity.

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Design and preparation of non-fullerene acceptor for photoinduced charge separation systems

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Donor(D)-acceptor(A) bulk heterojunctions (BHJ) of low bandgap oligomers and polymers with fullerene have been proposed, in the two last decades, as promising candidates for organic photovoltaic (OPV) devices, with external quantum efficiencies (EQE) as high as 70% [1]. However, this high EQE has not been entirely conveyed into high power conversion efficiencies (PCE) due to low absorption coefficients in the sunlight spectrum (low spectral overlap), thermal energy losses, exciton recombination losses, limited electron, and hole conductivity, among other reasons. As a result, the reported certified PCEs have stagnated at 11% for the last 15 years. Some of these drawbacks have been amended by the development of non-fullerene acceptors (NFA) with more flexible tuning of structural and electronic properties[2]. Recently, a series of NFA composed of a D-A-D S,N-heteroacenes backbone were developed resulting in the outstanding Y6 family, presenting PCEs of about 15-18% when blended with PM6 polymer[3]. However, the synthesis of these compounds is complicated, costly, and polluting, prohibiting large scale applications. Oligomers and polymer of conjugated systems that can reproduce the Y6:PM6 features can be prepared by simpler and cleaner routes and can be produced in large scales. In this contribution, we propose new NFA based on S,N-heteroacenes for OPV devices. Using theoretical approaches, we have designed oligo-S,N-heteroacenes and oligo-phenothiazines as D-A heterojunctions. We have synthed monomers with an appropriate functionalization, oligomers, and prepared thin films. In addition, we report their structural, optical, and electro-optical properties.

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Development of Bioinspired Luminescent Langmuir-Blodgett Films Using Europium Complex and Tristearoyl Uridine for Advanced Probe Applications

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In nanoscience, techniques have been developed to investigate and manipulate biological components at the molecular level. Nanobiotechnology, in particular, centers on molecules of biological interest that self-assemble on nanostructures, generating significant interest in the scientific community. Among these self-assembling molecular systems, Langmuir and Langmuir-Blodgett (LB) films can be produced as mono- or multilayered structures with molecular precision. Langmuir monolayers, characterized by their molecular arrangement at the air-water interface, are ideal models for exploring the organization of biological membranes. In this study, we engineered Langmuir monolayers using 3',4', and 6'-tri stearoyl uridine (PNM2) for its potential anti-tumor properties and integrated the complex [Eu(tta)3(H2O)2] as a luminescent spectroscopic probe. The Langmuir and LB films were created using a mixture of the 0.5 mg/mL solutions in chloroform, combined in a 2:5 volume ratio. The characterization of these monolayers involved methods such as tensiometry, infrared spectroscopy, and microscopy, confirming the successful incorporation of the complex into the floating film. The monolayers were then transferred to solid substrates as LB films by vertically passing several times the substrate through the monolayer at a surface pressure of 30 mN/m, providing films with the number of layers, and consequently thickness, controlled by the number of passages of the substrate through the monolayer. We analyzed the resultant LB film using luminescence spectroscopy, revealing a high luminescent intensity when excited at 344 nm through antenna effect and a lifetime of 0.52 ms, offering valuable information on the molecular structure and local lanthanide symmetry. This research indicates that these monolayers hold promise for developing luminescent probes for medical applications, particularly in exploring and treating cell membranes.

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Development of glass and glass-ceramic substrates based on bismuth and vanadium phosphates for photocatalytic applications

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There is currently great concern about the increase in pollutants in water, called emerging pollutants and an alternative to treating organic pollutants is photocatalytic materials. However, these materials are usually difficult to apply because they are obtained as powder, in addition to having photocatalytic activity in the UV region, which is less available from sunlight. This study aims to develop glass and glass-ceramic with crystalline particles based on BiVO4 and BiPO4 for applications as photocatalytic material active with phases under visible light for degradation of pollutants [1]. To evaluate the phosphobismuthate glass and glass ceramic as a potential photocatalytic material, the synthesis of the glass composition of Bi(PO3)3-Bi2O3-Na2O-V2O5 was performed by melt-quenching varying the V2O5 content, and the glass-ceramics were prepared using a heat-treatment with different temperatures. Their characterization was made using Differential Scanning Calorimetry (DSC), x-ray diffraction (XRD), Raman and UV-Vis spectroscopy. It was possible to verify the reduction of Bi2O3 by surface plasmon resonance at 455 nm and the presence of the vanadium ions when the samples were analyzed in UV-vis region. With DSC was possible to observe the increase in the glass transition temperature as V2O5 was introduced into the composition. The Raman spectroscopy showed a gradual depolymerization of phosphate network into pyrophosphate and vanadate-based network. The XRD patter diffraction shown the coexistence of the BiVO4 and BiPO4 phases in glass ceramic samples. Therefore, it was possible obtain glasses with good stability evaluating the changes coming from the addition of vanadium in the composition. Furthermore, to obtention to crystals phase with promising potential as photocatalytic material in visible light region.

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Development of glass-persistent composite by direct incorporation of $Sr_2MgSi_2O_7$:Eu^{2+},Dy^{3+} into phosphate glass

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Oxide glasses are a condensed state of matter that present structural disorder from the 2nd sphere of coordination, in addition to the presence of glass transition temperature (T_g). Due to the high characteristic temperature of conventional silicate, phosphate-based glasses are studied in applications that require milder temperatures, such as for the incorporation of crystalline materials. Crystals with persistent luminescence (PeL) properties depend on a host matrix to be widely applied, which provides improved mechanical properties and chemical resistance [1,2]. The production of a 'persistent glass' by incorporation of the crystals into the glass synthesis requires the addition of PeL microparticles at temperatures above the melting temperature (T_m), which introduces the problem of corrosion of the microparticles by the melt, even using a matrix with low characteristic temperatures such as in phosphates. In this scope, the commercial blue persistent $Sr_2MgSi_2O_7$:Eu^{2+}, Dy^{3+} was incorporated into a glass matrix of composition K_2O-Li_2O-P_2O_5-Nb_2O_5 at a temperature close to the T_m of the already synthed glass. UV-vis absorption indicates the transparency of the final composite from 350 to 800 nm. Raman and SEM-FEG coupled with EDX analyzer confirm the non-interaction between the incorporated particles and the glass matrix. Additionally, micro-CT findings corroborate the homogeneous dispersion of the crystals in the glass volume mixed in a planetary mixer. The absolute persistence measurement in cd/m^2 shows the same non-interactive the luminescent behavior when compared with pure PeL microparticles. That said, the corrosivity of the matrix can be assessed by additional heat treatment varying dwell time and temperature.

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Development of luminescent materials for solar energy conversion

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Under laboratory conditions or testing in standard situations - which involve solar radiation of 1000W/m², temperature of 25°C, and solar spectrum AM=1.5 - with current technology, it is feasible to produce individual crystalline silicon cells with an efficiency greater than 26%. However, commercially, the efficiency ranges between 15% and 20% [1]. Considering that these solar cells achieve mostly visible light conversion, the main objective of the project is the development of luminescent materials that can convert the ultraviolet (UV) and infrared spectrum of the Sun, which are not efficiently absorbed by commercial photovoltaic cells, into visible light to increase efficiency in the photovoltaic energy generation process. For UV to visible conversion, transparent matrices have been developed using different materials such as sodium polyphosphate with aluminum chloride coacervates, sol-gel glass or transparent polymers like acrylic, containing doped CdS quantum dots that are responsible for UV light absorption and visible light emission. The conversion of infrared to visible is being evaluated through optical upconversion processes using amorphous transparent materials doped with lanthanide ions. Initial studies will allow the development of suitable materials for this purpose, but conversion will require further studies and the use of solar concentrators due to the low quantum efficiency of upconversion processes. The materials will be evaluated by their absorption and emission spectra.

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Development of oxyfluoride glass and glass-ceramics with luminescent properties

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The oxyfluoride glass were studied with the aim of obtaining glass-ceramics with luminescent properties. After the synthesis of glasses using the melting-cooling method under established conditions, the samples were thermally analyzed by DSC (Differential Scanning Calorimetry), treated at Tx1 (first temperature at which crystallization begins) to obtain a glass-ceramic and subsequently crystalline phase was identified. It was possible to observe, from XRD, the formation of KLaF4 crystals in the glass sample. The glasses were doped with europium (Eu3+) and co-doped with erbium and ytterbium (Er3+/Yb3+), remaining transparent, thus demonstrating good hosts for these elements. Subsequently, these obtained samples were heat treated to obtain glass-ceramics. From the heat treatment it was possible to obtain transparent luminescent glass-ceramics with the phases KLaF4. By studying luminescence spectroscopy, a reduction in symmetry around the europium ion in doped glass-ceramics was observed, due to the increase in the emission intensity of the band at 594nm. An increase in the emission intensity related to the transition at 539nm in the glass ceramics of the 15K30LaErYb precursor glass was also noted. It was observed in the energy upconversion spectrum of the sample co-doped in the system with K2O, splittings of the Stark levels in the glass-ceramics suggesting that the Er3+ ion is in a crystalline environment. Furthermore, an increase in the emission band in green compared to red in glass-ceramics was also observed, also indicating lower phonon energy associated with the presence of crystals in the glass matrix. The lifetime of glass-ceramics doped with Eu3+ was reduced in relation to glass samples and it is believed that this may be related to the higher asymmetry ratio of these samples. Finally, it was possible to obtain luminescent and transparent glasses and glass-ceramics with a high molar percentage of LaF3, achieving the main objectives of the work.

Development of plasmonic thin-layer chromatography for the separation of graphene quantum dots

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The use of focused laser light to manipulate particles at micro and nanometer scales has garnered significant interest for applications like organic molecule crystallization, nanomaterial classification, and cell manipulation [1]. Graphene quantum dots (GQDs) have unique properties that are adjustable by their and chemical composition. This work aims to use thin layer chromatography (TLC) and plasmonic trapping to separate GQDs according to its s and optical properties. Silica gel TLC plates were previously prepared by depositing a strip of Ag nanoparticles (NPs) 10 mm above the GQDs spot, that was located 10 mm from the base of the plate. Ag NPs were synthed from a solution of silver nitrate (AgNO3), dimethylformamide (DMF) and polyvinylpyrrolidone [2]. A solution of 25%vol. DMF and 75%vol. of ethyl alcohol was used as the chromatography eluent. During the chromatography process, the Ag strip was irradiated using a 405 nm CW laser diode, operating at 500 mW. TLC plates were characterized by photoluminescence (PL) characterization. TLC results without irradiation indicated that GQDs could be separated into 3 components, with retention values (RF) of approximately 0.45, 0.70 and 1.0. TLC performed under laser irradiation showed a strong PL signal associated to the GQDs in the Ag strip, suggesting that plasmonic entrapment is occurring.

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Doped hybrid matrices and functionalized acrylate polymers employed as active materials for random laser systems

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Random laser systems have been widely investigated for several technological applications, ranging from integrated photonics to medical diagnosis [1]. Random lasers can be classified in two classes according to its feedbacks mechanism: (i) non-resonant feedback and (ii) resonant feedback. The emission in this kind of lasers can be observed when an external light source is focused on an optically active material, which contains in its interior scattering centers with on order of few micro and/or nanometers, distributed in a disordered way in its volume. There are large varieties of samples that can be employed in random lasers experiments. In this work, we prepare different optically active samples and investigate its application in random laser systems. First, we produce solid polymeric materials functionalized with xanthene dye and SiO_2 nanoparticles. The polymeric samples are photopolymerized using a UV lamp. These samples are prepared using equal proportions of two three-acrylate monomers, tris(2-hydroxyethyl) isocyanurate triacrylate and ethoxylated(6)trimethylolpropane triacrylate and one photoinitiator, ethyl-2,4,6-trimethylbenzoyl phenyl-phosphinate, compound responsible to absorbs the light and generates free radicals to start the UV polymerization process. We also use different SiO_2 concentration to prepare the samples, aiming change the number of scattering centers into the bulk. Finally, we prepare doped aerogels via sol-gel process using organic/inorganic hybrid matrices. Through the control of chemical reaction, we are able to produce aerogels bulks with different porosity, an import feature to change the number of scattering centers inside the sample. Our results show that the prepared samples are promising materials for application in random lasers experiments.

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Effect of Mg^{2+} doping concentration on thermoluminescence properties of $CaAl_2O_4:Ce^{3+}$

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This study investigates the influence of varying concentration of magnesium ions (Mg^{2+}) co-doped with cerium-doped calcium aluminate ($CaAl_2O_4:Ce^{3+}$) by thermoluminescence (TL) analysis. TL is a powerful technique used for ionizing radiation dosimetry, involving electron excitation by radiation and subsequent light emission upon thermal stimulation [1]. Solution combustion synthesis was employed to synthe $CaAl_2O_4$ samples, both doped and co-doped. $Al(NO_3)_3$, $Ca(NO_3)_2$, and CH_4N_2O were used as starting materials, with urea acting as a fuel for the combustion, while $Ce(NO_3)_3$ and $Mg(NO_3)_2$ provide the doping ions. The concentration of Ce^{3+} ions was maintained at 0.15 mol% whereas Mg^{2+} concentrations were varied in 0.1, 0.5, and 1 mol %. The reagent mixture was transferred into a preheated muffle furnace at 500 ºC and kept for 5 min. After combustion, the crystalline powder formed was crushed in an agate mortar to obtain the fine powder. TL measurements were conducted using the Risø reader (model DA-20) equipped with a beta source ($^{90}Sr/^{90}Y$) for irradiating the sample and a Hoya U-340 filter. Samples were exposed to a beta radiation dose of 0.1 Gy and TL glow curves were obtained at a controlled heating rate of 5°C/s up to 500ºC. Preliminary results showed three intense TL glow peaks at 110, 340, and 450°C. The variation in the concentration of Mg^{2+} ions resulted in a decrease in the intensity of the lower temperature TL peak (110ºC). On the other hand, there was an increase in the intensity of the two TL peaks at higher temperatures (340 and 450°C), which are more thermally stable and hold potential for investigating dosimetric characteristics. Thus far, it can be concluded that incorporating Mg^{2+} ions as a co-dopant in $CaAl_2O_4:Ce^{3+}$ samples show potential for dosimetry applications.

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Encapsulated optical humidity sensor for agricultural production

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Measuring humidity levels is paramount in ensuring optimal conditions for agricultural production. In this study, we investigated a humidity sensor based on optical fiber technology, specifically designed for agricultural environments, particularly those displaying particulate pollution. The sensor reported herein employs thin polymeric films deposited onto optical fibers. Fluctuations in humidity levels induce changes in the refractive index and thickness of the polymeric film, enabling humidity measurements through spectral analysis of the device. To ensure the functionality of the sensing platform in environments with particulate pollution, we encapsulated the sensor within a custom-designed 3D-printed capsule featuring pores of adjustable s [1]. This encapsulation procedure shields the sensor from particulate pollution while maintaining gas permeability, thereby ensuring accurate readings in challenging agricultural conditions and contributing to extending the device's lifetime. In this context, the compact and adaptable design of our sensor facilitates its integration into agricultural applications, from open-field cultivation to food production. Therefore, the encapsulated optical humidity sensor reported in this work represents a relevant advancement in optical fiber technology for agriculture, with promising results for improved productivity and sustainability in modern farming and food production practices.

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Engineering Near-Infrared Responsive Branched Gold Nanostructures

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When metallic nanostructures are irradiated, the conduction band electrons undergo a collective and coherent oscillation in resonance with specific frequencies of light, resulting in increased absorption and scattering of the electromagnetic field, known as localized surface plasmon resonance (LSPR) [1]. Following optical excitation, plasmon can decay into an electron−hole pair, generating the so-called hot electrons, which can favor photothermic and photocatalytic processes. Morphological changes in metallic nanostructures are responsible for direct modifications in their optical properties, allowing the development of systems with tunable absorbance from visible to the near-infrared region (NIR) of the spectrum and optimized generation of hot electrons. Here, we propose a novel nanomaterial that combines the optical properties of gold nanorods and high reactive sites of branched structures. Gold nanorods were synthed by a seed-mediated method, followed by the subsequent branch growth. We have obtained highly branched nanostructures that have optical responses at the NIR region and are good candidates for sensing, photothermal and photocatalytic applications. We demonstrate that the branched structure growth and stability are dependent on the nanorod surface coating and reduction rate, resulting in structures with different morphologies and tunable optical properties. Also, coalescence with smaller particles was also observed during the growth, resulting in highly asymmetric structures around the nanorod surface with high surface area and slits that can act as high reactive spots.

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Enhanced Photocatalytic Performance of Titanium Dioxide-Carbon Composite Coatings Embedded with Silver Nanoparticles

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In the quest for efficient solutions for environmental remediation, titanium dioxide-carbon (TiO2-C) composite coatings with silver have emerged as promising candidates due to their nanostructural, morphological, and photocatalytic properties under visible light irradiation[1]. This study investigates the synthesis, characterization, and photocatalytic performance of these coatings, produced using the sol-gel technique followed by heat treatment at 500°C for 30 minutes. The uniform application of the coatings onto a glass substrate was confirmed through scanning electron microscopy (SEM) analysis, which demonstrated a homogeneous dispersion of the metal across the expanded graphite surface.The integration of silver into the coatings, achieved through immersion in a silver nitrate solution and subsequent exposure to ultraviolet (UV) light, resulted in a significant enhancement of photocatalytic activity. Photocatalysis curves showed up to 80% degradation of methyl orange dye under visible light irradiation over a period of six hours, with substantial degradation observed within the first two hours. This rapid degradation kinetics underscores the practical potential of these coatings in wastewater treatment and environmental remediation processes.The characterization techniques employed, including X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), and Raman spectroscopy, provided insights into the crystal structure, chemical composition, and functional groups present in the coatings. The results indicate the successful incorporation of silver into the TiO2-C matrix, which may lead to the formation of silver nanoparticles or silver oxide species, known for their photocatalytic properties.In conclusion, the comprehensive analysis of the TiO2-C composite coatings embedded with silver suggests their potential as efficient photocatalysts for environmental remediation applications.

Enhancing Charge Transfer in Dye-Sensitized Solar Cells: Impedance Studies of the Nb_2O_5 Thin Film/Electrolyte Interface

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The niobium pentoxide (Nb_2O_5), a semiconductor oxide, has stood out as a gap-blocking layer (BL) and electron transporting layer (ETL) in perovskite cells, due to its physical and chemical properties such as good transmittance in the visible spectrum region, chemical stability, and energy band gap, indicating improvements in the cells' Voc [1]. In this context, there is an opportunity to examine its application in Dye-Sensitized Solar Cells (DSSCs), as a thin film between the photoanode/Fluorine-Doped Tin Oxide (FTO) interface. In DSSCs, various resistances, for example, R_s (surface resistance of FTO and cell contact) and R_{rec} (resistance to charge recombination at the FTO/photoanode/Electrolyte interface) are critical [2]. In this study, we amide to optimize the Nb_2O_5/electrolyte interface by varying the rotation speed (2500, 5000, and 7500 rpm) to obtain thin films of Nb_2O_5 using the Spin-Coating technique. The Nb_2O_5 solution was prepared by the sol-gel method, with $NbCl_5$ (0.5g), H_2O (0.6 ml), and CH_3CH_2OH (9.5 ml), stirred for 240 min. The films were then sintered at 500°C for 2 h. In this context, we evaluated the charge transfer resistance at the interface. UV-Vis-NIR transmittance spectroscopy analysis revealed the average transmittance in the visible spectrum of the samples: pure FTO; 2500; 5000; and 7500 rpm, with results of 82.96%, 79.88%, 82.32%, and 81.59%, respectively. The film produced at 5000 rpm showed a transmittance very close to that of pure FTO. In characterization by electrochemical impedance spectroscopy, , films at 2500, 5000, and 7500 rpm exhibited R_s values of 23.89, 36.37, and 25.65 (Ωcm^{-2}), respectively, and R_{rec} values of 16.50, 32.50, and 23.01 ($k\Omega cm^{-2}$). Preliminary results suggest higher R_{rec} at 5000 rpm, prompting further research including TiO_2 layer addition and more analyses.

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Erbium (Er3+)- and ytterbium (Yb3+)-doped calcium phosphate

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Calcium phosphates(CPs) are widely employed as biomaterials because their characteristics resemble the characteristics of natural bone tissues. Their excellent biocompatibility minimizes the chances of rejection after they are implanted. In addition, CPs display bioactive properties that promote interaction between the biomaterial surface and the bone, facilitating osteconduction and playing a crucial role in bone regeneration [1]. The calcium (II) ions(Ca2+)in the CP structure can be partially replaced with erbium (III) ions (Er3+) or ytterbium (III) ions (Yb3+). Here, we evaluate the effect of doping CP with 1% Er3+ and 10% Yb3+ aiming to identify properties that might contribute to innovative approaches for detecting or treating diseases [2]. X-ray diffraction of the doped material revealed peaks at 2θ = 34.5, 31.2, 29.8 and 27.9o, corresponding to card n001-0941, attributed to CP. Figure 1 shows the energy up-conversion spectra of the doped material upon excitation at 980 nm. Yb3+ acts a sensitizer, transferring the absorbed energy to Er3+, which acts as activator and emits radiation in the visible region (green). The bands at 525 and 553 nm correspond to the 2H11/2→4I15/2 e 4S3/2→4I15/2 transitions, respectively (thermally excited states). Intensified emission of the band at 525 nm in relation to the emission of the band at 553 nm indicates that the temperature of the system increased and can be attributed to heating promoted by increasing laser power. The spectra also display a less intense band at 650 nm, in the infrared region, which is due to the 4F9/2 → 4I15/2 transition [3].

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Europium(III) complex fluorescence enhancement by silver nanoparticles: a potential luminescent sensor

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The development of sensors for analytes detection which humans and the environment are exposed to can be optimized by optical sensors studies. These are devices that make the detection of a substance of interest giving a visible analytical sign, like a color change, light emission or luminescence quenching [1,2].The present work investigated the intensification of $[Eu(bmdm)_3(H_2O)_2]$ (bmdm = avobenzone, 1-(4-Methoxyphenyl)-3-(4-tertbutylphenyl)propane-1,3-dione) complex emission by Metal-Enhanced Fluorescence (MEF). The AgNPs were synthed in aqueous solution using pectin as reducing and capping agent and were confirmed by UV-Vis spectroscopy and TEM [1]. The particles obtained were between 10 and 50 nm, depending on the synthesis conditions. The complex was synthed with 1:3 molar ratio of Eu:bmdm, stoichiometry was confirmed by complexometric titration, the coordination by FT-IR and the visible emition by photoluminescence spectroscopy [2]. The emission spectra profile change in function of complex and nanoparticles ratio. The MEF effect was observed in some conditions due to nearby metal nanoparticles. The presence of Cu^{2+}, Fe^{2+}, Fe^{3+}, CrO_4^{2-}, $Cr_2O_7^{2-}$, $H_2PO_4^-$ in the dispersion exhibited a clear quenching in the emission, with the analytes being detected between 10 and 100 µmo/L. These results suggest that the combination of these materials has a great potential for the development of devices for detection and quantification of some inorganic ions in aqueous dispersions. Incorporating this system in polysaccharides thin films is being considered for the development of a detecting device.

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Evaluation of Luminescent Properties of Y3Al5O12:Tb3+ for Luminescence Thermometry

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Luminescence thermometry, a promising technique based on the use luminescent properties of materials that vary with temperature, offers an accurate and non-invasive method for measuring temperatures across various scales. Exploiting the thermal sensitivity of luminescent emission from lanthanide ions, this approach is applicable from nanomedicine to the optimization of microdevices. Despite the advancements, challenges such as the need for materials with greater sensitivity and resolution persist. This work aims to overcome these limitations by exploring the potential of new materials doped with Tb^{3+}, with a specific focus on Y3Al5O12 (YAG). The YAG:Tb3+ with different dopant concentrations were synthed by the Pechini's method and sintered using a CO2 laser as the main heating source. The resultant ceramics exhibited a high relative density of about 98–99 ± 1%, good microstructural homogeneity as verified by scanning electron microscopy, and a single cubic crystalline phase as determined by X-ray diffraction. Photoluminescence properties were probed from 20 to 320 K and the thermometric parameters determined.

Exploring the shape-induced enhanced Raman scattering (SIERS) effect in silicon V-shaped microchannels for detection of environmental contaminants without metallic nanostructures.

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Raman spectroscopy is a powerful tool for identifying compounds, providing specific vibrational information for each molecule. However, the Raman scattering signal is inherently weak, and several strategies have been developed to improve its detection against analytical methods. Our research group recently demonstrated that V-shaped microchannels on silicon substrates (Si-V) can intensify the Raman signal without metallic structures. This effect was called shape-induced enhanced Raman scattering (SIERS) [1]. Based on that, we evaluated the SIERS effect performance in the absent metallic nanostructures with a class of molecules of environmental control interest. Herein, the SIERS performance was performed in comparison with Raman analysis using Si-V and Si flat, with target molecules of atrazine, 2,4-D, fipronil, and benzo(a)pyrene in a concentration range of 10-3 to 10-8 mol L-1. For this, the Si-V substrate was positioned with a 5° tilt, and 10 µL of target molecule solutions were dropped onto the Si-V, and dried at room temperature (~25°C). This process was repeated three more times, totaling 40 µL of solution for each mentioned molecule; the same process was performed for flat Si. The results reveal that the Si-V substrate shows a spectral profile as a function of signal/noise more defined than Si flat, provided by the Si-V geometric shape. Specifically, the Raman signal for Si-V substrates of all molecules is in media intensified 5-fold than Si flat, which is associated with the stronger electromagnetic field and light confinement into the Si-V microchannel, corroborated by simulation with infinite elements. From a practical point of view, Si-V substrates show great promise for commercial applications once their reusability is the main advantage, in addition to the improved Raman signal free of metallic nanoparticles.

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Exploring Vibrational Changes with CARS and Raman in Tilapia Gills and Livers Exposed to Pesticides

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The study aims to investigate the impacts of pesticides on biological systems (on the gill and liver tissues) of fish of the species Oreochromis niloticus (Tilapia). The increased use of pesticides has resulted in irreversible damage to human health, including the induction of carcinogenesis, and to the environment, with contamination of the soil and, particularly, groundwater and water sources. According to a report by the United Nations (UN), it is estimated that approximately 200,000 people die each year in the world from acute pesticide poisoning. Therefore, this research evaluates the effects of pesticides on aquatic organisms, using the CARS (Coherent Anti-Stokes Raman Spectroscopy) microscopy technique and Raman scattering. The results revealed that exposure to pesticides caused serious morphological changes in the livers and gills of fish. Furthermore, it was found that the effect of pesticides is not influenced by the period of exposure (24h and 96h), indicating that animals exposed to pesticides for a short period suffer irreparable damage to their gill tissues. In short, it can be inferred that the damage caused by pesticides results from the contamination of the aquatic system by these substances. Therefore, water quality is crucial for the preservation of ecosystems. This research provides valuable information for environmental management and public health, highlighting the urgency of measures to mitigate the harmful effects of pesticides on aquatic life and human health.

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Fiber optics-based refractive index sensor for water quality monitoring

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Efficient monitoring of water quality is vital for safeguarding human health and ecological integrity. In this context, optical fibers, due to their capability to be set as compact and highly sensitive sensing platforms, emerge as a key enabling technology for the design and development of new sensors for water quality assessment. Measuring water quality can be addressed through measuring different physical and chemical parameters such as turbidity, temperature, pH, and refractive index. In this context, in this work, we investigated an optical fiber sensor capable of detecting refractive index variations, thus contributing to the efforts on water quality assessment. The sensor reported herein utilizes multimode interference inside a singlemode-multimode-singlemode (SMS) configuration and polymer-coated optical fibers for detecting the refractive index variations in the medium external to the fiber aiming at having better resolution than that achieved with typical self-image phenomenon-based SMS sensors [1]. By investigating the sensor's performance, including its sensitivity and resolution, we demonstrate its potential to act as a robust tool for addressing water quality monitoring needs. We understand that our results contribute to advancing sensor technology and underscore the potential of optical fibers to act as platforms for the development of new water resources monitoring devices, hence contributing to human health and ecological sustainability efforts through efficient water quality assessment.

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Fine structural characterization of nanoparticles based on electron diffraction: Gathering morphology, atomic arrangement, and strain using low dose experiments

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Metal nanoparticles play important roles in basic and applied research. The tunning of their physicochemical properties can be obtained by controlling structural aspects (, shape, atomic arrangement, etc.) and chemical properties (composition, alloying, chemical gradient or core-shell structure, etc.). This has been extensively studied in plasmonics to control surface plasmon resonance or in catalysis to improve selectivity, sensitivity, and activity of catalysts. Precise control of NPs formation is usually achieved with wet-chemical synthesis, a high throughput affordable method, but which may demand complex multistep procedures. Synthesis optimization demands precise characterization approaches; transmission electron microscopy (TEM) is certainly one of the most utilized methods due to its intrinsic high spatial resolution. It was usual to consider TEM as a very useful but qualitative atom resolution imaging tool for materials science, but it must be emphad that Angstrom resolution images may require a rather high electron irradiation dose what may induce significant sample modifications. Instrumentation associated with TEM has shown a remarkable progress including many different aspects such as electron optics, automation, reproducibility, and detectors. Here, we will discuss novel advanced structural TEM tools based on electron diffraction (ED) which can be applied to obtain morphology and details of atomic structure for very complex multidomain or multibranched particles. These recent ED approaches are particularly interesting because the require low electron irradiation doses in the range of 10-200 electrons per square Angstrom. We will discuss the use of the so called 4D-STEM (spatially resolved ED mapping), electron-based Pair Distribution Function (ePDF) and Precession Electron Diffraction (PED). We aim to show how these new methods open a wide range of opportunities to solve the structural characterization of nanomaterials to gather quantitative informatio

Fundamental Study of Tungsten Phosphate Glass for Applications in Photonics and Scintillators

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Glassy materials have several advantages over crystalline materials, such as stoichiometric flexibility in your compositions. When doped with earth rare ions (RE), they have various photonics applications due to their intrinsic properties, such as optical sensors, lasers, etc. [1]. Phosphate glasses contain alkaline/alkaline earth and have characteristics, including low melting and glass transition temperatures, a wide transmission in the UV to infrared range, and high coefficients of thermal expansion. The glass system $NaPO3-Ba(PO3)2-Ga2O3$ with different Na/Ba ratio compositions have been prepared using the conventional melting-quenching method. Thermal properties were investigated by DSC. The replacement of NaPO3 by Ba(PO3)2 leads to a decrease of Tg and thermal stability from crystallization parameter (Tx-tg). Additionally, the structural study was monitored by Raman scattering and Infrared spectroscopy (FTIR) and Solid-state NMR. The Raman scattering has shown that the increase of Tg is followed by a decrease of the intensity of the band at 870 cm-1 characteristic of P-O-P bonds which suggests a depolymerization chair phosphate units. Infrared spectroscopy has shown the same behaviour also was observed, the intensity of the P=O stretch band decreases and the intensity of the P-O- asymmetric stretch increases, showing the increase of different terminal groups P-O-. These results were confirmed by 31P NMR spectra, where the phosphate chair depolymerization, resulted in a reduction of P2 units and an increase in P1 formation.

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Guided Luminescence in Waveguides written by Femtosecond Laser in Quantum Dots-doped Phosphate Glasses

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Quantum dots (QDs) have been widely studied due to their electronic, optical, and structural properties [1], and glasses doped with this type of nanoparticles have been used in applications in optoelectronics, solar cells, optical amplifiers [2], and resonant nonlinear optical devices [3]. In this work, we report on guided-wave luminescence in buried waveguides written by femtosecond lasers in QD-doped phosphate glasses. The guiding properties of the waveguides have been investigated by end-face coupling of free-space light. Under the optical pump laser at 405 nm, guided-wave luminescence of QDs at visible light range has been realized through the waveguides. Two types of waveguides were written, one with a single track, and another formed by five adjacent tracks. We compared the intensities of the guided-wave luminescence observed in these two types of waveguides, the optical losses and the guided profile.

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Highly active MOF/carbon nitride-based heterojunction in the of rhodamine B dye photodegradation under visible light.

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In the world, around 700,000 tons of synthetic dyes are produced and used in various sectors [1]. In light of this, researchers have been developing methods that can change this scenario, with one highly studied branch being the production of catalysts that can be active in degrading organic dyes [2]. This work aims to present the development of a photocatalyst formed from the heterojunction of a Metal-Organic Framework (MOF) and graphitic carbon nitride (g-C3N4). The lanthanide MOF (EuBDC) was obtained through the reaction of europium nitrate and terephthalic acid organic ligand (C6H4(COOH)2), in the presence of g-C3N4 previously synthed from urea, to generate EuBDC/g-C3N4 composite with different mass ratio. The heterojunction was characterized by X-ray diffraction (XRD), FT-IR, and diffuse reflectance spectroscopy in the UV-visible region. Photocatalytic assays were conducted with a sample containing a 50/50 mass ratio of EuBDC and g-C3N4 in a solution of rhodamine B dye (50 mL, 10 ppm), using a conventional 30W LED lamp, monitored using UV-VIS spectroscopy. The photodegradation percentage of 94.30% and a rate constant of 7.31 x 10-2 min-1 were observed, superior to the pristine components. The results were satisfactory when compared with the literature on the degradation of rhodamine B dye using other photocatalysts.

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High-precision glass refractive index dispersion curve determination by optical transmittance measured in commercial spectrometers

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It is well known that, in the absence of absorption, the linear refractive index dispersion curve of a glass slab can be obtained from its optical transmittance curve [1]. However, in practice, the transmittance curves are not common for high-precision refractive index measurements and they are only used for an approximate determination. Despite the sample and sample preparation defects such as internal scattering, poor surface parallelism, and surface imperfections, for instance, even for very good and well-prepared samples, inexact dispersion curves can be obtained from the transmittance curves. Considering that standard commercial UV-Vis spectrometers are very common in many laboratories, it is interesting to take advantage of this fact and find the necessary requirements that can lead to obtaining good dispersion curves with a reliable index of refraction magnitude. In this context, in order to understand why an imprecise refractive index curve is obtained and how to overcome it, we perform systematic transmittance measurements in several well-known optical glasses [2] with different thicknesses. Preliminary results, obtained using a UV-Vis spectrometer (UV 1800 from Shimadzu), have shown that sample thickness and linear absorption are the main constraints to be considered. For example, when measuring the transmittance curve of good samples with different thicknesses, we found that the least square method can be used to reduce the thickness and absorption issues. Furthermore, employing a standard two-arm spectrometer, we discovered that adjusting the sample position (in either the sample or reference arm) also contributes to obtaining improved transmittance curves.

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Hydrothermal synthesis of alkali niobates for photocatalysis

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Nanoparticle alkali niobates have photocatalytic properties, which allows their application in the decomposition of organic pollutants [1]. In this work, sodium niobate ($NaNbO_3$) and potassium niobate ($KNbO_3$) were synthed by the hydrothermal method under the following reaction conditions: temperature 160 and 200°C and time 6 and 24 hours. The samples obtained were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM) and the BET adsorption method. As a result of the XRD analyses, a single phase of sodium niobate was obtained in the monoclinic phase for both synthesis conditions and a single phase of potassium niobate with an orthorhombic crystal structure. As for their morphology, the SEM images showed the sodium niobates to be cubic in shape and approximately 3 to 5 micrometers in . For potassium niobates, the images obtained showed agglomerates of small, regular particles in the order of micrometers. The BET method characterization of $KNbO_3$ showed a larger surface area than $NaNbO_3$.

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Improvement of white light generation from triply Nd^{3+}-Eu^{3+}-Yb^{3+} doped TZN glasses by surface plasmon resonance

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The massive use of cellphones, personal computers and even the graphical interfaces present in the new generation's vehicles, it boosts the demand for high definition screens. The use of light-emitting diode (LED) as a more efficient and commercially feasible light source which replaces the incandescent light bulb and great part of the flash lamps, it also contributes in the development of such screens, due the performance of the white light emitted by this device. Nevertheless, there is an increasing concern to develop screens and lamps that are agreeable for the user's vision and it diminishes modifications of the sleep's patterns from those that are exposed for long periods of such light sources. An alternative white light source designed by researchers for the achievement of this goal, it was generate this source from the combination of emission bands in the visible region of spectrum, as a result of photoluminescence from lanthanides ions embedded to vitreous matrices, with the intensities of each band controlled primarily by the concentration of ions into the glasses, but it also driven by the power of excitation beam that initiates the photoluminescence process. Despite the promising progress in white light generation through lanthanides ions doped glasses [1], the small absorption cross-section of lanthanides ions and low luminescence efficiency caused by mediated electric dipole 4f-4f transitions are the main challenges that may hinder their integration in future applications. The present work presents an alternative that provides the boost and/or control of the intensities from photoluminescence

bands of trivalent lanthanides ions in triply doped Nd^{3+} - Eu^{3+} - Yb^{3+} tellurite-zinc-sodium (TZN) glasses, as the consequence of surface plasmon resonance effect due to the add silver nanoparticles (Ag) into the glasses.

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Incorporation of graphene quantum dots into silica substrates obtained by the sol-gel process

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This work aims to incorporate graphene quantum dots (GQDs) into silica substrates, obtained through the sol-gel process, in order to develop a solid nanocomposite material. GQDs were obtained from the carbonization of refined sugar with sulfuric acid. After filtration and dilution in alcohol, four different GQDs suspensions were obtained. Silica xerogel nanocomposites containing GQDs were obtained by sol-gel synthesis. Xerogels were also submitted to heat treatments up to 1200 ºC. Tauc plots indicated direct bandgaps of ~5.0 and 3.5 eV for all the samples, associated with π-π* and n-π* transitions, respectively [1,2]. Photoluminescence (PL) was recorded under excitation at 473 nm. A broad PL band, between 500 and 800 nm, was observed for all the nanocomposites. The PL intensity was not linear, in respect to the GQDs concentrations, indicating the formation of aggregates during the synthesis. However, the PL intensity presented an enhancement superior to 100% after heat treatments. Solid nanocomposites congaing GQDs are, thus, promising materials for applications in the field of photonics and/or random lasers.

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Influence of blue luminescence on ozone sensor response of ZnO:Co thin films

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Ozone is considered as one of the main pollutants present into the atmosphere [1] and is frequently utilized in disinfection processes due to its potent oxidative capacity [2]. This gas negatively impacts human health, and may causing serious respiratory illness depending on its concentration (> 120 parts per billion) [1]. Therefore, the development of low-cost materials with higher sensitivity, fast response and recovery, and also fair stability, is important. Cobalt-doped zinc oxide thin films obtained by spray pyrolysis technique have shown promise in ozone gas sensing to exhibit a good sensitivity at low concentrations (21 ppb) and high selectivity [3]. In this study, we investigated the influence of defects induced and tuned by Co incorporation and controlled atmosphere annealing, respectively, on the ozone sensor response of cobalt-doped zinc oxide thin films. The samples were grown on Si substrates using a simple acetate-based route by spray pyrolysis technique. Structural and morphological characterizations, and chemical surface analysis were performed. Room-temperature photoluminescence measurements and ozone gas sensing evidenced a notable enhancement in sensor response towards ozone, particularly, in samples exhibiting a defect band emission at approx. 2.7 eV. The improved sensor response is attributed to an increase in the number of actives sites, originated from the presence of defects associated with blue luminescence, such as Zn_i. These defects can act as active sites on the surface of the films, enabling an increased adsorption of oxygen species.

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Influence of cerium as a reducing agent on the optical and magneto-optical properties of Tb^{3+}-doped borogermanate glasses

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Typically, magneto-optical (MO) devices are based on crystalline materials. However, the growth of single-crystals is time-consuming, expensive, and results in materials with limited s and shapes. When compared to crystals, glass is one of amorphous materials with advantages such as durability of optical and mechanical properties with the chemical composition and possibility of being produced in the form of optical fiber. Terbium is the most popular rare-earth in magneto-optical glasses due to its large magnetic moment and small absorption coefficient in the visible and IR regions. However, it is well known that terbium in a glass exists mainly as Tb^{3+}, usually being accompanied by a small amount of Tb^{4+}, and the ratio of these two ions is strongly dependent on the composition of the matrix glass host and the melting atmosphere [1]. In this work we report the influence of cerium oxide as a reducing agent in the optical and magnetic-optical properties of the Tb^{3+}-containing borogermanate glass compositions with potential application in the construction of magnetic field and electric current detection devices. Borogermanate magneto-optical glasses doped with terbium and cerium oxide with a chemical composition (100-x-y $(41GeO_2\text{-}25B_2O_3\text{-}4Al_2O_3\text{-}10Na2O\text{-}20BaO)\text{-}xTb_4O_7\text{-}yCe_2O_3$ were prepared by a conventional melt quenching method and their physical properties, magneto-optical effect, luminescent properties were studied.

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Influence of the PVP on the ZnS colloidal nanoparticles for photonic applications

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Zinc sulfide (ZnS) is an efficient inorganic semiconductor with a wide band gap (3.5–3.9 eV) tunable in the UV absorption spectra and self-organization of three-dimensional (3D) periodic structures with different symmetries [1]. The ZnS nanoparticles offer remarkable applications in photonics, such as optical cavities and photonic crystals. In this study, we investigated how the molecular weight and concentration of polyvinylpyrrolidone (PVP) affect the particle and polydispersity of the ZnS. ZnS nanoparticles were synthed using the homogeneous nucleation process. The methodology used is close to the procedures outlined by Wu et al. [2]. To modulate particle growth, organic stabilizers as PVP with different molecular weights (K10 and K40) were introduced on the wet-chemical synthesis by varying concentrations for ZnS^{2+}: S^{2-} mass ratio of 3:1. The morphology is entirely dependent on the PVP concentration. In both molecular weights of PVP for the concentration of 60 mg/mL, the average diameter of the resulting ZnS colloidal nanoparticles was approximately 175 nm with a polydispersity of 8%. The molecular weight of PVP K40 stabilized the system and resulted in the production of smaller nanoparticles, around 130 nm, regardless of the PVP concentration. For concentrated suspensions (60 mg/mL) of PVP K10, the average diameter increases to 226 nm, followed by a discernible reflection wavelength of 640 nm. Notably, it further exceeds the PVP K10 concentration of 78 mg/mL, and the average diameter achievs a reduction. The suitable distribution of the spherical ZnS nanoparticles obtained from potential low-cost production and upscaling protocols enable a variety of possible applications of technology, including colored photovoltaic panels, functional pigments, and plasmonic sensors.

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Investigation of Graphene Quantum Dot Synthesis via Laser Irradiation

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Graphene quantum dots (GQDs) are particles that usually have a size smaller than 10 nm and exhibit photoluminescence (PL), which depends on the structure of the particle [1,2]. There are several synthesis methods presented in literature for GQDs, which can be obtained from natural precursors, such as carbohydrates and cellulose for example [1,2]. The objective of this work is to investigate a new synthesis route for GQDs, using laser irradiation to obtain nanometric particles, a method not previously explored in the literature. In this work, sucrose was initially carbonized with sulfuric acid. The resulting suspension was evenly divided into two beakers. One of the solutions was subjected to irradiation with a 405 nm CW diode laser operating at 500 mW. The laser beam was focused inside the beaker containing the suspension, which was kept under agitation and heated to 60°C in a water bath. The other beaker was heated with agitation under the same conditions but was not subjected to laser irradiation. The absorbance at 337 nm, corresponding to the $n \rightarrow \pi^*$ transition of the GQDs, was monitored during the process. Results showed that the concentration of GQDs increased during the irradiation procedure. The morphology of GQDs was also analysed by TEM. The new methodology proposed in this work was promising for the synthesis of GQDs from carbonaceous materials.

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Low absorption measurements in transparent solids using Optimized Thermal Lens Spectroscopy

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The determination of very low absorption in solids is very important for several subjects, such as optical fibers, laser cooling and special experiments like detection of gravitational waves, petawatt lasers, etc. Several techniques have been applied to solids such as laser calorimetry, interferometry, photoacoustic (PA), photothermal deflection (PD), and TL. In this paper we used the TL technique in different vitreous hosts. Marcano [1] proposed a TL configuration with a focused excitation beam and an expanded and collimated probe beam. He showed that in this configuration the TL signal can be maximized. In the steady state it reaches its maximum value f(z,∞) → Pi/2. Moreover, this arrangement makes the TL signal almost independent of the beam's waists and positions, therefore increasing the experiment accuracy. The experiments were performed using cw lasers as excitation beams, such as Ar+ (360, 457 – 515 nm), Nd3+:YAG (1064nm) and Er3+ fiber tunable laser (1535 – 1565 nm). The excitation beam was focused by a 20 cm focal length and the HeNe probe beam (633 nm) expanded and collimated to ~8 mm diameter. For the fused silica rod (vitreous quartz from Heraeus) with L= 5cm and 4 cm diameter at 1535 nm, we obtained the thermal diffusivity, (D = 8.3 10-7 m2s-1) and also the absorption coefficient (A = 1.8 10-4 cm-1, ~78 dB/Km). This absorption is possibly due to OH-group vibration, a broad band centered at 1383 nm. Similar measurements were obtained in BK7 borosilicate glass, A=1.8 10-4 cm-1, and Nd3+ doped laser glasses (Q-98 and Q-246, Kigre) with A = 4.3 10-3 cm-1 and 1.8 10-2 cm-1, respectively. In conclusion, the experimental setup is very simple and provided excellent results, with good accuracy and high sensitivity, even using relatively low excitation powers (~1 W) for this kind of measurement.

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Luminescent and magnetic behavior of Eu3+ - doped lanthanum magnetite after slow cooling

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LaMnO3 is a compound with a perovskite structure that is ordered antiferromagnetically below 150 K. In pure lanthanum manganite, the transition metal atom is predominantly in the Mn3+ state, and when the substitution of a divalent ion (such as Ca2+, Ba2+, or Sr2+) on the rare-earth site occurs, an equal number of Mn4+ ions are created at the expense of Mn3+. The magnetic behavior of this material is determined by the nature of the interactions among the mixed-valence Mn ions [1]. When the divalent strontium ion is inserted, Curie temperatures between 305 and 348 K are obtained if a relative fraction of Sr2+ reaches values between 0.33 and 0.35 [2]. This is desirable for the development of thermomagnetic motors that use water as a refrigerant liquid. In literature, some studies are devoted to analyzing the effect of the Eu3+ presence on manganites [3]. In our study, the effect of Eu+3 on the magnetic, optical, and structural behavior of the slow-cooled La0.7Sr0.3MnO3 and La0.4Eu0.3Sr0.3MnO3 manganites was investigated using magnetization measurements as a function of the applied field, X-ray diffraction, scanning electron microscopy, energy-dispersive X-ray spectroscopy, and photoluminescence (PL). Synthesis was carried out by a solid-state reaction route. The results showed that the addition of Eu+3 decreases the saturation magnetization of the manganite, exhibit the R-3cH space group and the presence of Eu+3 increased the unit cell volume of the manganite and decreased the saturation magnetization. The PL showed the emission of Eu3+ ions when excited through charge transfer band and two-lifetimes were determined suggesting two different local environments of Eu3+ ions from La0.4Eu0.3Sr0.3MnO3 and EuMnO3

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Multimode optical fiber containing Tb^{3+} ions for magneto-optical applications

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In recent years, magneto-optical materials such as optical fibers have gained interest for applications such as optical isolators, transducers, and sensors [1]. Developing thermally stable glass compositions for manufacturing these fibers presents a significant challenge. This work presents the results of manufacturing a multimode magneto-optical fiber based on borogermanate glasses with high concentrations of Tb^{3+} ions. The core and cladding glass compositions were BGB-9%Tb_4O_7 and BGB-8%Tb_4O_7, respectively. The core and cladding exhibited ΔT higher than 200°C, with softening points (T_s) at 628°C and 650°C, coefficients of thermal expansion ($\alpha_{25\text{-}500°C}$) at 10.02 and 10.20 x 10^{-6} K^{-1}, and refractive indexes at 532 nm of 1.7609 and 1.7514, respectively. The Verdet constant (V_B) values for the core and cladding compositions are -55 and 57 $radT^{-1}m^{-1}$, respectively. The glass preform was fabricated in three steps: (1) Core preform: a 4 cm long and 4 mm diameter glass rod was prepared using the melt-quenching method at 1400°C; (2) Cladding preform (tube): a 6.0 cm long and 4.2 mm diameter glass tube was manufactured using the rotational casting method at 1400°C; (3) The multimode glass preform was created by inserting the core into the tube (rod in tube). Subsequently, the multimode glass preform was drawn in an optical tower at 740°C and coated with methacrylate polymer. Optical images revealed a core diameter of 190 µm and a cladding thickness of 40 µm. The numerical aperture (NA) value for the multimode fiber was 0.183, and the calculated acceptance angle (θ_a) was 10.5°. The attenuation loss, measured using the cut-back technique, achieved a high value of 13 dB m^{-1}. In conclusion, the manufacturing of a multimode magneto-optical fiber opens possibilities for the development of new Faraday rotators in the future.

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Nanophotonics properties of Low-dimensional Sn3O4 nanobelts with Synchrotron Infrared Nanospectroscopy

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Phonon polaritons (PhPs) result from coupling electromagnetic fields and crystal lattice vibrations, creating bosonic quasi-particles analogous to photons confined at the crystalline lattices interfaces with opposite signs of permittivity. They exist from THz to mid-IR spectral frequencies within Reststrahlen bands (RBs), between transversal (ω_{TO}) and longitudinal (ω_{LO}) optical phonon frequencies. PhPs enable light confinement beyond the diffraction limit in nanostructured polar dielectric materials, facilitating applications such as super-resolution imaging, thermal emission, and data storage. Their advantages stem from inherently higher quality factors and lower optical losses than plasmon polaritonics. In the far and mid-infrared regime, particular attention has been drawn to strongly confined phonon polaritons (HPhPs) observed in materials like h-BN[1], α-MoO3[2], and SnO2[3] due to their natural hyperbolicity and enhanced waveguiding properties. In the scope of photonics, Sn3O4 exhibits negative permittivity within specific spectral ranges, from far to mid-IR, where various polaritons coexist. This work introduces low-dimensional Sn3O4 nanobelts as a lithography-free nanophotonic platform suitable for the cavity confinement of infrared radiation. Leveraging scattering scanning near-field optical microscopy (s-SNOM) in conjunction with Synchrotron Infrared accelerator-based sources, we used broadband Infrared Nanospectroscopy (SINS) to access PhPs cavity modes experimentally.

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Nonlinear optical characterization of a GaP crystal: origin and polarization dependence studies

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Gallium phosphide (GaP) is one of the most promising materials for integrated nonlinear photonics, due to its fundamental properties such as high refractive index (>3), indirect band gap (2.24 eV), good transparency over a broad spectrum (0.55-11 µm), very high nonlinear refraction (NLR) and absorption (NLA), etc. [1] However, only a few studies on nonlinear optical characterization of this semiconductor were made so far. For example, it is crucial to determine the figure of merit for ultrafast all-optical switching (AOS). Materials with high NLR are not necessarily good candidates for AOS if the NLA is also high. Furthermore, such zincblende semiconductors can have nonlinearities from different origins and values depending on laser wavelength, beam polarization, pulse repetition rate, crystal orientation, and so on, which need to be understood. In this way, here, we propose to explore two experimental measurements, Nonlinear Ellipse Rotation (NER) [2] and Polarization Resolved Z-Scan (PRZS) [3], which are capable of determining the material NLR and NLA and, more importantly, providing clues about the origin of the nonlinear effects. To do so, a femtosecond laser system Carbide (from Light Conversion) is operated at 1030 nm with pulses of ~216 fs and tunable repetition rate (from ~1 kHz up to 1 MHz) to characterize a GaP crystal (100 cut, 500 µm thickness). So far, preliminary results indicate that the crystal orientation affects both the NLR and NLA, with mean values around 4.5 x 10^{-18} m^2/W for nonlinear refractive index and 0.6 x 10^{-11} m/W for two-photon absorption coefficient.

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Obtaining nanostructured ferrites for application in advanced oxidation processes

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This work aims to develop a floating photocatalyst to be used to remove organic contaminants present in wastewater [1]. For this purpose, the use of nanostructured ferrites such as cobalt and manganese ferrites, synthed via Pechini and placed under blocks of autoclaved cellular concrete (CCA). This junction aims to unite the magnetic properties of ferrites with those of CCA to float in water, in order to obtain a floating and magnetic photocatalyst that is easy to remove at the end of the tests, and to eliminate the need for agitation of the system [2]. Diffuse reflectance characterizations were carried out in solids to be able to measure the band gap, the x-ray diffraction of the ferrites in powder form and the apparent density measured by Archimedes' principle of each of the blocks covered with the ferrite resin. The tests were carried out with each of the ferrites, and using the dye indigo carmine as a model molecule for organic contaminants without and with the incidence of ultraviolet light (UV-C). In both tests, cobalt ferrite achieved a higher removal percentage than manganese.

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Optical waveguides in perovskite particles embedded tellurium-zinc glass for photonic applications

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Integrated optical devices are at the forefront of enhancing miniaturization and integration with microelectronics through the use of nonlinear optical materials (NLO) for a broad spectrum of photonic applications and the development of precise systems. Techniques such as femtosecond-laser waveguide writing have opened new avenues for detailed and versatile fabrication methods. This research delves into the potential of tellurite-zinc glass (TZ) and perovskite $BaTiO_3$, tri-doped with Er/Yb/Zn and embedded in TZ glass (TZ-NP),1 aiming to advance the functionality of NLO materials within integrated optical systems. The focus is to explore the unique properties of pure TZ and TZ-NP glasses, prepared through the melt-quenching technique, for applications involving integrated optical systems. Chemical surface and internal structure analyses were conducted using X-ray Photoelectron Spectroscopy (XPS) and High-resolution Transmission Electron Microscopy (HR-TEM). The study also focuses on optimizing femtosecond laser (fs-laser) direct writing for creating microstructured waveguides in TZ-NP glass with low propagation loss. An end-face coupling experimental setup measured the waveguide near-field mode intensity. Kelvin Probe Force Microscopy (KPFM) was also used to assess the electrical properties crucial for photovoltaic devices. The possibility of a 14-fold increase in surface potential providing a highly homogeneous response using the KPFM compared to the pure TZ glass has been shown. The propagation loss was reduced to 1.35 dB/cm in optical waveguides of TZ-NP without introducing additional scattering. It has been demonstrated that embedding perovskite particles in glass significantly improves the response of optical and electric properties through enhanced light-matter interactions, potentially leading to the development of optical waveguide components and photovoltaic devices for photonics.

pH dependence of the SERS spectra of the natural product 4-methylesculetin

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Coumarins are abundant in diverse plant species, particularly aromatic, culinary, and medicinal plants. Among the vast array of over 1300 identified coumarins, the derivative 4-methylsculetin (4-ME) has exhibited noteworthy efficacy in in vivo models of intestinal inflammation1. The chemical groups present on the 4-ME molecule not only influences its biological activity but also allows its application as an analytical tool in biomolecule detection using surface-enhanced Raman spectroscopy (SERS). In this study, we examined the pH dependence of the 4-ME SERS signal on Ag nanoparticles (reduced by hydroxylamine). Our analysis revealed changes in Raman band intensities primarily as the pH shifted from 5 to 7.5. Moreover, the intensity of the peak associated with the ring breathing vibration mode, at 1147 cm-1, surged by 40 times at pH 12 (dominated by anionic species) compared to pH 5.5 (predominantly neutral species). Variations in SERS signal intensities at different pH levels may result from changes in interactions between the charge of 4-ME molecules and the adsorption of molecules on the silver surface2. These findings underscore the enhanced capability, dependent on pH, in detecting 4-ME in terms of SERS signal intensity.

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Photodegradation of methylene blue using the FeBTC/FeS hierarchical compound

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Metal organic networks (MOFs) are crystalline hybrid solids of metal ions interconnected by organic ligands, forming porosity and highly accessible surfaces.[1] An important application of MOFs is in water remediation. Fe-based MOFs such as FeBTC have been widely studied because they have a bandgap directly excited under visible light, in addition to being applied in Fenton processes, which improves their photochemical performance.[2] This work aims to modify FeBTC MOFs with sulfide ions to produce FeBTC/FeS hierarchical compounds and perform their structural and photocatalytic evaluation. Electrosynthesis was carried out using iron and platinum as the anode and cathode, respectively. H3BTC was used as a ligand in TBABF4 solution, where was applied a constant current of 30 mA during 3 h. FeBTC was activated under 170 °C for 2 h. The FeBTC/FeS was prepared using FeBTC with 2 mL of Na2S solution at different concentrations. The structures were characterized by scanning electron microscopy. The FeBTC MOF shows the formation of clusters of 1 –2 um. Interaction with HS- ions partially breaks down the structure of MOFs, presenting irregular and porous surfaces. FeBTC/FeS was analyzed by EDX image mapping, showing the presence of the Fe, O, C and S elements, homogeneously distributed over all the composite surfaces. The materials were evaluated under different conditions for photocatalysis using a methylene blue solution. The FeBTC MOF shows adsorption of 20% in the absence of light. In the presence of light, its bleaching performance increases to 40%, while modified (FeBTC/FeS 3) reaches 80% after 120 min of irradiation. When H2O2 is added, the performance of the MOFs reaches 98% of decolorization in 120 min. It can be demonstrated that using HS- ions for modifying photocatalysts based on Fe MOFs is effective in achieving 100% discoloration of MB.

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Polymer-Noble Metal Nanoparticle Composites: Investigating Ideal Temperatures for Production of Gold Nanoparticles in a Polymer Matrix

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We have explored potential optimal temperatures for synthesizing gold nanoparticles (NPs) within a polymer matrix, aiming to establish a cost-effective and scalable approach for fabricating polymer-noble metal nanoparticle composites. We analyzed the influence of temperature and exposure duration on the nanoparticle production process. For the polymer matrix we used a combination of two acrylic resins, Sartomer SR-368 and SR-499. Upon polymerization this mixture yields a rigid and durable material which is used in many research papers for producing polymeric microstructures [1]. Notably, this polymer does not possess a glass transition temperature which makes it particularly suited for studies involving thermal treatments. Our main goal was to identify the temperatures at which gold atoms had sufficient mobility to enable NP formation to be observed and measured.

Nanoparticles were synthed within a polymer matrix by incorporating the metal ion precursor HAuCl4 into the base resin and then the samples were subjected to thermal treatments at temperatures between 120°C and 300°C for durations ranging from 5 to 120 minutes. The polymer matrix serves a dual role, both reducing the metal ions through electron donation and stabilizing the nanoparticles to regulate their growth. The results demonstrated that nanoparticle (NP) formation reaches an optimal level at a temperature of 180°C. This value probably is closely linked to the inherent properties of the polymer. Future studies should explore NP formation within various polymeric matrices. By manipulating exposure time and temperature, we achieved significant control over the amount of nanoparticles produced, as evidenced by the absorption spectra of the samples.

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Preparation and characterization of N,N'-bis(3-triethoxysilylpropyl)-1,4,5,8-naphthalenediimide(NDI) molecular crystal and NDI mesoporous organosilicas for durable organo-electronic systems

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Naphthalene tetracarboxylic diimides (NDIs) are efficient skeletons as electron acceptors due to their high electron affinity. They are applied in heterogeneous catalysis and organic-electronics. We report for the first time the synthesis of N,N'-bis(3 triethoxysilylpropyl)-1,4,5,8-naphthalenediimide (NDI-silane) molecular crystals obtained from recrystallization in petroleum diethyl ether solution. The compound is stable in air conditions and chloroform solution. Its molecular structure and stability were confirmed by liquid-state nuclear magnetic resonance (NMR) spectroscopy. Its crystal indexing and structure were determined by X-ray powder diffraction (XRPD) in combination with Laue patterns obtained by transmission electron microscopy (TEM) and molecular dynamic calculations in the framework of the density functional theory (DFT). Stable NDI-silane crystals were used to obtain mesoporous 100% NDI-based organosilica using the ionic liquid 1-butyl-3-methyl imidazolium-tetrafluoroborate as templating and sol-gel catalytic agent. These materials show a well-formed organosilica network as probed by ^{13}C and ^{29}Si solid-state NMR spectroscopy. The mesoporous materials were characterized by thermogravimetric analysis (TGA), N_2 adsorption isotherms, and TEM images, demonstrating that they are highly thermally stable, being stable up to 450 ºC. N_2 adsorption isotherms and TEM images demonstrate microporous and mesoporous structures associated with narrow slit-like pores of about 4 nm with surface areas of about 40 m^2g^{-1}. These materials are prominent candidates as durable platforms in organo-electronic applications.

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Preparation and characterization of zinc niobium phosphate glasses and glass-ceramics for photocatalytic application

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ZnO is an important material due to its photocatalytic properties. Usually, it has been investigated in powder form or as thin film/coatings on some substrate, but it may present some limitations. Glasses generally do not provide photocatalytic activity, but that may be induced by obtaining photocatalytically active crystals in the glass, obtaining a glass-ceramic. Transparent ZnO nanocrystals in silicate glass-ceramic was already reported, but the melting temperature was very high (~1600°C). Phosphate glasses are known for low cost and by melting at low temperature. Also, alkali niobium phosphate glasses present high thermal, chemical and mechanical stability, wide transmission window and low phonon energy [1-3]. So, in this work was prepared glasses with molar composition: (70-x)KPO3-30Nb2O5-xZnO (x=0 to 25 mol%) by melt-quenching method. Glasses were then analyzed by X-ray diffraction (XRD) and Differential Scanning Calorimetry (DSC), in which with ZnO content higher than 15 mol% occurs the appearance of a crystalline event that decrease temperature as zinc are incremented. So, glass-ceramics were prepared from pristine glass containing 20mol% ZnO with heat treatment occurring in the onset of this peak varying time by 2h30, 5h and 10h. By DSC is observed that occurs the crystallization of this crystalline phase since that disappear after treatments, but also an increasing of a second crystalline peak is observed, that might be related to a higher temperature event associated to a niobium crystalline phase. The crystallized phase of glass-ceramics might be related to zinc, as it appears with its increment. Considering that, these glass-ceramics are being considered to be tested as a photocatalytic material for degradation of rhodamine B.
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Preparation of Fe-$MoSe_2$ nanosheet photoanodes aiming at photoelectrocatalytic degradation of organic dyes

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Photoelectrocatalysis (PEC), an advanced electrochemical oxidation process, has been applied as one of the promising environmental remediation techniques [1,2] Two-dimensional (2D) materials have been extensively studied in PEC, such as photoelectrocatalysts, co-catalysts for bandgap tuning or support matrices for catalysts [1,3]. Molybdenum diselenide has great potential as a photoanode to improve visible PEC processes, but its performance is limited by active sites and recombination of photogenerated electron-hole pairs [1,3]. Therefore, many researchers have investigated the use of doped photoanodes for the PEC degradation [1]. In this study, Fe-$MoSe_2$ compounds were synthed by a microwave-assisted solvothermal method. To understand the physicochemical structure, X-Ray Diffraction (XRD), Raman Spectroscopy, UV–vis Spectroscopy, Field Emission Scanning Electron Microscopy and photoelectrochemical tests have been applied and investigated in detail. Preliminary results of Scanning electron microscopy revealed flower-like $MoSe_2$ nanosheets microstructure with diameters of 200 to 300 nm. The XRD analysis of the samples confirms the obtaining of the hexagonal phase 2H-$MoSe_2$ (JCPDS: 29-0914). The most prominent peaks are the Raman active A_{1g} and $E_{2g}{}^1$ modes at 240 and 281 cm^{-1}, respectively, indicating that the prepared $MoSe_2$ samples are composed by 2H-$MoSe_2$. The doping of $MoSe_2$ has proven to be an effective strategy to increase the conductivity and photosensitivity. Furthermore, the samples are going to be analyzed through electrophotocatalytic degradation experiments.

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Production and optical characterization of thin films of organic polymers and 2D materials for application in OPVs

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With the technological development, the energy demand is always increasing. Also, with climate change, there is a growing need for renewable energy sources. In this context, there is demand for new materials for application in energy conversion, in particular for solar cells. The addition of 2D materials to organic polymers has been subject of studies in recent years, both due to the properties of these materials as higher electron mobility or adjustable bandgap, and the modifications that they cause in the morphology and crystallinity of the polymers [1]. In this work, we characterize thin films of organic polymers as PEDOT:PSS and 2D materials as GO for application in solar cells. The films were produced by solution processed and deposited using blade coating. Film thickness was obtained using a Profilometer. We performed optical characterization of the films using Spectroscopic ellipsometry, and a model was used to extract the optical properties consisting of the real and imaginary part of the refractive index as a function of the wavelength from 190 nm to 2100 nm. The film morphology was also analyzed using scanning electron microscopy. Results from samples with and without the 2D materials added were compared. Changes of the light absorption, refractive index and morphology were correlated with the addition of the 2D materials. The results show that these films can be applied on solar cells, and suggest that the correct application of these 2D materials can help to improve power conversion efficiency.

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Quantum-plasmonic coupling in Er^{3+} doped hybrid thin films for nanophotonic devices

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The investigation of rare-earth (RE) ions embedded within glass matrices interacting with surface plasmon polaritons and localized surface plasmon resonance (plasmon modes) in the realm of strong coupling presents significant potential for advancements in nanophotonics devices. The exploration of the fundamental interplay between these components is ongoing, fostering novel concepts and deepening our comprehension of quantum plasmonics. This study centered on the fabrication of hybrid thin films composed of Er^{3+}-doped nanoglasses embebed on polymethyl-methacrylate (PMMA). These films were produced via the spin-coating technique onto an array of Au nanoslits, forming a plasmonic metasurface. With a thickness of approximately 100 nm, the close proximity of an Er^{3+} ion to an plasmonic metasurface facilitated a robust interaction between them. Consequently, when the Er^{3+} ion emits light, its emission merges with the plasmon modes generated on the metal-dielectric interface. This collaborative effect amplifies the local field around the plasmonic metasurface, significantly enhancing luminescence and improving the radiative emission rate of Er^{3+}, thereby reducing its radiative lifetime. Understanding these intricate dynamics is crucial for the advancement of innovative nanophotonic devices leveraging these coupling phenomena.

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Sensitive SERS sensor by inkjet printing of gold nanoprisms on paper

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To achieve its full analytical potential, Raman Spectroscopy needs to be enhanced. One of the most studied and promising ways to improve the Raman signal is through Surface-Enhanced Raman Spectroscopy (SERS), which commonly uses gold and/or silver nanoparticles. Several strategies to obtain SERS substrates have been developed, such as on rigid and flexible substrates. In this sense, the development of flexible substrates could help to disseminate and broaden the applications of SERS. In this regard, it is desirable that the manufacturing procedure of the substrate is reproducible and easily scalable. In such a manner, inkjet printing is a promising method as it is automated and capable of local production of the substrate by depositing an ink composed of metallic nanoparticles onto paper, allowing for highly sensitive and specific analysis [1].Thus, the aim of this work is the synthesis and evaluation of gold triangular nanoprisms (AuNPrs) inkjet printed paper-based SERS substrates. A wide plasmonic excitation band centered around 650 nm marks the extinction spectra of the obtained colloidal suspension. The electron micrographs of the AuNPrs presented homogeneous nanoparticles. Chromatographic paper was selected for the printing process using a commercial printer, because of its low fluorescence intensity. The substrate performance was evaluated by the acquisition of SERS spectra of crystal violet (CV) in different concentrations when altering the number of printing cycles. The SERS intensity, the reproducibility of measurements, and the detection limit was balanced against the number of printing cycles to decide on the best substrate. The optimization of the manufacturing process by the use of CV as a model molecule permits the development of a substrate for the analysis of a molecule with environmental or biological interest.

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SERS-active platforms using silver and gold nanoparticles to investigate the selective enhancement mechanism of rhodamine 6G and rhodamine-B

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Understanding the selective enhancement mechanism of the SERS effect and carefully selecting SERS-active platforms and probe molecules, to achieve the high-sensitivity SERS measurements in various applications, such as biological and chemical sensing to surface analysis.[1] The choice of SERS-active platforms depends on their ability to generate strong electromagnetic fields and provide a suitable surface for molecular adsorption.[1] In this way, the combination of microfluidic deposition to silicon (Si) substrate functionalization and metallic nanoparticle adsorption is very promising to obtain SERS-active platforms with more reproducibility deposition, due to deposition flow control. Herein, we developed of microfluidic system based on 3D-printed structure to deposit metallic nanoparticles, silver and gold (AgNPs and AuNPs) to investigate the selective enhancement mechanism of rhodamine 6G and rhodamine B (Rh6G and RhB). A Si substrate is embedded in a 3D-printed structure composed of two parts: a top structure having inlet and outlet entries, with a microchannel having 200µm width and 0.5 mm length; and the bottom part possessing a sample holder for exactly the Si substrate. Then, flow injection deposition in Si substrate functionalized with (3-mercaptopropyl)trimethoxysilane (MPTMS) or (3-aminopropyl)triethoxysilane solution, followed by AuNPs or AgNPs immobilization. An effective AuNPs and AgNps synthesis is confirmed by UV-vis spectroscopy with plasmon bands at 531 and 409 nm, corroborated by STEM micrographs with a good homogeneity distribution. The results reveal the dependence of SERS enhancement signal with metallic nanoparticle composition, i.e., Au or Ag, in the Rh6G and RhB spectra. Achieving selective enhancement in SERS-based applications is important because it can detect and identify target molecules with high specificity.

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Spectroscopic study of mixed aluminum and gadolinium oxide doped with lanthanide ions

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We prepared the mixed aluminum and gadolinium oxide matrix doped with optically active ions by the non-hydrolytic sol-gel route aiming to synthe a material displaying up- and down-conversion of energy. We conducted a spectroscopic study of the matrix containing different lanthanide ions, namely Er^{3+}, Yb^{3+} at 1:10 molar ratio and Er^{3+}, Yb^{3+}, and Eu^{3+} at 1:10:1 molar ratio. The excitation spectra displayed the typical Er^{3+} and Eu^{3+} ions transition bands and a broad band between 250 and 400 nm, attributed to charge transfer (CTB). The bands at 379 and 487nm refer to the Er^{3+} transition from the ground state $^4I_{15/2}$ to the excited states $^4G_{11/2}$ (379 nm) and $^4F_{7/2}$ (489 nm). Also we can see the typical bands of the Eu^{3+} transition from the ground state $^7F_0$ to the excited states $^5L_6$ (394 nm) and $^5D_2$ (463 nm) [1,2]. The emission spectra presented bands in the infrared region due to Er^{3+} (980 and 1540 nm) and Yb^{3+} (980 nm). When excited at 980 nm, the samples emitted in the green region (525 and 545 nm) of the electromagnetic spectrum (energy upconversion), corresponding to Er^{3+} emission.

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Structural and optical properties of boron-tellurite glasses with heavy metals and doped with rare earth ion

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Borate glasses belong to a class of materials widely used as a base for optical devicesdesigning. In this work, borate glass were manufactured containing heavy metals into their composition and doped with Neodymium ions. The glasses were structural and optically analyzed via X-ray diffraction, Raman spectroscopy, UV-vis optical absorption, photo-luminescence, and time-resolved photoluminescence. The material analysis is further accomplished by the calculation of Judd-Ofelt parameters, and laser parameters (saturation intensity, emission cross-section, and figure of merit). Focus is given on how the ratio Te⁄(Bi+Te) affects the structural and optical properties of the samples. It is observed a reorganization of structural units which provokes a decrease of phonon energies in function of the increase of Bi content, resulting in a 5.3 % reduction in the 1060 nm emission lifetime of the Nd3+. All doped samples can be used as a gain medium since the experimental branching ratio, , achieved values between 69 % and 72 %. The samples present quantum efficiencies of 76.31 %, 51.20 %, and 47.30 % for 1, 0.6, and 0.2 ratios, respectively. Our findings indicate that the samples have potential to be used as a laser gain medium.

Structural and optical properties of ZnO:Eu under hydrostatic pressure

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The trivalent state of Eu ion holds particular importance in the development of optoelectronic devices due to its broad spectrum of visible emissions. Although the claiming of 4f electrons shielding effect in the lanthanide series, the changes in host crystalline structures have significant effects on optical emissions of Europium-doped ZnO thin films.
This research explores the influence of ZnO host crystallinity on optical emission of Eu^{3+} employing simultaneous X-ray Diffraction (XRD) and photoluminescence spectroscopy (PL) techniques performed at Sirius synchrotron facilities. The XRD measurements were performed at 25 keV up to 14.5GPa with PL measurements excited with a 532nm laser simultaneously. At 10.0GPa it is possible to identify a peak attributed in the literature to the cubic phase of ZnO at (200) direction. The complete change from the hexagonal to the cubic phase of ZnO was reported in the literature at pressures from approximately 9.0GPa [1]. In our film, this phase change was not abrupt. In addition, we observed a phase coexistence characterized by comparable intensity peaks within the pressure range up to 14.5GPa, indicating the presence of both hexagonal and cubic phases. The Eu^{3+} ions exhibited visible emissions characteristic of optical transitions between D0 and F levels with a significant decline in emission intensity observed at 10.0GPa. We discuss the correlation between the lattice structure of ZnO and the RE 4f-energy levels.

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Structural and Spectroscopic Studies of Rare Earth-doped Polyphosphate Coacervates

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The Coacervation process refers to the aggregation of colloidal particles in solution. In this case, the droplets of dense polymeric phase formed during liquid-liquid phase separation also called coacervates are extended by colloidal particles. An example of a material that can be formed by this process is polyphosphate coacervates, which have glassy characteristics. In this work, polyphosphate coacervates doped with paramagnetic Ln3+ ions (Ln = Dy, Ho and Tb) were prepared with the aim of obtaining materials in the form of films that present magneto-optical properties to be explored. The coacervation process was induced by adding a solvent with a high dielectric constant, such as ethanol, to a solution of Ln-polyphosphate. The materials obtained were structurally characterized via FTIR, XRD and Raman spectroscopy. Undoped coacervates generally have amorphous structures. XRD analyzes showed that after the addition of Ln3+ ions, the formation of ortho and pyrophosphate crystalline phases occurred. From Raman scattering, we identified that the precursor presents two main specific vibration modes at 743 cm-1 and 1009 cm-1, attributed to the symmetrical stretches in P-O-P (bridges) and P-O (terminal), respectively. For samples containing Ln3+, it was observed that the υs(P-Ot) band shifted from 1009 to 1017 cm-1. The spectroscopic properties of Ln3+ ions were evaluated via photoluminescence spectroscopy. In the emission spectra of samples containing Dy3+ and Ho3+ ions, it was possible to observe, in a more pronounced way, an emission band centered at 576 nm and 669 nm, referring to the transitions 7F9/2 → 6H13/2 and 5F5 → 5I8, respectively. The samples doped with Tb3+ ions showed atypically intense emission in the region close to 491, 546 and 686 nm, due to the transitions 5D4 → 7F6, 7F5, 7F4. In sequence, these materials will be evaluated for their magneto-optical properties via Faraday rotation angle experiment.

Structural characterization and luminescence properties of Er^{3+}-doped aluminophosphosilicate glass obtained by sol-gel method

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Rare earth (RE)-doped glasses are key materials for the fabrication of gain media for optical amplification [1]. Silica (SiO2)-based optical fibers exhibits a low solubility of RE ions in its matrix which leads to cluster formation, resulting in concentration quenching of luminescence [2]. The ternary system SiO2-Al2O3-P2O5 is of great interest for active optical devices since the Al and P incorporation increases the solubility of RE ions. The optical and structural characterization of 95SiO2-2.5Al2O3-2.5P2O5 glass composition Er3+-doped (0.05 to 1.0 mol.%) were investigated. The structural evolution from hybrid to glassy material was monitored at different heat-treated temperatures (80, 550, 600, 700, 800 °C in air and 900 °C under vacuum). The transmission window observed in the IR range for the Er3+-doped AlPSi glasses is similar to that observed for the pure silica glass. SEM images showed pores formation as the heat treatment temperature increases, attributed to the burning off of residual solvent and organics components. N2 physisorption indicated that the glass heat-treated at 800 °C still exhibited a high surface area value of 331.12 m2 g-1, which decreased to 78.06 m2 g-1 after heat treatment under vacuum, due to the densification of the matrix. UV-Vis-NIR spectra were evidenced by a decrease in the intensity of OH groups bands, which corroborated to Solid-State NMR data. Finally, the luminescence study demonstrated that the heat treatment under vacuum clearly promoted an increase in luminescence intensity and lifetime values. The results indicated an enhancement in luminescence properties up to 0.5 mol.% Er3+, however, it was observed a concentration quenching of luminescence for concentrations higher than this.

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Structure and nucleation mechanism in alkali and alkaline-earth diborate glasses

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Understanding the mechanisms and kinetics of crystallization processes is crucial in comprehending the glass-forming ability of undercooled liquids and the stability of glass. Glass devitrification can occur through either heterogeneous nucleation and growth triggered by catalysts, impurities, or surfaces, or homogeneous nucleation and growth throughout the sample volume. While any glass may undergo homogeneous nucleation under optimal conditions, heterogeneous nucleation is thermodynamically favored and can occur more rapidly. Previous studies in silicate and borate glasses suggest a correlation between nucleation mechanisms and structural similarity between glass and their corresponding isochemical crystal phase[1]. This research focuses on the structural characterization of diborate glass compositions (M(2)O.2B2O3, where M = Li, Na, Ca, and Mg) and their respective isochemical crystals. High-resolution Solid State Nuclear Magnetic Resonance spectroscopy is employed to analyze the structural environments of network-forming and -modifying species (6Li, 10B, 11B, 23Na). Additionally, changes in magnetic dipolar coupling strength between 23Na and 11B nuclei during the glass-to-crystal transition are characterized by rotational echo double resonance (REDOR) spectroscopy. The analysis confirms the correlation between nucleation mechanisms and the degree of structural similarity in short- and intermediate-range order between glass and their respective isochemical crystal phase.

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Structure and property of nano-heterostructure of Titanate decorated with bimetallic iron and silver nanoparticles

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Sodium Titanate nanotubes (NaTiNTs) are nanomaterials with wide relevance in several areas of science due to their physicochemical properties and possible applications in the environmental and biomedicine areas - textile effluent treatment and imaging [1, 2]. In this context, the objective of this work was to synthe by the conventional hydrothermal method NaTiNTs and perform ion exchange with metal ions: Iron, Silver, and bimetallic Iron and Silver and investigate the structure and properties of these nanomaterials. It was observed through Raman spectroscopy vibrational modes characteristic of Titanate nanotubes and additional modes of new iron phases as γ-FeOOH and α-Fe2O3 seen in the bimetallic nano-heterostructure, TiNT@FeAgNP. The X-ray diffraction confirmed the presence of iron oxides that are probably decorating the surface of the nanotubes. In addition, SEM analysis revealed that the nanotubes are gathered in interlaced clusters and EDS revealed the chemical elements present in the nano-heterostructures such as sodium, oxygen, titanium, iron, and silver. The measurements by UV-VIS indicated that the insertion of iron and silver ions caused the displacement of the absorption band from the ultraviolet region to the visible region, consequently causing the decrease of the band gap energy in these samples. Finally, it is emphad that Titanate nanotubes with iron and silver ions tend to have magnetic behavior which may have potential applications in textile effluent treatment and imaging.

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Surface-enhanced Raman scattering (SERS) as analytical tool to detect pesticide directly in fruit peel

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Surface-enhanced Raman scattering (SERS) provide a large signal enhancement being a promising tool of detection. One of limitations of technique is the signal fluctuations on the SERS intensity when the substrate is a solid and the spectra are collected point-by-point. Such behavior remains a challenge to obtain a linear regimen and build a calibration curve. Here, we propose apply SERS as tool of detection but instead to take the SERS intensity, take the number of SERS events to quantify thiabendazole (TBZ) pesticide. For this purpose, the detection was optimized using three synthesis of nanoparticles: silver reduced by hydroxylamine (AgH) or citrate (AgCT) and gold nanoparticles reduced by citrate (AuCT). These nanoparticles were deposited onto apple peel and applied as SERS substrates to detect TBZ pesticide using Raman mapping under 785 nm laser excitation. Previously, theoretical calculations was performed studying the torsion barrier of thiazole ring in relation to benzimidazole ring to investigate the conformer which presents lower energy for TBZ molecules. The trans conformer was the most stable, in agreement with XRD patterns. The extinction spectra present a maximum at 416, 435 and 521 nm for AgH, AgCT and AuCT, respectively. In presence of pesticide the maximum was red shifted for three nanoparticles and for AgH and AuCT arise a new band at longer wavelength, reveling the strong interaction between TBZ and AgH and AuCT. TBZ SERS spectra using AgH, AgCT and AuCT are similar each other with lightly differences among them which can be related to the different interaction between TBZ and nanoparticle surface. In terms of intensity, AgH showed the higher SERS signal to TBZ and it was chosen for the next experiments. The dependence of TBZ SERS spectra in different pH medium was investigated from pH 2 up to pH 12. While SERS signal was absent at pH 10 and 12, at lower pHs (2-8) the changes in SERS spectra are related to difference of states of protonation of TBZ

Sustainable technology: heavy metal oxide glasses and glass-ceramics containing Eu^{3+} and Tb^{3+} ions recycled from fluorescent lamps.

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Heavy metal oxide (HMO) glasses exhibit transparency in the infrared region, high nonlinear optical coefficients and high refractive indexes [1]. These glassy matrices have great potential to solubilize a high concentration of rare earth (RE) ions, enabling a wide range of interesting optical and magneto-optical (MO) applications. In this work, we present the synthesis and characterization of $40PbO\text{-}20GeO_2\text{-}25Bi_2O_3\text{-}15Ga_2O_3$ (PGBG) glasses and glass-ceramics containing Eu^{3+} and Tb^{3+} obtained from the recycling of fluorescent lamps. Samples based on the PGBGx%res (xres = 0, 1, 10, 20, 30, and 60 %m/m of residues) were synthed and characterized using Differential Scanning Calorimetry (DSC), X-ray Diffraction (XRD), Raman spectroscopy, and Photoluminescence (PL) measurements. DSC curves showed the typical Tg and Tx around 450 °C and 570 °C, respectively. XRD analysis confirmed the noncrystalline behavior of the PGBG0% sample (glass), while the addition of lamp residues at different concentrations (%m/m) in the PGBG matrix induced the crystallization process of germanate crystals in the PGBG1, 10, 20, and 30%res samples (glass-ceramics). Additionally, SEM images showed the presence of cubic crystals with an average of 25 µm in the glass-ceramic samples. The Raman spectra showed a decrease in the intensity of the vibrational modes assigned to the BiO_6 and Pb-O species centered at 185 and 260 cm^{-1}, respectively. This behavior indicates that the addition of lamp residues at different concentrations (%m/m) changes the glass network. The emission spectra of the glasses and glass-ceramics exhibited bands attributed to the electronic transitions of Tb^{3+} and Eu^{3+} ions at 514 nm ($^5D_4 \rightarrow {}^7F_5$) and 615 nm ($^5D_0 \rightarrow {}^7F_2$), respectively. In conclusion, the preliminary results suggest the potential for developing glasses and glass-ceramics for optics and magneto-optics, especially as Faraday rotators.

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Synergism between the Photocatalysis and Adsorption in Tetracycline Removal and their Inactivation for Water Treatment Using Cerium-doped TiO_2 and Sepiolite

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As the global population increases, so does the demand for pharmaceuticals, including antibiotics such as Tetracycline (TC)[1]. These compounds can contaminate water, affecting aquatic ecosystem health and potentially reaching drinking water sources. Sepiolite (Sep) is a clay mineral, and the property of Sep makes it an excellent material in adsorption applications. Titanium Dioxide (TiO_2) is a prominently studied photocatalyst known for its advantages, including non-toxic, photo-stability, chemical stability, and cost-effectiveness. The main objective of this study is to improve the efficiency in the degradation and inactivation of tetracycline through Ce-doped TiO_2 with Sepiolite nanocomposites. The synthesis of the photocatalysts was carried out via hydrothermal sol-gel. The samples were varied in weight.% Ce at 0, 1, 2.5, and 5% were characterized by XPS, TEM, DRS, photodegradation, and inactivation tests. XPS results revealed that Ti and Ce were incorporated into sepiolite. Ti4+ and cerium were observed in the oxidative state Ce^{3+} and Ce^{4+}, the former being in greater quantity. TEM images confirmed the results obtained by XPS. From EDX-STEM images, titania is preferentially located at the edges of the clay material. In contrast, Ce is more homogenously dispersed on the sepiolite, with a smaller particle. Photocatalytic tests showed that the $1CeTiO_2$-Sep sample achieved the highest removal efficiency of TC (40 ppm) at 70.45%, demonstrating the efficiency of the synergistic effect of the two removal techniques. ThroughThe growth of the *E. coli* bacteria confirmed the inactivation of the drug in the solution. Therefore, the synergistic effect between adsorption and photocatalysis proved to be an efficient means for removing organic pollutants. Acknowledgements: Capes, Fapepi, CNPq

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Synthesis and Characterization of Cadmium Selenide Quantum Dots in Glass

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The rapidly evolving field of nanotechnology has identified quantum dots as promising materials with unique optical and electronic properties. Quantum dots, particularly cadmium selenide (CdSe) nanocrystals, exhibit high quantum efficiency, chemical stability, and tunable luminescence. These characteristics make quantum dots ideal for various optoelectronic applications, including LEDs, solar cells, sensors, and biological markers. Despite recent advancements, challenges such as large-scale synthesis and enhanced encapsulation techniques to improve stability and efficiency remain [1-3]. The primary objective of this work is to fabricate glasses with suitable optical properties for CdSe quantum dot growth using a simple ZBLAN matrix. This involves the controlled growth of CdSe quantum dots in the glass matrix through thermal treatment. Detailed optical analyses will be conducted using optical absorption and photoluminescence techniques to assess the quality of CdSe quantum dots. The study aims to investigate and optimize the optical properties of quantum dots embedded in glass matrices for application in optoelectronic devices.

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Synthesis and characterization of compounds based on titanium and zinc oxides

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Research on inorganic semiconductor materials has been increasing due to their various applications, driven by distinct optical, electrical, and photoelectronic properties compared to insulators and conductors. The advantage of these materials lies in their high surface area, with many active sites, intensifying catalytic activity [1]. Their properties depend on factors such as crystalline phase, particle , surface area, and degree of crystallinity. For photocatalytic applications of titanium and zinc oxides, low crystallinity in an amorphous or semicrystalline state can be problematic. High-temperature calcination can collapse the structure, leading to a loss of surface area[2]. In the synthesis of TiO_2G1 and TiO_2/ZnO, delicate thermal treatment balanced crystallinity, porosity, and particle . The study focused on thermal (TG, DTA), structural (XRD, FTIR), and morphological (SEM) analyses to optimize production, treatment temperature, and morphology. A temperature of 400 °C for 2 hours in a muffle furnace produced crystalline anatase TiO_2 and zinc-titanium overlap, confirmed by XRD, while SEM revealed materials with aggregates and interstices beneficial to catalysis. Finally, FTIR spectroscopy identified traces of carbon, which may be capable of affecting photocatalysis.

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Synthesis and Characterization of Glasses and Fibers for Ultra-Sensitive Magneto-Optical Sensors

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]Oxide glasses with magneto-optical (MO) properties have gained significant attention in various scientific fields and industrial applications, including magnetic and electrical current sensors. The LAVIE group (IQAr-Unesp) has been investigating new glass compositions with high concentrations of paramagnetic ions, particularly Tb^{3+}, for application in MO glasses. This study discusses the synthesis and characterization of boron-aluminate glasses containing 8 to 13 mol% of Tb_4O_7, as well as the development of optical fibers. The boron-aluminate glasses were melted using the fusion method followed by thermal shock and characterized using Differential Exploratory Calorimetry (DSC), Raman spectroscopy, UV-Vis-NIR absorption spectroscopy, and Faraday rotation for the calculation of Verdet constants (VB) at 632 nm. The synthesis results of the glasses indicate that they are thermally stable, with glass transition temperature (Tg) and crystallization onset temperature (Tx) values between 693-704°C and 850-942°C, respectively, and thermal stability parameters (ΔT = Tx-Tg) greater than 150°C. Additionally, the glasses exhibit high Verdet constants, good thermal stability, and a wide transmission window in the Vis-NIR region, making them excellent candidates for the production of MO fibers and the development of electrical current and magnetic field MO sensors. Regarding optical fibers, the methodology is being adapted from the Rod in tube method, and preform synthesis is being developed, with adjustments to parameters such as mold, fusion temperature, and piston descent speed, to minimize bubble formation and ensure diameter uniformity along the section.

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Synthesis and characterization of magneto-optical glass-ceramics containing TbAlO3 perovskite crystals

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In recent years, magneto-optical materials have attracted attention due to their potential applications as Faraday Rotators in the development of magnetic field and electric current sensors [1]. In this work, we present preliminary results of synthesizing and characterizing MO glass-ceramics with a borogermanate matrix (BGB) containing TbAlO3 perovskite crystals. The TbAlO3 crystals were synthed by solid-state synthesis using Tb4O7 and Al2O3 as precursors via thermal treatment at 1500°C for 75 hours in alumina crucibles. The crystallographic data are orthorhombic crystal system ($a = b = 5.236$ e $c = 7.465$ Å) and Pnma space group. Subsequently, the synthesis of BGB-xTbAlO3 were obtained by the conventional melt-quenching method at 1250°C for 2 hours. The BGB-xTbAlO3 glass-ceramics were characterized by Optical Microscopy, Differential Scanning Calorimetry (DSC), X-ray Diffraction (XRD), Raman and Photoluminescence (PL) Spectroscopies. Optical Microscopy images showed the presence of TbAlO3 crystals with average s between 20 to 50 µm dispersed in the glassy matrices. From the DSC curves, all typical temperatures such as glass transition (Tg), onset crystallization (Tx), ΔT were extracted. The values obtained were 533, 911, and 377°C, respectively. The emission spectra of the glass-ceramics (λexc = 377 nm) presented the most intense band at approximately 545 nm, attributed to the electronic transition 5D4 → 5F7 of the Tb3+ ion. In conclusion, the preliminary results demonstrate the successful incorporation of paramagnetic TbAlO3 crystals into a glassy and the potential for the development of new Faraday rotators.

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Synthesis and characterization of nanostructured luminescent materials with potential application in optical and optoelectronic devices

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The search for efficient light emitting materials, which are easy to synthetize using simple routes, is an important issue for the design of new optical and optoelectronic devices. In this sense, compounds such as, Ag-doped zinc sulfide, zinc silicate or strontium aluminates doped with Mn, have received notable attention for their fundamental features, including photoluminescent and electroluminescent properties, synthesis versatility, and potential application in several technological fields. In this work, we propose the synthesis and characterization of three different nanostructured luminescent materials, emitting in specific regions of the visible spectrum. Nanostructured materials are synthed with temperatures, processing times and heating rates appropriate to each system [1]. Nanocrystalline oxide materials (Mn-doped strontium aluminates – red emission) can be prepared by polymeric precursor method, which is based on the formation of an organic polymeric network obtained through the preparation of a viscous solution that is converted into a thermoplastic gel with the concentration of the solution. The goal is to reduce the mobility of cations by distributing them homogeneously in the polymer chain. In order to obtain the nanostructured phosphor materials, the co-precipitation method were used for Zn_2SiO_4:Mn systems (green emission). In this method, suspensions are obtained, based on the hydrolysis of an alkoxide or salt of the metals of interest. Finally, we use the conventional solvothermal method to synthetize Ag-doped zinc sulfide powder (blue emission). The prepared samples were characterized using optical spectroscopy techniques and scanning electron microscopy. These first results are promising for future applications in optics and optoelectronic devices.

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Synthesis and characterization of $(TbGd)_3Al_5O_{12}$ single crystals

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Single crystals like Terbium Gallium Garnet (TGG), Yttrium Aluminum Garnet (YAG) and Terbium Aluminum Garnet (TAG) exhibit unique properties due to their continuous, uniform, and highly ordered structure. TAG and TGG are commercially used as Faraday rotators, due to their magneto-optical properties [1]. Thus, as they exhibit emission in the green region of the electromagnetic spectrum (~575 nm) they are potential candidates for scintillators. These crystals are usually obtained by Czochralski methodology, which is an expensive and time consuming process. In this work we had proposed the synthesis of a series mixed crystals with formula $Tb_{3-x}Gd_xAl_5O_{12}$ (with $0.25 \leq x \leq 1.00$), using a glass as precursor media, as an alternative methodology. The chemical composition of the glass combines GeO_2-PbO-Bi_2O_3-Al_2O_3-(3-x)Tb_4O_7-xGd_2O_3. The glass batches containing 5 g of raw materials were melted at 1250 °C during 2 h and then, the liquid was quenched into the platinum crucible to room temperature. This procedure enables the growth of cubic single crystals with the formula $Tb_{3-x}Gd_xAl_5O_{12}$ which can be isolated by dissolving the glassy phase. The crystals were studied by X-ray diffraction, Raman spectroscopy, optical and electronic microscopies and the luminescence properties were studied to analyze the potential use of the materials as scintillators.

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Synthesis and characterization of the $(Gd_{0.2}Eu_{0.2}Tb_{0.2}Er_{0.2}Yb_{0.2})_2O_3$ oxide

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High-entropy oxides are part of the class of ceramic materials formed from a mixture of multiple oxides, resulting in an oxide composed of five or more cations in equiatomic proportion [1, 2]. These oxides tend to form a stable solid solution and may present different arrangements in their structure, resulting in a high configurational entropy, such as high-entropy oxides of the type $(\text{Rare-Earth})_2O_3$. These materials are being widely studied, mainly those composed of rare-earth oxides because they have interesting properties, such as luminescence, magnetism, structural, and electrical properties. It can be applied mainly to photosensors, magnetic sensors, solar cells, energy conversion, and piezoelectrics. Therefore, they are classified as functional and intelligent materials with high technological potential. 4f trivalent rare-earth ions with electronic configurations $[Xe]4f^n$ allow electrons to access different energy levels and some of them provide good luminescent properties across a wide range of the spectrum. Therefore, this work aims to investigate the $(Gd_{0,2}Eu_{0,2}Tb_{0,2}Er_{0,2}Yb_{0,2})_2O_3$ oxide focusing on its structural (X-ray diffraction), thermal (thermogravimetry), and luminescent (fluorescence around the visible spectra) characteristics. The simple oxides were mixed one after the other, starting from a binary composition to quinary. This allowed to understand the evolution of the material's properties with the addition of each oxide. Initial results indicated a change in color of the mixtures from white to brown. During thermogravimetric analyses, mass loss of no more than 6% was noted in all mixtures, without variations depending on the number of cations in the material, which indicates good thermal stability across all compositions.

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Synthesis and characterization of TiO_2 samples with surface modifications for applications in photocatalysis

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Photocatalysts based on titanium dioxide were synthed through the sol-gel method and subjected to hydrothermal heat treatment (TiO_2). Subsequently, this oxide had its surface modified by the incorporation of copper ions, using copper nitrate followed by photoreduction (5.0% of metallic Copper) [1]. The evaluation of the photocatalytic activity of these oxides was carried out through the degradation of the Ponceau 4R dye. Various characterization techniques, including TEM, XRD, specific surface area, ultraviolet/visible absorption spectroscopy and Raman spectroscopy, were employed. TEM analyses revealed morphologies composed of partially aggregated particles, with s ranging from 2 to 5 nm. According to XRD analyses, the crystalline anatase phase was predominant in all synthed compounds, with the presence of the brookite phase. The amount of brookite, as well as cell volume, deformation, lattice parameters, and crystallinity, were estimated by Rietveld refinement. The pure oxides and those with surface modifications maintained mesoporosity, with an average pore diameter between 47 – 56 Å. Raman spectroscopy data suggested the presence of anatase and active brookite modes in the structure. On the laboratory scale, the best photocatalytic performance was achieved using the TiO_2 oxide impregnated with 5.0% copper), resulting in 100% discoloration and 90% mineralization of the Ponceau 4R dye, using a high-pressure mercury vapor lamp, 400 W, and pH 6.9. In comparison, the TiO_2 achieved 100% discoloration and 73% mineralization for the same dye, under the same experimental conditions.

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Synthesis and characterization of vitreous matrix composed of metaphosphates

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The study of phosphate glasses holds significance from both a fundamental scientific perspective and for technological applications, as understanding their structure impacts mechanical, electrical, and optical properties. Additionally, these glasses exhibit substantial potential for technological applications and possess a simpler glass network to simulate. The research aims to investigate the vitreous system $0.95[x(NaPO_3) + (1-x)Zn(PO_3)_2] + 0.05\ Al(PO_3)_3$, with x: 0, 0.25, 0.5, 0.75, and 1, through structural characterization using Raman spectroscopy and NMR, primarily focusing on the effects caused in the glass network by the substitution of Zn with Na. The samples were characterized through Raman spectroscopy at UFLA and P-MAS, Na-MAS, andAl-MAS NMR spectroscopy at the Institute of Physics of São Carlos - IFSC/USP. Raman spectroscopy of the glass samples revealed typical glass pattern bands, while results for zinc metaphosphate aligned with a typically crystalline structure. NMR characterization also confirmed expectations for the glass material. ^{31}P-MAS spectra indicated the predominant presence of Q^2 phosphate groups, with small amounts of Q^1 groups, suggesting that the phosphate chains are not infinite, with these groups representing chain ends. It is concluded that the syntheses resulted in the expected materials, obtaining a crystalline material for zinc metaphosphate and entirely glassy samples. Future prospects involve additional structural characterizations using $^{31}P\{^{27}Al\}$ REDOR NMR, as well as density analysis, FTIR, DSC, and XRD.

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Synthesis and characterizations of the vitreous system Zn-Na-Al metaphosphates

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Phosphate glasses are materials with great potential for technological application, such as optical devices and sensors. The study of these systems is extremely important, as there is a close relationship between the structure of their network and their properties, such as ionic conductivity and chemical stability [1,2]. The objective of this work was to study the ternary vitreous system: 0.9[x(NaPO3) + (1-x)Zn(PO3)2] + 0.1 Al(PO3)3 with x = [0; 0.25; 0.50; 0.75; 1]. The structural characterization about the system was obtained using Raman spectroscopy performed at DFI/UFLA and Nuclear Magnetic Resonance (NMR) at IFSC/USP. Raman spectra of Zn(PO3)2 and glasses were obtained in order to verify whether there was adequate crystal formation in the first case, and amorphous structures in the second. Spectra were obtained using NMR in order to analyze the structural environments of network-forming and network-modifying species of 31P, 27Al and 23Na. As a result of the Raman characterization, it was possible to observe bands typical of a glassy pattern for the glasses and a solid solution behavior when replacing Zn with Na, while for the crystalline precursor it presented bands typical of a crystal. As for the characterization by NMR, as a result it was possible to observe the presence of Q1 phosphate groups, this fact indicates that the phosphate chains are not infinite, with such groups being extreme chain groups, the majority presence of different Q2 groups was also shown, as expected[1,2]. From this characterization, it was also possible to verify that there was no clustering of the ions in the network, and the increase in NaPO3 generated a positive increase in the chemical shift of phosphorus. It is therefore concluded that the preparation of the Zn precursor was carried out successfully, as well as the glasses showed an amorphous pattern.

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Synthesis and passivation of graphene quantum dots obtained by the controlled carbonization of sucrose for photonic applications

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Graphene quantum dots (GQDs) are fluorescent nanoparticles, usually with a of less than 10 nm. GQDs usually present wide photoluminescence (PL) spectra that may be tuned depending on excitation wavelength [1]. In this work, sucrose was employed and the main source of carbon. For the synthesis of GQDs, sulfuric acid (H2SO4) was added to aqueous solutions of refined sugar, in order to promote dehydration and carbonaceous formation. GQDs were obtained after vacuum filtration and dried at ~ 120 ºC. A suspension containing the GQDs in ethyl alcohol was prepared and subjected to dispersion by ultrasonic mixing for two hours. Subsequently, different ratios of tetraethoxysilane (TEOS) and deionized water were added to the suspension, in order to develop a passivation layer around the GQDs. Transmission electron microscopy (TEM) showed that multilayer GQDs were obtained. Photoluminescence (PL) of the GQDs was recorded for excitation wavelengths in the range of 250 – 700 nm. A tunable PL band was observed in the range of 400 – 600 nm. The results showed that passivation does not significantly alter the optical properties of GQDs. Nevertheless, after passivation a solid luminescent powder could be obtained, which is not achievable with the GQDs without passivation. Passivation is thus a promising method to obtain luminescent nanocomposites for photonic applications.

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Synthesis, characterization, and photocatalytic performance of nanostructured ZnO films under UV light

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The limited natural water resources have been contaminated by effluents originating from both the industrial and domestic sectors. A large portion of the available water is consumed in chemical processes in various industrial sectors, including textiles, paper, and leather. Also, the inappropriate disposal of pharmaceuticals and dyes on a large scale results in effluent contamination. Methyl orange is one of the most widely used azo dyes on a large scale. Photocatalysis is a promising green alternative for the removal of organic dyes in wastewater. This research aimed to synthe and characterize nanostructured zinc oxide films to obtain a UV-light-activated photocatalyst capable of degrading organic compounds. The films were obtained using the sol-gel method. Zinc acetate, MEA, and ethanol were kept under constant stirring for 60 minutes at 70°C. The solution obtained was sprayed onto cleaned borosilicate glass substrates by using an airbrush. The samples were then heat treated at temperatures of 450 and 500°C for 45 minutes. The characterization of the films was performed using X-ray diffraction (XRD), field-emission scanning electron microscopy (FE-SEM), UV-Vis spectrophotometry and wettability. The efficiency of the films was determined by the degradation of a 5 mg.L^{-1} methyl orange dye water solution at neutral pH, at constant temperature of 20°C, and under two sources of ultraviolet radiation (λ=352 nm) for 300 minutes. The films exhibited hydrophilic characteristics and superficial morphology consisting of spherical nanoparticles. The films showed photoactivity when exposed to UVA radiation, with the best performance in removing methyl orange dye being 48.6% for the film treated at 500°C. This removal value can be attributed to the improvement in the homogeneity of the morphology and thickness of the film treated at 500°C.

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Synthesis of gold-coated NaGdF4:Eu3+ nanoparticles for X-ray activated photodynamic therapy applications

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Nanoparticles offer exciting potential for medical applications as simultaneous agents for disease diagnosis and treatment, known as theranostics. X-ray photodynamic therapy (XPDT) uses X-ray absorption and offers potential for treating deep-seated tumors. Some materials can also emit light at different regions of the electromagnetic spectrum, such as the visible region, after being irradiated with X-ray. This process can enable imaging and is known as X-ray excited optical luminescence (XEOL) [1]. NaGdF4:Eu3+ nanoparticles have demonstrated great potential for XPDT and XEOL applications and, therefore, the aim of this study is develop NaGdF4:Eu3+ nanoparticles coated with metallic gold. Our focus is not only to improve the compatibility of the system with the gold shell, but also to investigate its effects on the optical properties of the NaGdF4:Eu3+ particles. First, NaGdF4:Eu3+, NaGdF4:50% Eu3+ and NaGdF4:30% Eu3+ were synthed and exhibited average diameters of 115 nm, 90 nm, and 75 nm, respectively. In our exploration of strategies for uniform gold shell coverage on nanoparticles, the single-step gold addition method, where gold layer is grown in situ during the synthesis of NaGdEuF4:Eu3+ nanoparticles, has been shown as a promising method. After the gold shell deposition, UV-Vis absorption spectroscopy reveals a plasmonic resonance peak at 550 nm, typical of gold nanoparticles. Fluorescence analysis, with excitation wavelength of 254 nm, revealed emission peaks characteristic for NaGdF4:Eu3+ structures at 590 nm, 615 nm, and 690 nm for both core and core@shell structures. These findings highlight the potential of our core-shell nanoparticle design for advanced applications in biomedical imaging and therapy.

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Synthesis of $SrAl_{12}O_{19}$:Mn phosphor by polymeric precursor method and photoluminescent properties

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Luminescent materials are currently receiving significant attention, holding great potential for various applications. Strontium aluminate is well-known for being an excellent host matrix for activator ions. Additionally, the presence of defects in the material's crystalline structure influences the luminescence intensity of the activator ion. Therefore, the synthesis method, doping, and component concentration in the sample are subjects of extensive and comprehensive research. In this study, pure SrAl12O19 and SrAl12O19 doped with Mn4+ ions were analyzed, as manganese ions are cost-effective and have minimal impact on human health and the environment. The material was successfully synthed using the polymeric precursor method, followed by annealing under various conditions, including a conventional atmosphere, N2, and a high heating rate. Regarding the structure, X-ray diffraction revealed that the N2 atmosphere condition combined with the high heating rate in the annealing led to a reduction in the formation temperature of SrAl12O19. It was concluded that Mn4+ ions were successfully inserted into the Al3+ sites under all synthesis conditions. Emission and excitation photoluminescence spectra showed bands corresponding to electronic transitions characteristic of the Mn4+ ion, with a strong emission ranging from pink to reddish. Thus, the ceramic material SrAl11.995Mn0.005O19 could be prepared successfully with a combination of the modified polymeric precursor method and a high heating rate in the annealing, exhibiting luminescent properties at a lower synthesis temperature.
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Synthesis of $TiNb_2O_7$ by microwave-assisted solvothermal route aiming at photocatalytic application.

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Brazil has the largest niobium reserve in the world, being responsible for ~ 90% of their global production [1]. Among them, niobium pentoxide (Nb_2O_5) is the most studied, mainly, due to its properties and applications as semiconductors in Grätzel cells and photocatalysts [2]. Titanium niobate ($TiNb_2O_7$) is a material derived from TiO_2 and Nb_2O_5 oxides, exhibiting characteristics that are poorly understood with few studies on photocatalytic applications [3]. The TiNb2O7 have been produced with different methods, the Microwave-assisted Solvothermal Synthesis (SAM) has stood out with advantages and benefits rather than other routes, especially in the synthesis of nanoparticles [3]. In this work, $TiNb_2O_7$ samples were synthed by the SAM route, aiming for its future application in photocatalytic systems. We used different proportions of the niobium to titanium precursor (1:1 and 2:1), different solvents (H_2O and ethanol), and synthesis temperatures (160-240ºC). Then, the samples were heat-treated in a muffle furnace at temperatures of 700-1000°C for 30 min. The X-ray Diffraction (XRD) analysis of the samples confirmed the attainment of the monoclinic crystalline phase of $TiNb_2O_7$. However, some additional peaks indicate the formation of crystalline rutile phase TiO_2. The results of Thermogravimetry (TG) analysis justify the temperature range applied in the heat treatment of all samples. Scanning Electron Microscopy (SEM-FEG) images revealed particles with irregular shapes and diameters ranging from 100 to 300 nm for all samples, which is the expected morphology of the material. Also, all samples are going to be analyzed through photocatalytic experiments.

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Synthesis using Cymbopogon citratus (DC) Stapf extract for obtaining ZnO nanoparticles for photocatalytic application.

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The use of semiconductors for environmental applications has been widely used in the face of the properties of these nanostructured materials. Green synthesis is an effective method for obtaining nanoparticles from metal oxides without the use of toxic reagents and therefore environmentally friendly. In this perspective the present work aimed to synthe ZnO nanoparticles from the alcoholic leaf extract of Cymbopogon citratus (DC) Stapf. Preliminary characterizations of the extract and nanoparticles were performed using Fourier transformed infrared spectroscopy (FT-IR) and X-ray diffratometry (DRX). The photocatalytic activity of NPs was evaluated by the degradation of the methylene blue dye under UV light irradiation. The characterizations showed the obtaining of ZnO and the photocatalytic activity was 45.91% in 120 min.

Tailoring the 1.53 µm Er^{3+} emission bandwidth via metallic nanorods coupling

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The Er^{3+}: $^4I_{13/2} \rightarrow {}^4I_{15/2}$ transition exhibits a wide bandwidth, which corresponds to the third optical communication window [1]. Several efforts were made to increase its bandwidth by co-doping with different rare-earth ions [2]. However, this last increases the complexity of the dynamics of the transitions between these rare-earth ions. Another alternative is the addition of metallic nanoparticles, but the control of the nanoparticle and shape is still challenging [3]. This research obtained a bandwidth increment of the $^4I_{13/2} \rightarrow {}^4I_{15/2}$ emission band in Er^{3+}-doped tellurite glasses via gold nanorods coupling. A set of 4 nanostructures was fabricated, which consisted of an array of 8×8 square nanorods (width of 500 nm) varying their separation distance. Micro-luminescence spectroscopy was carried out to measure the reflection spectra upon 980 nm excitation for the different nanostructures. The FWHM of the $^4I_{13/2} \rightarrow {}^4I_{15/2}$ emission band centred at 1530 nm calculated for the bulk glass is 60 nm, and the obtained with the nanostructures are about 103 nm. Such increment is ascribed to the population of the Stark levels of the $^4I_{13/2} \rightarrow {}^4I_{15/2}$ band due to the local field enhancement generated by the plasmon-Er^{3+} coupling. Further, varying the separation distance between the nanorods, the Stark levels' relative intensities vary, but the FWHM remains constant. Our system provides a straightforward way to expand the bandwidth and new directions toward engineering the Er^{3+} emission performance at the nanoscale.

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The influence of halide ions in the silver nanowires synthesis using polyol method

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Silver nanowires (AgNWs) have been studied due to their great optical and electrical properties, making them potential materials to be applied in transparent conductive films (TCFs). Halide ions, such as chloride (Cl-) and bromide (Br-), have been investigated in the synthesis of AgNWs by many researchers.[1] Cl- are commonly used to control the AgNWs growth by facilitating AgCl formation and controlling Ag+ in the solution thereby inhibiting the growth of silver particles (AgNP). Similarly, Br- are also being investigated as a capping agent due to their ability to adsorb onto the (100) crystal plane of Ag, analogous to the capping agent polyvinylpyrrolidone (PVP). In this study, we investigate the influence of Br- and Cl- ions in the synthesis of AgNWs using the polyol method, employing ethylene glycol (EG) as solvent and reducing agent, silver nitrate (AgNO3) as the metallic precursor and PVP as the capping agent. In the absence of halide salts, pyramids and rod structures were observed. When only Cl- is added in the reaction, a mixture of pyramids rods and wires were formed. The addition of Br-resulted in the formation of particles (d=133,7 ± 1,6 nm) attributed to the adsorption of Br- ions on the {100}, {110} and {111} crystal planes of fcc silver. The Uv-vis spectrum of sample with Br- exhibited a band at 430 nm, consistent with literature reports for AgNP. The spectra obtained for samples without halides and sample with Cl- are consistent with larger structures. However, when both halides are introduced in the reaction, longer and thinner AgNWs were produced,as observed through SEM, AFM and UV-vis, stating their important role in the silver nanowires growth. Enhancing our comprehension on the growth process and morphological control is important for optimizing the technological application of AgNWs, especially for TCFs.

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The influence of SiO2 nanoparticle morphology on scattering efficiency for Random Lasers

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In this work [1] we investigated the effect of the morphologies of silica nanoparticles in the scattering efficiency of light for random laser based on Rhodamine-6G (Rh6G) in an ethylene glycol (EG) suspension with quartzite or amorphous SiO2 nanoparticles. We characterized quartzite nanoparticles through electron microscopy and compared its morphology to those of amorphous silica. The results demonstrated a considerable increase in the random laser efficiency for lower scatterers' concentration due to the high reflectance of visible light in the particles face and the field scattering intensity in its sharp edges. We also did finite element simulations that further confirms those conclusions and presents new grounds for theoretically exploring the geometry of nanoparticles for random laser systems with natural nanomaterials. Our experimental results confirm that the full width half maximum as a function of excitation energy is lower for our nanoparticles, determining higher efficiency for the novel quartzite scatterers. The mean free path of the sample is optimal for concentration of 0.5mg/mL, with higher concentrations not offering enough interaction between scattered light and the fluorescent dye to further increase the lasing efficiency. The finite element method (FEM) simulations confirm that the sharp edges offer very good scattering for the smaller particles, with the far scattered field showing higher normalized intensities when compared to the incident light.

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Thermal Poling applied in a silver niobium phosphate glass

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Niobium phosphate glasses are low-cost materials with high chemical, mechanical and optical properties. The applications of glasses containing silver are related, among others, to its nature in the material [1-3]. Considering applications in Non-linear Optics, this work studied the effect of thermal poling in a sodium high-niobium phosphate glass with silver of molar composition $50NaPO_3$-$45Nb_2O_5$-$5AgNO_3$. The glass of 1mm thickness was placed in a thermal poling cell between two electrodes. In the anode side it was used an ITO electrode and in the cathode side it was used an n-doped silicon wafer and borosilicate glass to prevent the sample from adhering to the cathode. The process occurred at 300°C, under N_2 flow, and an applied DC voltage of 1 kV at a 150 $V.min^{-1}$ rate. The current curve versus time was collected during the test, and when the applied voltage achieved its maximum, the same took place to the current (~0.27 mA); then it started to decrease since ions migrate towards the cathode over the treatment time. After the current reached a value close to 0 mA, the temperature was reduced with the electrical voltage remained until to 80°C; then the voltage was turned off and the sample removed. Energy-Dispersive Spectroscopy allowed the identification of the elemental composition of the studied sample on its cross-section under the anode side. It was verified that not only occurs sodium depletion on the anode side, presenting a layer of ~2μm, but also silver was depleted and accumulated between the depleted layer and bulk region. In this sense, this depletion indicated the break of centrosymmetry of glass that may generate second harmonic, and also, the potential of the material for application such as planar waveguide.

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Thermoluminescence and photoluminescence of $BaMoO_4:Gd^{3+}$ and $BaMoO_4:Gd^{3+}/SiO_2$ core shell powders

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Rare earth-doped molybdates have been the subject of intense research owing to their promising technological importance in several scientific and technological fields [1]. $BaMoO_4$ is regarded as a self-activated luminescence material, with the main emission occurring at the green and/or blue spectral region at room temperature depending on its properties and on the adopted synthesis methodology which affects the defect structures [2]. This work investigates the structural, morphological, optical, and thermoluminescent properties of $BaMoO_4:Gd^{3+}$ and $BaMoO_4:Gd^{3+}$/core shell compounds, doped with different Gd^{3+} ions concentrations. The powders were synthed using the co-precipitation method associated with the microwave-assisted hydrothermal technique. The samples were characterized by employing powder X-ray diffraction (XRD), Raman, UV-Vis, Thermoluminescence (TL), Photoluminescence (PL), and Scanning Electron Microscopy (SEM). Thermoluminescence (TL) measurements were carried out for samples irradiated with a beta particle radiation dose of 3.0 Gy. The scheelite structure was observed from XRD measurements for all samples. The photoluminescence spectra show the effect of the gadolinium doping concentration and the adopted synthesis methodology and the selected excitation energy. The registered TL glow curves show that the maximum emission temperature, and the glow curve profile, change according to the gadolinium doping content. Results show the variation in the trapping parameters induced by the increase in the gadolinium doping concentration and synthesis methodology.

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Thermo-optical properties of carbon quantum dots produced from Orbignya speciosa biomass (babassu coconut).

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Investigating substances with high nonlinearities is a frequent and fascinating topic in the scientific community, as understanding such properties is crucial for advancements in various technological areas, such as data storage, signal processing, and information technology. Among these materials, those of organic and biological origin have stood out, exhibiting high nonlinearities due to the viability of low-cost and sustainable syntheses. Recent studies have demonstrated the potential of applying carbon dots (CDs) from biomass as materials with high optical nonlinearity values. However, there is still a need for in-depth studies of the thermo-optical properties of this type of material. In this study, the nonlinear optical properties under the thermal regime of CDs produced through a hydrothermal synthetic route using biomass from Orbignya speciosa (babassu coconut) as a precursor, a widely common plant in the “Mata de Cocais” biome in Northeastern Brazil, were investigated. The material formation was verified through UV-visible absorption spectrum analysis, revealing characteristic bands associated with π-π* transitions due to aromatic C=C bonds in the core of CDs and n-π* transitions of carboxylate groups present on the surface. Through thermal lens spectroscopy (TLS) with offset beams, using a continuous wave (CW) excitation laser at 532 nm and a CW probe laser at 633 nm, the material thermal diffusivity value as a function of dilution was obtained, with a maximum value of 2.03×10-7 m2/s. Using the Z-scan technique also under a CW regime with a wavelength of 532 nm varying the incident power from 10 to 23 mW, the highest n2(th) value was obtained, which reached -3.77×10-7 cm2/W for the highest intensity, through the analysis of phase shift from Z-scan was obtained the value for. The photothermal efficiency of the material was also quantified, yielding a value of 78.1% for absorption at 532 nm.

Triplet to Singlet: Enhancing Fluorescence in Organic Materials

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Energy transfer is crucial in optics, photonics, and optoelectronics. Usually, triplet excitons hinder device efficiency, notably in organic light-emitting diodes (OLED). Experimental studies showed simultaneous singlet-singlet (SS) and triplet-singlet (TTS) FRET from a single donor material (NPB) [1,2]. To explore this further, we used Density Functional Theory (DFT) to analyze the geometry and normal modes of NPB and the acceptor (DCJTB) molecules. By employing the nuclear ensemble method, we obtained the absorption and emission spectra for both materials. Additionally, we calculated the intersystem crossing (ISC) rates and phosphorescence spectra of NPB regarding the triplet excited state. Varying acceptor concentration affects the system's polarizability and fluorescence spectra due to dielectric constant dependency, altering ISC, emission, and transfer rates. To gain further insights into these dynamics, we developed a Kinetic Monte Carlo (KMC) algorithm based on electronic structure parameters from differently polarized systems. We investigated energy transferring, internal conversion, and non-radiative contributions as the acceptor concentration increased. The first mentioned experimental observations attributed exciton lifetime decay to non-radiative processes, but our results reproduced decay without considering non-radiative processes, highlighting TTS occurrence. Our study sheds light on the simultaneous SS and TTS transfers and provides valuable insights into energy transfer mechanisms, advancing OLEDs and related technologies.

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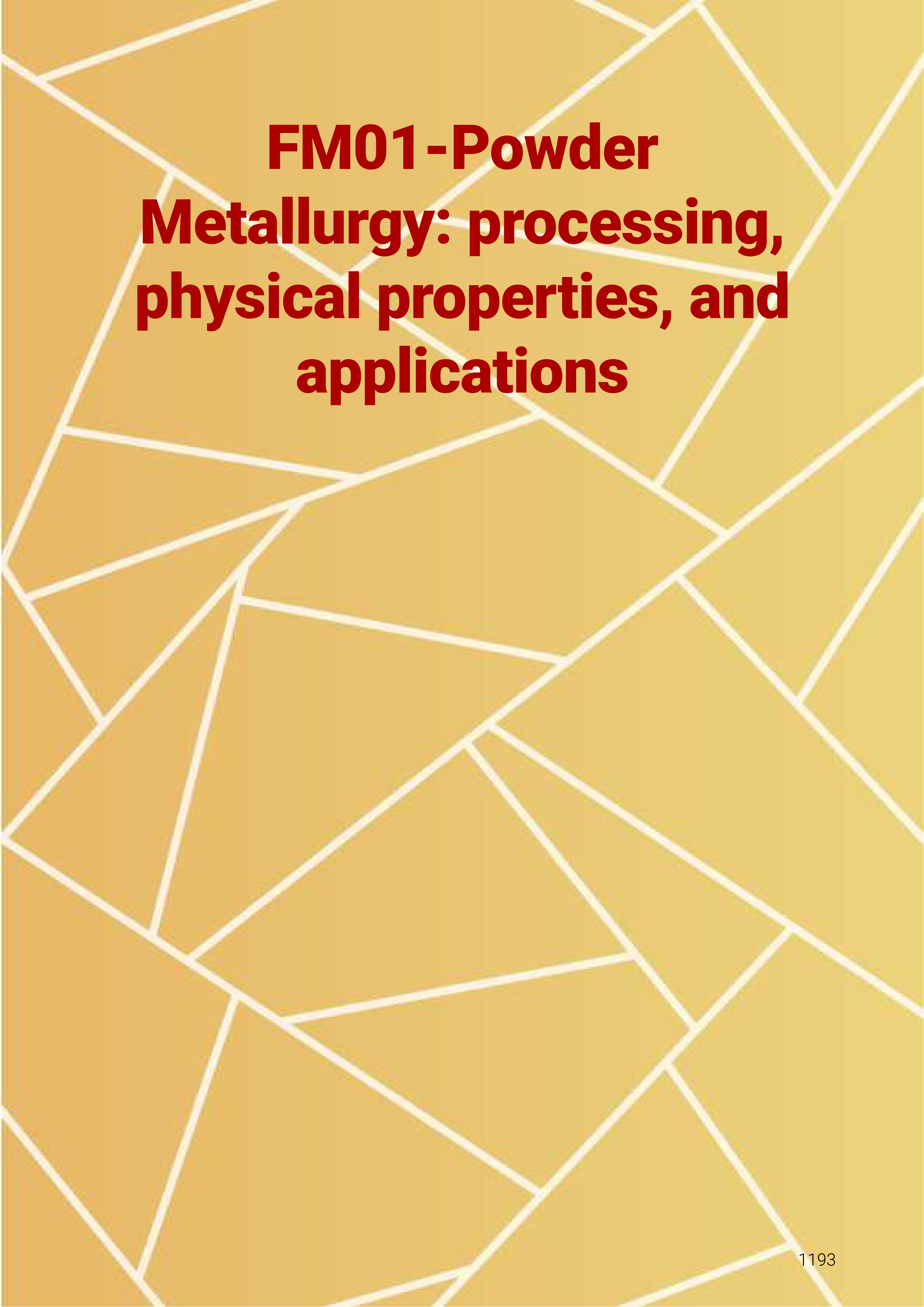

FM01-Powder Metallurgy: processing, physical properties, and applications

Macro and microtexture investigation of an Inconel alloy 625 produced by LPBF

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Additive manufacturing (AM) has gained significant attention from researchers worldwide [1]. Particularly, Inconel 625 alloys play a crucial role in various industries such as aerospace, petrochemical, and medical. This study focused on producing Inconel 625 alloy specimens through laser powder bed fusion (LPBF), with variations in key parameters, including hatch space, scan speed, and laser power, resulting in different volumetric energy densities (VED). The crystallographic components of seven specific VED conditions were evaluated using X-ray diffraction and EBSD techniques. Specifically, the changes in fiber textures, such as <100>//BD, <110>//BD and <111>//BD were explored and analayzed. These findings are significant as they shed light on the impact of LPBF process parameters on the texture components of Alloy 625 parts, ultimately leading to improved mechanical properties and wider application possibilities.

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Sinter-based additive manufacturing: basic concept, potential application and ongoing development

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Additive manufacturing (AM) is a disruptive technology that comprises a vast group of processing techniques where parts are manufactured adding material layer by layer. These very recent group of techniques is undergoing a remarkable evolution over the last decade. Nowadays processes for several classes of materials, such as polymers, ceramics and metals have been already proposed and studied. In metal additive manufacturing an important number of processing techniques uses metal powder as raw material to produce components, being classified as a new branch of powder metallurgy. Inside this group, sinter-based processes are those where the final properties of the part are obtained by sintering. Such processes offer several advantages over the processes involving metal fusion and solidification, such as flexibility of using a broad group of alloys, without concern of residual stresses. On the other hand, some drawbacks, like parts limitations and possible distortion during the sintering step, do also exist. The most known sinter-based metal additive manufacturing processes are binder jetting and material extrusion, but other process such as powder bed fusion, using special feedstocks, and photopolymerization are emerging. In this context the lecture starts by presenting the basic concepts to understand sinter-based additive manufacturing, presenting some cases and applications. Then, some results from the research developed by the authors will be presented. The discussion will be focused on material extrusion techniques, using solid feedstock (screw-based extrusion of powder injection molding like feedstock) and metal powder filled paste (robocasting). At the end, the main perspectives and challenges of sinter-based AM, from the point of view of the authors, will be presented.

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Chemical Debinding of MIM-based Material Extrusion Additive Manufacturing

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The metal powder injection molding process involves several stages. Firstly, metal powder is mixed with a binder system to form the feedstock, followed by pelletization or granulation, injection molding, extraction of the binder system through chemical and thermal processes, and finally, sintering. This technique presents challenges in producing parts with thick sections, due to the extended time to achieve suitable polymer extraction by chemical debinding. In an analogical way, Material Extrusion Additive Manufacturing (MEX), reproduces the same stages as MIM. However, instead of injection molding, MEX produces parts by deposing material from a nozzle in a path determined by the part design. Thus, MEX's greatest advantage lies in producing parts with complex geometry without the need for dies, as well as partial infill parts, with projected voids, thus reducing cross sections. Therefore, this study aims to compare the chemical extraction of cylindrical test specimens (height of 35mm and diameter of 21mm) produced via MEX with gyroid, cubic, and concentric filling patterns and internal fillings of 25% and 50%, with standard test specimens produced via MIM from the same feedstock (polypropylene, paraffin wax, EVA, and iron carbonyl). The analysis was conducted in two ways: i) by measuring the weight of the test specimens before and after 12-hour chemical extraction to determine paraffin wax mass loss; ii) by pycnometric densities before and after chemical extraction. The results revealed a superior extraction rate of the test specimens produced by MEX, especially those with gyroid patterns, due to their connected internal structure and low density which smooth the creation of the porous network during chemical debinding. This result opens up discussions about the application of additive manufacturing in contexts where large parts are required, with less restriction linked to the chemical debinding step.

Determination of a processing map for fabricating Inconel 625 by laser powder bed fusion through the variation of the scan parameters

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Superalloys are designed to be used in extreme environments in terms of high temperature and corrosion potential, since they maintain their properties, especially the mechanical strength, in these environments. Due to the difficulty in machining these materials, additive manufacturing has become an alternative manufacturing route. However, since the process introduces defects in the material, the most common one being the porosity, it must be minimized for metallurgical quality manufacturing, which is done by doing the correct parametrization of the equipment [1][2]. Initially in this study, the powder was characterized using XRD analysis, Laser Diffraction Particle Size Analysis, EDS and SEM. Then, in the OmniSint-160 equipment, the variation in laser scanning speed (750 to 1200 mm/s) and hatch spacing (0,08 to 0,11 mm) was used to analyze the fabrication of IN625 by laser powder bed fusion (LPBF), totaling 40 samples with different levels of energy density in the process, calculated using the formula Ev=P/(v.h.l), which is associated with the level of porosity, measured using ImageJ software after metallographic preparation. Of the 40 samples, 95% were found to have the conventional porosity level for the process (<0.5%), and the remaining had porosity, mostly being lack of fusion (LoF). Four samples were selected based on the energy density of the process and the level of porosity (highest and lowest energy density and porosity) for EBSD analysis, which showed microporosity in all of the samples and grain refining in the LoF regions. The results were complemented with microhardness and optical microscopy after chemical attack. This research contributed to the establishment of the parameters for manufacturing IN625 by LPBF, corroborated by the literature.

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Effect of the polymeric binder system content (wt%) on the shrinkage of samples produced by MEX

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Material Extrusion Additive Manufacturing (MEX), stands out for its low material waste, production of parts without the need for dies or molds, and low energy cost. In this process, metal powder (iron carbonyl) is mixed with a polymeric binder system (paraffin wax, polypropylene, and EVA), which allows the material to be molded by the 3D printer and ensures the green strength of the parts. After shaping via MEX, the parts undergo the binder system extraction by chemical and thermal process, and finally sintering, during which the parts shrink due to the polymeric binder removal and the metal powder sintering. In this context, the study aimed to produce test specimens via MEX in the shape of cubes (edges of 20 mm) and cylinders (height of 35 mm and diameter of 21 mm) with internal fillings of 25% and 50%, using a standard feedstock with binder system mass fractions of 6%, 7%, and 8%, to analyze the influence of these fractions in the shrinkage as well as on density and types of printing defects. First, the feedstock's pycnometers densities were analyzed, as well as their homogeneity by Scanning Electron Microscopy (SEM). Second, the weight and dimension of the samples were observed after the manufacture, the chemical extraction, and the sintering. Finally, to analyze the types and density of defects, cross-section metallography was conducted. The results revealed that the lowest mass fraction (6%) experiences less shrinkage during sintering, poorer processability, and higher defect density, due to the lack of the binder system in the feedstock. In contrast, the 8% fraction feedstock shows higher shrinkage, better processability, and lower defect density during printing. Lastly, the 7% fraction feedstock shows moderate effects compared to the other two.

Exploring the potential of an in-situ Fe-NbC metal matrix composite as a reinforcement for enhancing mechanical properties of powder metallurgy materials

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The metal matrix composite developed at LabMat combines the ductility of an Fe matrix with the toughness of NbC reinforcements, resulting in hardness values around 1000 HV, while being more cost-effective than traditional hard metals. Utilizing an in-situ processing method, involving the reaction between the intermetallic compound Fe2Nb and graphite, circumvents common defects found in ex-situ methods, such as uneven distribution of reinforcements and inadequate wettability between the reinforcements and matrix. This study aims to assess the composite's potential as an additive to enhance the hardness and toughness of other materials. Two types of commercially available iron powders were selected as base materials: a high compressibility die-pressing powder and a metal injection molding powder, chosen for their cost-effectiveness and wide range of applications. Samples containing 10%, 20%, and 30% by weight of the composite, corresponding to approximately 5%, 10%, and 15% by weight of NbC, were prepared. Two fabrication methods were employed: the first involved mixing the composite's precursor powders - Fe2Nb and graphite - with the iron powders, and the second involved mixing the heat-treated composite - consisting of NbC and Fe - with the iron powders. The samples were mixed, uniaxially pressed, and sintered in a vacuum furnace. Subsequently, they were analyzed using scanning electron microscopy (SEM) to evaluate the distribution, , and shape of the carbides, as well as the microstructure of the matrix. Additionally, the hardness and yield strength of the samples were measured and compared to those of the unreinforced base materials. The results have demonstrated that both the addition of the precursor powders and the heat-treated composite are capable of significantly improving the mechanical properties of the materials, indicating the potential of the composite as an additive for other alloys.

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In situ production of Fe + NbC composite powders for the development of sintered components.

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This study investigates the synthesis, properties, and processability of ferrous matrix composites reinforced with niobium carbide. The development of ferrous matrix composites incorporating second-phase ceramic particles is of interest for a wide range of applications due to their mechanical performance coupled with economic viability. The chosen approach involves the production of ferrous matrix composite powders reinforced with submicron niobium carbide particles formed in situ through thermochemical treatments. The in situ formation of reinforcements, which involves the formation of reinforcement particles within the matrix through the reaction of precursor materials, aims to improve the interface quality between the matrix and the reinforcement compared to traditional methods. The functionality of this technique relies on the reactions among raw materials towards thermodynamic equilibrium. For this reason, thermodynamic simulation tools via Thermo-Calc® software were employed to validate the working premise and design the selected process, aiming to reduce experimental volume and thus enhance time and resource utilization. Once the premise of in situ phase formation was validated, the feasibility of using different reaction temperatures was studied. The goal was to assess the impact of these parameters on the microstructure and, consequently, the mechanical properties. The macro and microhardness of carburized samples produced by uniaxial compaction followed by sintering are 533 HV10 and 553 HV0.05, with 8% porosity.

Production an Characterization of Ti-Nb alloys in Molten Salt

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Titanium and its alloys have unique characteristics when compared to other metals, such as low density, high mechanical strength, high corrosion resistance and biocompatibility. Titanium alloys have properties varying over a wide range, which makes them interesting for different applications, especially for aerospace and biomedical industries. Ti-Nb alloys have been studied as an alternative to replace of biomedical implants, because their mechanical properties are close to those of human bone. The present work investigated an alternative to conventional sintering, with lower cost and shorter processing time. The sintering in molten salt of Ti-Nb alloys samples produced by warm compaction of MIM feedstocks was investigated. MIM feedstocks were produced with three different compositions: Ti-10Nb, Ti-16Nb and Ti-22Nb using Ti and Nb elementary powders. Subsequently, the feedstocks were warm compacted and underwent the extraction of binders. Sintering was carried out in a molten salt atmosphere and in a vacuum for comparison. TiNb parts sintered using a molten salt shield showed properties similar to alloys used in biomedical implants. However, they have a lower densification when compared to samples sintered in vacuum. Microstructural and mechanical properties of Ti-xNb parts were evaluated. The results obtained in this work demonstrate that molten salt sintering is an alternative route for manufacturing porous titanium alloys.

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Study of inconel 718 cryogenic deformation produced by laser powder bed fusion

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Inconel 718 (IN718), a nickel-based superalloy used in high-temperature (HT) applications, offers good weldability and high strength, making it promising for additive manufacturing (AM) in complex geometries. Despite numerous studies on HT applications, its literature at cryogenic temperatures (CT) is limited [1]. Thus this study compares the mechanical behavior IN718 made by AM at room temperature (RT) and CT. It was used recycled powder IN718 with a morphology spherical with satellite particles. Plate dog-bone tensile samples (50mmx10mmx1.5mm) were fabricated for testing. Printing parameters were: power 217W, speed 1m/s, hatch spacing 8µm, layer thickness 4µm, and a 67° rotation of the laser beam between layers. Samples were polished to minimize stress concentration points. X-rays fluorescence confirmed the expected chemical composition [1]. Optical microscopy, with metallographic preparations, revealed the cohesion of melting pools and a porosity 0.09%. Tensile tests at RT and CT (-197ºC) with a crosshead speed of 0.3 mm/min. At CT, there was an increase in 30% ultimate tensile strength and 68% elongation. A possible explanation is that for CT the predominant deformation mechanism changes from dislocation slip to strain-induced martensite transformation. Thus the austetitic matrix of IN718 changes to hexagonal closed-packed or body-centered tetragonal structure [2]. Analysis of fracture surfaces via SEM revealed the presence of refined dimples in all tests, indicating no change in fracture mechanism but a shift in deformation mechanism. Brittle fractured particles were visible, possibly from solidification or previous prints [1]. Thus, it can be concluded that besides HT applications, IN718 is a promising material for use at CT.

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The Effect of Reduced Graphene Oxide on the Microstructure, Magnetic Properties, and Corrosion Resistance of NdFeB Magnets

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This work investigates the effect of adding reduced graphene oxide (rGO) as a milling agent on NdFeB magnets' microstructure, magnetic properties, and corrosion resistance. RGO was incorporated into NdFeB powder via mechanical milling for 7, 15, 30, and 45 minutes. X-ray diffraction (XRD) confirmed the presence of the Nd2Fe14B3.1 phase in all composites. Transmission electron microscopy (TEM) revealed that rGO adhered to the NdFeB particles as thin flakes, potentially hindering corrosion. Magnetic characterization showed a significant improvement in remanence (Br), intrinsic coercivity (iHc), and maximum energy product (BHmax) for magnets produced with longer milling times (30 and 45 minutes). Notably, magnet-3 (30 minutes milling) achieved a Br of 1.10 T, iHc of 972.59 kAm^{-1}, and BHmax of 221.62 kJ m^{-3}, exceeding those of other samples and approaching values reported in the literature [1]. Electrochemical Impedance Spectroscopy (EIS) analysis demonstrated superior corrosion resistance in magnets fabricated with longer milling durations, likely attributable to the protective influence of rGO. This research underscores the potential of utilizing rGO as an environmentally friendly and efficient milling agent to increase the performance of NdFeB magnets

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Ultra-fast High Temperature Sintering (UHS) Of Ni-NiO Composites

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Powder metallurgy and sinter-based additive manufacturing are cost effective routes for manufacturing high value metal alloys and metal matrix composites such as Ni based alloys used in the aerospace and energy industries. Despite the development of these manufacturing techniques in recent years, the sintering step remains a challenge due to its high energy consumption and long dwell times. Ultrafast High Temperature Sintering (UHS) has emerged as an alternative capable of sintering metal alloys in just a few seconds. In this study, we evaluate the UHS sintering of Ni-NiO composites. The effects of UHS current and dwell time on the microstructure and mechanical properties of Ni-NiO was investigated. UHS should facilitate the development and manufacture of metal alloys and composites from metal powders.

Additive Manufacturing of Fe-6.5Si Alloy: A New Route to Improve Electric Motor Components

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The demand for more efficient electric motors necessitates advancements in materials and manufacturing processes to achieve lower energy consumption and reduced costs [1]. Traditionally, electric motor cores comprise thin sheets of Fe-Si alloys stacked with an electrically insulating material to mitigate losses from parasitic currents [2]. However, the addition of 6.5 wt. % silicon to electrical steels, while enhancing the electrical and magnetic properties, poses challenges due to forming the brittle B2 and D03 phases, rendering conventional production techniques inadequate [3]. Laser Powder Bed Fusion (L-PBF), an Additive Manufacturing (AM) technique emerges as a promising alternative route due to its ability to employ high cooling rates and hindering the formation of such fragile phases [3]. This work represents the initial phase of an ongoing investigation. The primary objective is to explore the production of Fe6.5Si (wt. %) alloy by L-PBF, aiming for high densification. Relative densities ranging from 84% to higher than 99% were achieved, with volumetric energy densities between 35 J/mm3 and 720 J/mm3. Notably, denser regions exhibited more pronounced cracking, underscoring a critical aspect for further investigation. Structural analyses, including X-ray diffraction (XRD) and scanning electron microscopy (SEM), provided valuable insights into the microstructural features. Subsequent steps of the study will encompass magnetic and mechanical behavior analyses, aiming to deepen our understanding and potentially validate L-PBF as a viable production method for Fe-Si alloys with high silicon content.

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Adsorption of the tetracycline antibiotic by $CoFe_2O_4$ nanoparticles

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Antibiotics are indispensable for human and animal health. However, their widespread use presents consequential environmental risks, due to toxic effects and the potential development of resistant bacteria. Hence, effective removal of antibiotics from waste water and the environment is imperative [1,2]. In this work, cobalt ferrite ($CoFe_2O_4$) nanoparticles (NPs) were investigated as an adsorbent for the antibiotic tetracycline (TCN). $CoFe_2O_4$ NPs were synthesized by coprecipitation, annealed at 623 K and characterized by X-ray diffractometry (XRD), Fourier transform infrared spectroscopy (FTIR), Mössbauer spectroscopy (ME), vibrating sample magnetometry (VSM), electrophoretic light scattering and gas adsorption. The experimental data confirmed the formation of the partially inverse spinel phase of $CoFe_2O_4$ with crystallite size of 4 nm, superparamagnetic behavior, low saturation magnetization and coercivity, isoelectric point close to pH 7 and mesoporous structure. The non-linear equilibrium data better fit the Freundlich model, suggesting a heterogeneous surface of the adsorbent. Adsorption measurements in the time range 5-2880 minutes showed a greater suitability of the Elovich non-linear kinetic model, often associated with chemical adsorption processes. Additionally, FTIR showed a shift from 1580 cm^{-1} to 1590 cm^{-1} in the v(C=O) absorption band, indicating that this group may have acted as a binding site for TCN molecules. The maximum adsorption capacity (42 $mg.g^{-1}$) occurred at pH 7 and room temperature, favoring the industrial application of $CoFe_2O_4$ as adsorbent.

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Al/CNT composite deposits produced by selective laser melting.

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Selective laser melting (SLM), and particularly the materials deposition, layer by layer (Additive Manufacturing – AM) has been extensively used in production of several metallic components in titanium alloys, special steels, and aluminum alloys. However, the use of such technology to produce metal matrix composites is still very incipient, due to the complexity of processing simultaneously a material based in two very distinct phases.

In the present work, an Al/CNT (carbon nanotube) composite was deposited on an aluminum ally substrate to promote a surface strengthening effect. The CNT were previously coated by TiO2 by the sol-gel technique. The resulting TiO2 coated CNT were mixed to aluminum powder (2/98 w%) and spread over the substrate to be melted using CO2 and fiber Nd-YAG lasers in successive tracks. The resulting microstructure can be controlled by the heat input [1] and the high heating/cooling rates [2] decreases the risk of CNT to degrade. Furthermore, the Marangoni effect [2] can also improve the dispersion of the reinforcing phase.

The results show that a good metallurgical bond between the deposit and substrate can be obtained, but the heat input is a key parameter and must be optimized to reduce the porosity level in de deposit. Furthermore, oxidation of the liquid aluminum is a concern, as it increases the balling effect.

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Analyzing the quality of our drinking water: by examining the presence of total coliforms and e. coli.

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The project draws attention to a severe issue with Brazil's poor sewage treatment system, which results in a large amount of sewage being dumped improperly — often into a black cesspit beneath the surface. Sewage not disposed of properly can contaminate groundwater, which is used for various purposes, and can cause significant health issues. Mainly, children are more susceptible to illnesses from contaminated water, with diarrhea being one of the primary reasons for hospital stays [1]. This study aims to accurately and realistically diagnose the presence and level of total coliform and Escherichia coli (E. coli) contamination in the urban and rural areas of Ilha Solteira, SP, Brazil [2]. In the event of contamination, the findings must act as an alert and encourage local efforts to enhance cleanliness. Furthermore, the research aims to create a titanium dioxide ($TiO2$) photocatalytic filter that can clean water tainted with germs that pose a health risk to humans. Solution Blow Spinning (SBS), a promising method for producing nanofiber materials with a wide range of applications in water purification and pathogen elimination, was selected to make the filter [3].

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DEVELOPMENT OF TEACHING NOTEBOOKS FOR THE DISSEMINATION OF KNOWLEDGE AND PRACTICES IN THE AREA OF ADDITIVE MANUFACTURING

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The development of teaching notebooks on additive manufacturing, processes and machinery was carried out within the GMAT UFSM (Materials Technology and Mechanics Group of the Federal University of Santa Maria), with the aim of helping undergraduate Mechanical and Aerospace Engineering students develop your research. The material prepared covers the different types of additive manufacturing, the basic step-by-step guide to creating digital models and instructions on how to prepare the files that will be taken for manufacturing, a brief review of the most used materials, as well as a manual for using the machines available during the production and characterization process of the parts: 3D printers, ovens, cutters, polishers, among others. From the use of teaching notebooks, it was found that this material helped students participating in the GMAT UFSM, perpetuating knowledge and serving as quick reference material, in addition to promoting the dissemination of additive manufacturing knowledge to other undergraduates interested in the area, enabling , also, the development of individual applied projects.

Evaluation of laser sintering parameters of copper-graphene composites aimed at manufacturing additive

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Pure copper has high values of electrical and thermal conductivity, on the other hand, it has low mechanical resistance, making it almost unfeasible for some applications, among them a component for high power magnet coils. The development of materials for application on these magnets is limited by the characteristics of their conductors, which must have high values of mechanical resistance and electrical conductivity. However, obtaining these high simultaneous properties is still an obstacle due to the mechanisms of increased resistance causing attenuation in the electrical properties. Alternatively, the manufacture of copper-based composites with different reinforcement materials, such as graphene, has been studied. In this study, the behavior of the powder of copper composites reinforced with reduced graphene oxide was investigated through a laser sintering aiming at future production by additive manufacturing. For this, the composites were produced by a mixing route between copper powder and graphene oxide, giving rise to the composite powder. The reduction of the composite powder was carried out under a hydrogen reducing atmosphere. Laser sintering was performed using Yb:Fiber laser with a wavelength of 1064 nm under optimized power of 445 W and different scan speed and laser beam diameters. The microstructural results showed the appearance of the tracks after irradiation and it was possible to lead to an optimal processing speed for this study. Through FTIR it was observed that during the laser processing functional groups were reduced and through analysis of nanohardness vickers an increase in the hardness was observed after irradiation to laser thus suggesting possible preliminary parameters to be applied in manufacturing additive.

Evaluation of microstructure and tensile properties of Inconel 625 produced by laser powder bed fusion after stress-relieving and solubilization

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The Inconel 625 nickel-based superalloy (IN625) performs excellently in high-temperature applications and is resistant to corrosion and oxidation [1]. In addition, due to its good weldability, it can be processed through additive manufacturing (AM) by laser powder bed fusion (LPBF). This advanced manufacturing route makes it possible to produce complex components without the need for multiple steps, through the sequential deposition of material layer by layer [2]. Although the LPBF technique has several benefits, high residual stresses and anisotropy of mechanical properties are associated with it. This could be due to the rapid cooling rates that follow the rapid heating during layer deposition [2]. Because of this, heat treatments are necessary after deposition in order to develop the desired microstructure and mechanical properties. In this study, stress-relieving (SR) and solubilizing (SB) heat treatments were carried out together, and their influence on the microstructure and tensile properties of the alloy was analyzed. Tensile tests at room temperature were carried out on the samples, followed by fractographic and EBSD analyses. The tensile strength limits found were greater than 1 GPa, and the fracture surface revealed the presence of small dimples, characteristic of a ductile fracture.

Acknowledgments

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Influence of calcination time and temperature on the properties of TiO2 photocatalyst supported on Laponite RD

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In the field of wastewater treatment processes, a technology that has been attracting considerable interest is Advanced Oxidation Processes (AOPs), applied in photocatalysis systems. Oxides of semiconductor metals like titanium dioxide (TiO_2) in the presence of radiation can release reactive oxygen species, which have the property of degrading organic compounds. In this aspect, these properties are enhanced when the oxides are supported on substrates, such as Laponite RD clay [1]. This work aimed to determine the influence of calcination temperature and time on the photocatalytic properties of TiO_2 supported on Laponite RD. The compounds were prepared by adding the desired amount of oxide to an aqueous dispersion of Laponite RD [2]. Subsequently, the mixture was calcinated at desire temperature ranging from 400°C to 900°C. The time study was conducted at temperatures of 600°C, 700°C, and 900°C, from 2 to 6 hours. The materials were characterized by X-ray fluorescence (XRF) and Fourier Transform Infrared (FTIR) spectroscopy, observing variations in the composition of different samples and characteristic bands of the oxides and clay. It was noted that the incorporation of the oxide does not significantly alter the structure of Laponite RD.

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Influence of Cryogenic Straining on the Mechanical Behavior and Work Hardening of AISI 304 Austenitic Stainless Steel

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The metastable austenite of austenitic steels can produce strain-induced martensite, which directly affects the material's mechanical behavior and work-hardening values. This study aims to investigate the influence of cryogenic straining on the mechanical behavior of AISI 304 austenitic stainless steel. The material underwent isothermal tensile tests, using synchrotron X-ray diffraction (XRD) in situ at cryogenic temperature (93 K) and room temperature (298 K). It obtained the stress-strain curve and diffraction pattern for each condition at several stages of material straining. The modified Crussard-Jaoul analysis was employed to identify different work-hardening stages related to the different deformation mechanisms at each temperature. The results indicated that the volume fraction of α' strain-induced martensite (SIM-α') increased with the strain level, mainly in the sample tested at cryogenic temperature. Furthermore, cryogenic straining resulted in higher rates of SIM-α' transformation and a significant increase in yield strength and tensile strength, with a slight decrease in uniform elongation compared to the room temperature test. The kinetics of strain-induced martensitic transformation at cryogenic temperature significantly influenced the mechanical behavior and work-hardening of AISI 304 austenitic stainless steel.

Mechanical and tribological properties of self-lubricating composite with ferrous matrix containing MoS2, NiO, and graphite

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Graphite and MoS2 are utilized as lubricant that works as substitute of oil in mechanisms that oil cannot or it is hard to be apply such as in aerospace parts and elevated temperature process parts. Utilizing powder metallurgy is possible to integrate graphite and MoS2 in components granting them auto lubricity proprieties that usually is not possible by other way of production. This study focuses on the production of self-lubricating composites using MoS2, NiO and graphite dispersed in an iron matrix. Samples were produced by powder metallurgy with different sintering temperatures (850 °C, 950 °C and 1050 °C) for 1 hour in atmosphere of 95% Ar + 5% H2 on a tubular furnace. The samples evaluation comprised tensile tests to assess resistance and yield stress and reciprocating sliding tests to evaluate the tribological behavior of the samples. Microstructural characterization of the samples was conducted. Previous research has shown that MoS2 and graphite can react with iron matrices during sintering providing good tribological proprieties [1]. This study aims to explore those results by adding NiO in the matrix to provide more mechanical resistance and maintaining good tribological properties. The results indicate that adding NiO increase the strength and delay the reaction between MoS2 and iron. By carefully controlling the lubricant's particle , composition, and processing parameters, the study was able to create self-lubricating iron-based composites with good mechanical behavior and low friction coefficient (<0.1) and wear rate.

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Mechanical properties of Inconel 625 fabricated by laser powder bed fusion in different temperature conditions of testing

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Additive manufacturing (AM) has been attracting interest due to the advantages it can provide, such as the manufacture of complex geometry components near-net shape with less human interference during the stages of production. Superalloys are materials that are used in conditions considered extreme in terms of temperatures and corrosion potential of the environment, and they are able to withstand these conditions and still maintain their mechanical properties. One example of the application of superalloys in these conditions is in the offshore oil industry [1]. The aim of this study was to evaluate the tensile strength of IN625 at different temperatures. The specimens were manufactured by powder bed fusion (PBF) in the OmniSint-160 equipment with a combination of parameters providing a level of porosity (<0.5%). The as-built specimens were tested at room temperature (RT) and cryogenic temperature (CT). The tests were carried out in duplicate for both temperatures. The samples tested at TC had a 20% increase in ultimate tensile strength (UTS) compared to those tested at RT, with also an increase in yield strength but a reduction in fracture toughness. The fractography of the samples after testing was carried out in SEM, and for both temperatures the presence of dispersed dimples of micrometric could be seen, characterizing ductile fracture. For the samples tested at TC, the deformation mode can be associated with the Transformation Induced Plasticity (TRIP) effect, which explains the increase in the mechanical properties [2]. This study has highlighted the increase in mechanical strength for the superalloy under study, which mainly has an austenitic structure as the matrix, also occurs when the manufacturing route is by MA.

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$NiFe_2O_4$ nanoparticles for tetracycline removal using alternating magnetic field

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In environmental remediation area, magnetic nanomaterials are used as adsorbents and are known for separation using an external magnetic field. However, recent research shows improved contaminant removal efficiency with magnetic nanoparticles (MNPs) under an AC magnetic field [1,2]. This may be related to the MNPs heat generation capacity, the increase in the diffusion rate of soluble molecules, the endothermic nature of many processes, and the thermal instability of contaminants [3]. In this work, nickel ferrite ($NiFe_2O_4$) MNPs were used to investigate the removal of antibiotic tetracycline (TCN) under AC magnetic field. The MNPs were synthesized by hydrothermal method and characterized by X-ray diffractometry, gas adsorption, thermal analysis, infrared spectroscopy, transmission electron microscopy, Mössbauer spectroscopy and vibrating sample magnetometry. TCN removal tests were carried out comparing effects produced at the same temperature by an AC magnetic field (300 A; 222 kHz) and by a heating plate. The results evidenced the MNPs spinel phase (≈ 25 nm), saturation magnetization of 54 emu.g^{-1} and specific surface area of 50.92 m^2.g^{-1}. TCN removal occurred by endothermic adsorption, with an increase in removal efficiency from (51.4 ± 2.1) % to (99.1 ± 0.1) % when comparing heating under an AC magnetic field to the use of a heating plate. These results were associated with greater homogeneity of heat generated due to magnetic induction heating mechanisms. The MNPs reuse was evaluated, and a removal capacity significant loss was observed only after the fourth adsorption cycle. Therefore, the $NiFe_2O_4$ MNPs are suitable candidates for use in antibiotic removal processes under AC magnetic field.

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Optimization of the scan parameters for laser beam powder bed fusion of Inconel 718

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Aeronautical, aerospace, and nuclear industries increasingly rely on Ni-base superalloys like Inconel 718 (IN 718) for their mechanical properties at high temperatures; the alloy operates effectively up to 700°C [1]. The difficulty in machining this alloy makes additive manufacturing (AM) a more suitable fabrication method. Optimizing AM parameters, such as laser power, scan speed, and layer thickness, enhances both the microstructure and mechanical properties of components produced via laser beam powder bed fusion [2]. Therefore, this study aims to determine the optimal printing parameters for IN 718 using the OmniSint-160® Selective Laser Sintering 600W machine. Recycled IN 718 powder, supplied by Sandvik, with a mean particle of 40.30 µm, was used. SEM analysis showed spherical powder shapes with occasional satellite particles. Constant parameters included a laser power of 200 W and a layer thickness of 0.04 mm. The laser spot was 0.09 mm, and the scanning direction rotated by 67° after each layer. Samples were fabricated with scan speeds from 750 mm/s to 1200 mm/s and hatch spaces from 80 µm to 110 µm, resulting in 40 samples. The combination of parameters that resulted in the sample with the lowest porosity was a scan speed of 1000 mm/s and a hatch spacing of 80 µm. The porosity range varied from 0.08% to 3.24%. High speeds with increased hatch spacing resulted in porosity due to a lack of fusion, on the other hand lower speeds combined with reduced hatch spacing led to keyhole porosities. SEM images and EBSD maps contribute to a more comprehensive analysis of the types of defects found.

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Performance and corrosion resistance of nickel coating in salt spray

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The interposition of a barrier between the metal and the environment, i.e. a protective coating, is an alternative to minimize the corrosion in metallic materials exposed to aggressive atmospheres. This is a challenge associated with the expansion of brazilian power sector, specially for transmission towers from wind farms generation. These structures are made of galvanized steel due to the high incidence of the lines in coastal, urban and industrial zones. Frequently, this material has adequate corrosion resistance, but in the North and Northeast regions of Brazil there are high salinity aerosois, winds, temperatures above 30 °C and relative humidity of around 75% [1] which implicates the study of new corrosion resistent materials. This investigation aimed the evaluation of the corrosion resistance of chemical nickel coatings, which are widely used in deepwater oil exploration [2], compared to the tradional galvanized steel. The study was carried out on 1020 carbon steel coupons, coated with a high-phosphorus nickel bath (13%) compared to hot-dip galvanized (100 µm), traditionally applied to power transmission towers. These were exposed in a salt spray chamber (3.5%), in a standardized cyclic test [3], for up to 450 h, and the corrosion rate was verified by gravimetric method. The results indicated the proposed Ni coating showed a loss of mass of 11.13 µm/year, which were up to 83% lower than galvanized steel, that presented 69.16 µm/year. The materials were subsequently characterized by scanning electron microscopy and it was verified the formation of a compact oxide over the entire surface of the Ni coupon, without exposing the substrate, which justified the enhanced performance.

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Synthesis and characterization of new molecular sieves as made from metallurgical slag.

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The present work has been developed within the startup AGA – Consultancy and Development of Technical-Scientific Projects and is based on an aspect of the well-established national industry in Brazil, the metallurgy industry, casting and machining of special copper alloys. First stage of the work consisted of treating solid waste from the special copper alloy industries and using this treated waste as raw material in the synthesis of molecular sieves on a nanometric and micrometric scale, thus adding value to the waste generated. In the second stage, the materials synthed from the treated residue were characterized by various physicochemical techniques, mainly in the solid state, such as powder method x-ray diffraction, energy dispersive x-ray spectroscopy, absorption spectroscopy in the infrared region, nitrogen physisorption, scanning electron microscopy and optical atomic emission spectroscopy with inductively coupled plasma. From the synthesis and characterization of the materials, it was demonstrated that slag from the metallurgical industry can be a raw material for the production of new molecular sieves containing copper[1] in their crystallographic structures.

Synthesis and characterization of TiO_2 and ZnO photocatalysts supported on Mg-Al LDH applied in the photocatalytic degradation of methyl orange dye

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Layered double hydroxides (LDHs) are hydrotalcite-type anionic clays with a layered structure, which can be synthetic or natural. They have great potential for application in several areas due to their structural, chemical, electronic, ionic and optical versatility. LDH is an excellent adsorbent, and when combined with TiO2 and ZnO oxides in presence of light can degradete organic pollutants. The aim of this work was synthesis and characterization of TiO2 and ZnO photocatalysts supported on Mg-Al LDH applied in the photodegradation of methyl orange dye. In a typical sol-gel method, the precursors MgCl2.6H2O and AlCl3.6H2O were solubilized in distilled water, followed by the addition of citric acid and ethylene glycol under heating to gel formation. The gel was subjected to a termic treatment at 300°C for obtained the LDH powder. The incorporation of the oxides was carried out by adding an ethanolic suspension of the oxides to the LDH, followed by calcination at 500°C. The material was characterized by Fourier Transform Infrared (FTIR) and powder X-ray Diffraction (XRD), where the characteristics of the layered structure of Mg-Al LDH were confirmed. The synthed material was subjected to photocatalysis tests using the methyl orange dye. Photodegradation tests confirmed the presence of photocatalytic activity in the synthed compounds, resulting in a more proiminent degradation of the dye when compared to the pure oxide.

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The effects of debinding and sintering on Binder jetting of Ti-6Al-4V alloy

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Binder jetting of Ti-6Al-4V alloy is a promising approach for manufacturing biomedical implants. Fabrication of Ti-6Al-4V components with high-density and mechanical properties similar to the ones achieved by powder injection molding (PIM) has already been demonstrated. However, the oxygen and carbon uptake is still higher than the standard level for biomedical application (ASTM F2885). In this study, the effect of debinding and sintering parameters on the carbon and oxygen uptake and microstructure was investigated. Optimizing debinding and sintering can decrease interstitial uptake in Ti alloys. However, just optimizing debinding and sintering cycles may not be suitable for achieve ASTM standard for biomedical applications, for that new binder system should be developed.

Ultra-fast high-temperature sintering of niobium-based alloys

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Ultra-fast High-temperature Sintering (UHS) is an innovative technique that has emerged as a promising technology for sintering high-melting temperature materials such as ceramic materials. This method uses high heating rates (up to 105°C/min), through an electric current and short residence times at high temperatures to obtain densification, allowing sintering in just a few steps. It has recently been demonstrated that this technology can be adapted for the sintering of metallic alloys, being especially attractive for the sintering of high-temperature alloys such as niobium alloys. In this study, we explored the influence of sintering parameters such as current and residence time on the final microstructure and mechanical behavior of sintered niobium alloys through optical, electronic and microhardness microscopy tests. The results demonstrate the potential of UHS as a cost-effective and time-efficient method for producing high-performance niobium alloy components for aerospace, automotive and other advanced engineering applications.

Ultra-fast High Temperature Sintering (UHS) Of Aluminium

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Aluminum is the second most utilized metal globally, playing a crucial role in modern engineering projects aimed at developing lighter structures. Besides its low density, aluminum offers several benefits, including the capacity for infinite recycling without any loss in its physical-chemical properties. Given the increasing demand for aluminum, advancements in more efficient manufacturing processes are essential.

In the manufacturing of samples, aluminum powder is compacted in a hydraulic press. A specific amount of powder and binder are added and then pressed into the matrix cavity using two punches, upper and lower, at room temperature. Subsequently, sintering occurs in a vacuum atmosphere.

This study introduces Ultra-fast High Temperature Sintering (UHS) as an alternative to conventional sintering, featuring a significantly shorter processing time. Tests indicate that metallic aluminum powders consolidate in just a few seconds using the UHS technique. During this process, a green sample is placed inside a carbon felt and heated by Joule effect until aluminum sintering is achieved. The effectiveness of this process will be evaluated through analysis using a scanning electron microscope (SEM) and microvickers hardness tests. The results obtained so far suggest that UHS is a promising alternative for manufacturing aluminum alloys.

Use of Graphene for the Reinforcement of Metal-based Materials Composites – MMCs

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Use of Graphene for the Reinforcement of Metal-based Materials Composites – MMCs

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The use of nanofillers derived from carbon compounds has been an increasingly explored alternative for the reinforcement of metal alloys, mainly those developed from powder compounds. Among these nanofillers, Graphene has been highlighted by its remarkable properties of yield strength, Young Modulus, thermal conductivity, high surface area, that justify its use in several metallic composites (Metal-based Materials Composites – MMCs).[1,2] Based on such properties, Graphene's use has been evaluated in combination with different metals in the most diverse applications as automotive parts, aerospace industry, electronic devices, equipment for energy conversion and storage, sensors and biosensors, and others [2,3]. Considering the growing interest in the application of this nano reinforcement, the present paper brings an overview of the current status of these composites, highlighting the most recent developments, methods of dispersion, characterization analyses, the most recurring applications and the main challenges for their dissemination in powder metallurgy.

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Validation of Digital Image Correlation Analysis Applied in Miniature Tensile Specimens

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While the tensile test is crucial for characterizing the fundamental mechanical properties of a material, some circumstances, such as insufficient inputs or the need to sample machines in service, may make it impossible to produce test specimens standardized by conventional standards. Therefore, miniaturized specimen testing is a viable alternative in these situations [1-3]. This study aimed to validate the miniaturized tensile test, applied in conjunction with the Digital Image Correlation technique, by studying the behavior of a 316L stainless steel sample produced by Wire Arc Additive Manufacturing, allowing the analysis of the deformation distribution of the specimen as well as defining the inherent anisotropic properties of this manufacturing process explored in the longitudinal, transversal and diagonal directions. Using the technique, it was possible to validate the application of digital image correlation on miniaturized samples and verify the mechanical behavior in more detail, allowing its correlation with the microstructure of the material.

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FM02-Design of 3D structural functional materials: synthesis, processing, properties, and applications

3D printing of functional composites for energy, automotive, aerospace and biomedical applications

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Additive manufacturing opened a new world of possibilities for the industry. The combination of the versatility of 3D printing techniques with specially designed functional materials allows to find new solutions for technological challenges in a wide range of fields. In this work, we present recent developments in the production and application of functional (nano)composite 3D printing filaments composed of engineering thermoplastics, nanoparticles and other fillers, including graphene, carbon nanotubes, carbon fibers, bioglass, among others. In particular, we have focused on specific properties, such as electrical conductivity and biocompatibility, combined with the improvement of mechanical properties. Functional nanocomposites were obtained via twin screw extrusion and other related polymer processing techniques, and 3D printing filaments were then produced. The rheological, mechanical and functional properties of these materials were tested, as well as their printability. The resulting composites were then explored for different applications, including special uses for the automotive and aerospace industries, including their use in fuel cells and other energy-related applications. Another set of materials were studied for use in implants and related biomedical applications.

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Bioprinted Conductive Biomaterials for Cardiac Bioengineering

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Cardiovascular diseases are the leading cause of death, and there is a need for new treatments. The scarcity of heart donors and the difficulty of cardiomyocyte (CM) regeneration present challenges. Tissue Engineering (TE) offers potential solutions, with 3D bioprinting emerging as a promising approach. One of the major hurdles in cardiac TE is the low maturation of CM [1]. To address this, materials with electrical conductivity have been incorporated into hydrogels to create a conducive environment for CM [2]. In this study, natural biopolymers were used, either with carbon nanotubes (CNTs) or MXenes. These served as carriers for CM as bioinks for extrusion-based bioprinting. The constructs were then subjected to electrical stimulation. Preliminary tests were conducted to measure conductivity, rheological properties, and printability before cell culture. Then, cell viability and metabolic activity were assessed. The results indicated that CNTs and MXenes enhanced CM metabolic activity without compromising cell viability. However, 3D bioprinted CM did not display clear signs of maturity, remaining round-shaped within the hydrogel matrix without spreading. Nevertheless, when these bioprinted constructs were electrically stimulated, those containing conductive materials demonstrated increased metabolic activity. Incorporating CNTs and MXenes into biomimetic hydrogels could enhance the maturation of CM. This is achieved by improving the physical properties of these biomaterials and facilitating electrical stimulation, thereby promoting CM activity.

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3D graphene-based hydrogel as a binding layer in o-DGT samplers

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Three-dimensional graphene-based materials (3D-rGO) have unique properties for contaminant sampling. However, to date, no studies have applied them to passive sampling of contaminants in water. A widely used type of passive sampling device is the diffusive gradient in thin films (DGT, or o-DGT when applied to organics). They use two layers superimposed on support: i) a diffusive phase, usually agarose; and ii) a binding phase, which aims to absorb and/or pre-concentrate the analyte. Usually, the binding layer has been replaced by different materials, with 3D graphene-based hydrogels being promising binding agents due to their sorptive properties previously reported. Thus, this work aimed to develop an o-DGT device with a binding layer modified with a 3D-rGO to sample atenolol in water. The synthesis of the material was carried out using an environmentally friendly and low-cost route[1]. The boundary conditions were determined by the diffusion coefficient and the influence of pH and ionic strength on the sampler's operation. Then, the sampler was applied to a tap water sample. The device calibration results showed that the sampler was able to absorb atenolol linearly with time. The pH did not influence the functioning of the device, but the ionic strength influenced the elution in the sampling stage. This interference can be overcome by adjusting the ionic strength in the binding layer before assembling the sampler. In the real sample, the device performed well, with 92% atenolol recovery. The results obtained were promising and the unprecedented use of 3D-rGO in o-DGT samplers proved to be favorable, especially considering that it is obtained in an environmentally friendly way that consolidates its environmental application, making it ideal for this purpose.

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3D printing of monolithic titania pieces using Pechini resin as organic and inorganic binder

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Additive manufacturing (AM) is relatively new method of fabrication that enables new applications and developments which were harder to achieve through the traditional manufacturing processes. The main challenge for the AM of ceramics resides on the high temperatures needed to melt those materials. Therefore, the extrusion method, called Direct Ink Writing (DIW), has emerged as one of the primary techniques for ceramic AM. The formulation of the ceramic paste for DIW is one of the central aspects of research for this technic [1]. Ceramics can be obtained by polymeric precursor, which consist in the synthesis of a resin with cations on its chains, allowing a great stoichiometric control [2]. Thus, the use of Pechini resin with titanium cations can behave as an organic binder, adjusting the rheology of the ceramic paste, and subsequently as an inorganic binder after heat treatment when combined with P25. The nano titania, which is formed from the resin, has a high surface energy, allowing its sintering at lowers temperatures, aiding in the consolidation of the structure [3]. Samples were printed and heat treated at 350°C. The characterizations through plates rheometer, BET, XRD and SEM indicate the interaction between the P25 and the titania from the resin. The paste present pseudoplastic and thixotropic. BET results show a slight change on the surface area of the material after heat treatment, while the XRD display a noticeable increase of the rutile crystallite without a significant change on phases proportions. The detailed results are still being worked on and will be shared and discussed at the conference.

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Accessing Open Metal Sites and Exploring the Photophysical Properties of a Family of Rare-Earth Cluster-Based Metal-Organic Frameworks

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Nearly thirty years after the first use of the name metal–organic framework (MOF), this class of materials is receiving more attention than ever, being considered by many as the future of materials science. These distinguished materials are composed of metal ions or clusters bonded by organic linkers, giving rise to three-dimensional network structures. Because of their very interesting characteristics, which often include extensive porosity, crystallinity, and structural tunability through controlling the metal and the organic linker building units, more than 100,000 different MOFs have so far been reported. Nevertheless, the research regarding this class of materials is still relatively young. In recent years, MOFs have been studied for a large number of applications including gas storage, drug delivery, chemical separations, light-harvesting and energy conversion, catalysis, sensing, and adsorption.

Due to the special characteristics of rare-earth (RE) elements, which include scandium, yttrium, and the whole series of lanthanoids, promising new RE-based MOFs have been obtained in the past years. Among these characteristics, it is worth mentioning the high coordination numbers and distinct optical properties of RE ions, which can lead to the generation of materials with interesting photophysical and photochemical properties and unique crystalline structures.

In this work, a series of RE-MOFs based on the archetypical zirconium MOF-808 were obtained through a *de novo* synthetic approach. A series of studies were carried out in order to optimize the synthetic conditions, focusing on a balance between high purity, yield, and suitable crystallite sizes. The final materials are fully characterized by PXRD, SCXRD, N2 sorption, TGA, DRIFTS, SEM, ICP-MS, NMR, and studied regarding their photophysical properties through DR-UV-vis and photoluminescence spectroscopy.

Adapting the Metallurgical Industry to Advanced Foundry Sand Mold Manufacturing

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Binder jetting is an additive manufacturing process (3D printing) that enables the production of casting molds and cores from a digital model, typically stored as an STL file. In this method, intricate geometries are achieved by precisely binding sand particles through controlled application of a Binder (typically furanic or phenolic resin) onto the desired geometry, consolidating the sand particles with micrometric precision. The process is executed layer by layer until the final part, matching the CAD model, is fully realized.

In traditional foundry practices, silica sands are commonly used in mold and core manufacturing without controlled particle and shape. However, in the realm of binder jetting, the specific characteristics of the raw material become crucial, impacting various aspects such as layer deposition accuracy, geometric resolution, mold surface finish, and the interaction between sand particles and the binder.

In Brazil, the adoption of binder jetting for sand mold production signifies a significant leap forward, fostering innovation and enhancing competitiveness within the domestic metallurgical sector by harnessing local resources effectively. This research project aims to comprehensively assess various parameters, including mechanical strength, apparent density, deformation characteristics under elevated temperatures, layer-by-layer filling quality, and adherence to the CAD model specifications. The evaluation encompasses molds manufactured through both conventional methods and additive manufacturing processes, utilizing three distinct types of silica sand with varying particle s, along with two commonly employed resins in foundry operations: furanic and phenolic.

Additive manufacturing of the multi-material consisting of metallic glass and titanium alloy

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Multi-material additive manufacturing (AM) possess enormous potential to extend the design space beyond complex geometries. In particular, the ability to manufacture parts from multiple materials using AM technologies enables optimization of the mechanical properties of the parts or/and to provide additional functions for the final parts. Different materials combinations, including materials from different classes (e.g., metal-polymer, ceramic-metal, etc.) and various AM technologies, have already been explored to create customized multi-functional objects to suit many needs.

In this study, a multi-material composed of a CuZr-based metallic glass and conventional titanium alloy was synthed by laser powder bed fusion (LPBF). Metallic glasses (MG) are amorphous materials characterised by glass transition. These feature outstanding strength but extremely limited tensile plasticity. Commercial titanium-based alloys are typically very tough and can affectively arrest crack propagation. At the interface of this multi-material two materials mix forming new phases affecting the performance of the multi-material. The interface of the multi-material has been studied in details. The resulting bimetallic composite can be used as a promising material for various applications requiring high strength and toughness along with an excellent corrosion resistance.

analysis of the electronic properties of n-acetyl-d-glucosamine via dft

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N-acetyl-d-glucosamine (NGD) is a basic monomer found in glycoproteins and chitosan. This molecule has several specific biological activities and plays an important role in the structural regulation of animal tissues, as well as being widely used in various industries, such as pharmaceutical, biomedical and chemical [1,2]. However, its electronic properties, which make it bioactive, are still not fully understood. In this work, we have characterized the charge distribution and electronic density of NDG. The initial coordinates of the molecule were obtained from the Pubchem database, under ID 439174, and optimized using the Density Functional Theory (DFT) method for 3D geometry. The calculations were carried out using a hybrid functional (B3LYP), base def2-TZVPP and auxiliary base def2/J. An energy of -819.86 Eh, HOMO -7.39 eV, LUMO -0.05 eV and band gap of 7.34 eV were observed, with regions of zero electronic density in the LUMO. NGD has an asymmetric charge distribution, presenting a large dipole moment (5.18098 Debye), which may be one of the factors behind the bioactivity of this molecule. Further studies need to be carried out to predict the regions in which the monomer can undergo nucleophilic, electrophilic and radical attacks.

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Antimicrobial and Rheological properties of photopolymerizable resin modified with Graphene Oxide

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Polymers, such as components of photopolymerizable resins, have biocompatible characteristics and are widely used in the biomedical field, mostly originating from renewable and biodegradable sources [1]. Graphene oxide (GO) is the oxidized form of graphene, which has carboxylic, carbonyl, and hydroxyl groups in its structure, facilitating interactions with biomolecules and inducing bacterial death without an intracellular process [2]. The insertion of nanostructures into polymers offers the possibility of new properties and can enhance the potential applications of the material in the biomedical field [3].This work proposes the functionalization of a commercial photopolymerizable resin compatible with SLA printing with GO to create an antimicrobial surface for new implantable devices created by 3D printing. The work involves prototype design using Fusion 360 software for an auricular device for stenosis treatment, GO synthesis by the modified Hummers-Hoffman method, and analysis of GO's influence on the rheology and thermal properties of the resin. The GO sheets were analyzed by scanning electron microscopy, transmission electron microscopy (TEM), Raman spectroscopy, dynamic light scattering (DLS), and Zeta potential, showing a size around 2.0 µm and negative charge due to the presence of functional groups. The comparison of the resin alteration with and without GO addition is mainly conducted through rheology and differential scanning calorimetry (DSC) techniques. The antimicrobial activity of GO and resin/GO is being tested against gram-negative bacteria (Escherichia coli).

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Biological scaffolds fabricated via two-photon polymerization to evaluate the bacterial cellulose growth

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Biomimetic systems with miniaturized dimensions have been employed in several experiments, achieving fast results and with great accuracy, similar to analyses performed in macroscopic environments. Microenvironments require specific architectures that can be reached using laser micromachining techniques, such as two-photon polymerization (TPP) [1]. This technique has many advantages, allowing the production of environments with specific features and without shape limitation. In this work, aided by the TPP technique, we produce different arrays of microstructures, fabricated using acrylate-based materials, in order to evaluate the growth and development of the *Komagataeibacter xylinus* bacteria, the micro-organism responsible for producing bacterial cellulose (BC), a natural polymer with several biological applications. As result [2], we obtained films with different thickness, depending how long the bacteria were inoculate on the platforms. All formed biofilms were characterized morphologically and structurally by scanning electron microscopy, infrared spectroscopy and Raman spectroscopy. BC grown in microenvironments presents similar features to those of biofilm formed in macroenvironments, maintaining their attractive properties. Using BC as a flexible substrate in TPP experiments, the natural polymer did not change by laser irradiation, maintaining its original features until the end of the photopolymerization process.

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Biophysical characterization of 3D printed silver-doped α-TCP scaffolds for bone repair

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The possibility of nosocomial microbial infections, which can result in several difficulties and severe health hazards for the patient, especially from antibiotic-resistant strains, is one of the main risks connected with orthopedic implant surgery. Bone grafting has recently become a viable option for replacing and mending broken bones, and 3D printing makes it possible to customize the procedure to each patient's unique requirements. For this purpose, the current study attempts to create a self-setting ink made of AgPμ microparticles-loaded alpha tripolyphosphate (α-TCP), which will give the antibacterial activity of the 3D-printed matrix. Scanning electron microscopy (SEM), Fourier transform infrared (FTIR) spectroscopy, X-ray powder diffraction (XRPD), and differential scanning calorimetry (DSC) are used in the biophysical characterization of α-TCP scaffolds. α-TCP-AgPμ's antibacterial efficacy is assessed against Gram-positive Staphylococcus aureus and Gram-negative Escherichia coli. 3D printed AgPμ-containing α-TCP scaffolds show strong antibacterial activity against both bacteria.

Development of Vascular Devices in 3D Printing: Driving Innovation in the Medical Field

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3D printing has emerged as a technology with the potential to create complex and customized structures for medical devices, matching design criteria related to precision and processing speed.[1] In the context of vascular diseases, personalized manufacturing plays a crucial role, as long as the anatomical particularities of each patient are considered for prostheses used in arteries, veins or even the heart. 3D printing involves layer-by-layer deposition of material to create three dimensional structures. This approach allows for precise customization and efficient manufacturing of vascular prostheses. However, challenges related the biocompatibility, durability, functionality, and structural conformity of medical devices are latent. This study is ongoing, and the experimental phase involves the production of vascular tubes using commercial polymers tritan, nylon, ABS, TPU flex, and PLA. The choice of these materials was based on properties such as biocompatibility, mechanical, chemical, and thermal resistance, easy processing, flexibility, high transparency, low cost, and adaptation to different anatomies. The initial vascular tubes showed a need for improvement in internal dimension, as well as printing parameters to ensure dimensional accuracy and surface quality, to ensure adequate blood flow and reduce the risk of thrombosis. This work will advance to more complex devices, such as grafts for lower limb revascularization and vascular bifurcations for aneurysms and peripheral arterial diseases. Therefore, studies like these are important to understand the interaction in the environment and the durability of other types of prostheses when integrated into the circulatory system [2]. The main expected contributions include enabling cost reduction for Brazil's single healthcare system and reducing hospital readmissions for the treatment of patients affected by vascular diseases. References: [1] DATTA, Sudipto; BARUA, Ranjit (2024), [2] Mirzababaei et al.(2024).

Effects of the formation of 1-D and 3-D ZnO/NiO heterostructure on the selectivity towards toxic gases

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The detection of toxic gases has become increasingly important in the last decades, as the rapid industrialization of the modern world poses a threat to human and environmental health. Among gas sensing materials, semiconductor metallic oxides (SMO) have emerged as promising gas sensors due to their exceptional physical and chemical properties. Particularly, ZnO (n-type) stands out amongst SMOs because it presents high electron mobility, high thermal and chemical stability, and can be synthesized in different morphologies, including 1-D and 3-D particles. However, ZnO presents limitations concerning selectivity, which can be improved by associating ZnO with other SMOs, forming a heterojunction. 1-D NiO (p-type) has been reported to enhance selectivity and sensor response when combined with ZnO. In the present study, 1-D ZnO rods (R) and 3-D ZnO hollow spheres (HE) were synthesized via the precipitation method and were combined with 1-D NiO in a hydrothermal reaction, forming an n-p heterojunction. The gas sensing properties of 1-D and 3-D ZnO and heterostructured 1-D and 3-D ZnO/NiO samples were evaluated when exposed to O3, NO2, NH3 and CO gases. Both 1-D ZnO and 3-D ZnO samples did not exhibit selectivity towards any of the studied gases. On the other hand, 1-D and 3-D heterostructured ZnO/NiO samples showed an improvement in the selectivity towards oxidizing gases. The 3-D HE-ZnO/NiO sample presented a better selectivity towards NO2 gas, albeit with a lower sensor response compared to 3-D HE-ZnO. This better selectivity was attributed to a p-type response due to the bending of the valence band on the material's surface. Therefore, the association of 3-D ZnO and 1-D NiO has improved the overall selectivity of the evaluated sensors.

exploratory analysis of vibrational and electronic properties of the alliin molecule via dft

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Alliin is the main chemical constituent of garlic, compartmentalized in mesophyllc cells [1]. It is part of a set of organosulfur compounds that have several bioactive properties to be explored, including potential antifungal, anticancer, antithrombotic, antiviral and antioxidant activities [2]. This research aims to analyze vibrational and electronic properties through Density Functional Theory (DFT). The initial coordinates of the molecule were obtained from the Pubchem database, under CID 9576089, and optimized the 3D geometry using the DFT method. Calculations were performed using a hybrid functional (B3LYP), def2-TZVPP base and def2/J as auxiliary base. No negative frequencies were observed. Total energy of -913.724 Eh and Gibbs energy of -913.59433881 Eh were observed. The calculated molecular orbitals showed the values HOMO -6.349 eV, HOMO (-1) -7.154 eV and HOMO (-2) -7.284 eV, LUMO -0.596 eV, LUMO (+1) -0.328 eV and LUMO (+2) - 0.312 eV, with a 5.753 eV band gap. Pronounced absorption peaks were observed at 3073, 1800 and 1145 cm^{-1} in infrared exposure, associated mainly with the carboxyl and sulfoxide groups [3]. Furthermore, it is necessary to compare this spectrum with experimental data, because harmonic vibrations were considered. It was possible to identify a region with low electron density in this conformer. Our initial analysis suggests the presence of sites favorable for chemical reactivity, yet further calculations are required to ascertain the types of electrophilic, nucleophilic, and/or radical attacks to which allicin may be susceptible.

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From Detoxifying Chemical Warfare Agents to Treating Nuclear Wastewater: Adventures in the Synthesis of Metal-Organic Frameworks

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Metal–organic frameworks (MOFs) are structurally diverse, porous materials comprised of metal nodes bridged by organic linkers. These scaffolding-like structures can be thought of as atomically precise molecular sponges. Through careful choice of nodes and linkers to build the scaffold, the chemical and physical properties of MOFs can be elegantly tuned and materials with high surface area and porosity can be obtained. As a consequence, MOFs have been explored for many potential applications including, but not limited to, gas storage and release, chemical separations, catalysis, drug delivery, light harvesting and energy conversion, and the detoxification of hazardous analytes. In addition to these promising potential applications, MOFs offer an interesting platform for studying fundamental concepts in inorganic materials chemistry. In the Howarth group at Concordia University, we are particularly interested in the study of MOFs comprised of metal cluster-based nodes, in part, because of the high and variable coordination chemistry and connectivity of metal clusters, which allows several unique and intricate MOF topologies to be designed and synthed. In this presentation, zirconium and rare-earth cluster-based MOFs are explored from design and synthesis to potential applications in the detoxification of chemical warfare agents and nuclear wastewater treatment.

Microstructural and Mechanical Characterization of the AA2017 Alloy Produced by Laser Powder Bed Fusion with the Addition of TiC Nanoparticles

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The application of Laser Powder Bed Fusion (L-PBF) for processing Al-Cu alloys presents a notable challenge because of their extensive solidification interval, often resulting in hot cracks in the as-built sample. Aiming to avoid this problem, the objective of this work was to process the AA2017 alloy, which is the oldest and best known alloy of the Al-Cu system, by L-PBF with the addition of 1 wt.%, 2 wt.%, and 4 wt.% of TiC nanoparticles, which acts as heterogeneous nucleation sites during the solidification. Optical microscopy, scanning electron microscopy, and electron backscatter diffraction showed a microstructure of the AA2017 alloy characterized by the typical α-Al columnar grains along the building direction and Al_2Cu precipitate. The addition of TiC nanoparticles and the increase in its concentration led to a refinement of the microstructure and an increase in ultimate tensile strength (UTS) and elongation at fracture. The grain measured by optical microscopy gradually decreased from 64±27 µm in the as-built AA2017 alloy to 17.3±6.8 µm, 3.1±1.2 µm, 2.6±0.5 µm with 1, 2, and 4 wt.% of TiC nanoparticles, respectively. The UTS and elongation at fracture obtained by tensile tests increased from 314±47 MPa and 8±6% in the as-built AA2017 alloy to 346±13 MPa and 10±2%, 366±13 MPa and 14±5%, and 355±13 MPa and 9±2% with 1, 2, and 4 wt.% of TiC nanoparticles, respectively. X-ray diffraction and transmission electron microscopy were used to complement the characterization of the microstructure.

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Polyamide-6 nanocomposites reinforced with lignin nanocarbon: effect of the PP-g-MA/polypropylene as a compatibilizer

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Nanocomposites based on polyamide-6 (PA-6) reinforced with carbon nanofillers have been the subject of intense research due to their special characteristics, offering significant industrial applicability across various sectors including civil construction and automotive industries. Studies focusing on these nanocomposites, typically aim to enhance their mechanical and thermal properties. Rocha et al. [1] has developed a new nanocarbon material from lignin, similar to graphene nanoplatelets named as "lignin nanocarbon" (LNC). The aim of this study was to manufacture an alternative PA-6 3D-quaternary nanocomposite, using a 2D material as a filler, changing the LNC content from 1 to 3 wt.% into PA-6 polymer matrix. Results from prior investigations indicated a slight increase in Young's modulus with the incorporation of LNC filler, but no improvement at the tensile strength was observed with the addition of LNC by itself. Therefore, we included maleic anhydride-grafted polypropylene (PP-g-MA), as a compatibilizer, and polypropylene (PP) homopolymer as an interfacial polymer, at the PA-6/LNC formulations, aiming the enhancement of the interaction between different phases, favoring the tensile transference from the matrix to the filler at the interface region [2]. The extrusion of the PA-6/PP/PP-g-MA/LNC masterbatches were performed using (25.5 wt.% of PP, 5.0 wt.% of PP-g-MA, 59.5 wt.% of PA-6 and 10.0 wt.% of LNC) and shows good processability were the specific mechanical energy (SME) during the processing was 80 J with PA-6 and 15 J with the PA-6/PP/PP-g-MA/LNC. The decrease of the SME when the compatibilizer was incorporated into the nanocomposite formulation, probably occurs due to the decrease of the viscosity of the molten polymer provided by the compatibilizer diffusion.

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SILOXANE-POLYETHER NANOCOMPOSITES WITH IRON OXIDE NANOPARTICLES FOR FUTURE APPLICATIONS AS MAGNETO-RESPONSIVE DRUG DELIVERY SYSTEMS

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In this work hybrid Siloxane-Polieter nanocomposites containing iron oxide nanoparticles functionalized with organic groups to acquire an hydrophilic or hydrophobic character were synthed. Transmission Electron Microscopy (TEM) and Dynamic Light Scattering (DLS) analyses revealed monodispersed and spherically shaped nanoparticles, with 9.71 ± 1.88 nm (hydrophobic NP) and 5.49 ± 0.80 nm (hydrophilic NP) hydrodynamic radius, suitable for magnetic hyperthermia application. X-ray diffraction (XRD) revealed the spinel structure of maghemite or magnetite, consistent with results from Vibrating Sample Magnetometry (VSM), which demonstrated the superparamagnetic behavior of the particles. The structure and properties of the particles were preserved in the nanocomposites whereas Small-Angle X-ray scattering (SAXS) measurements evidenced the three-dimensional structure of the hybrids, consisting of a network formed by polymer chains crosslinked by siloxane nanoparticles, in which the iron oxide particles are dispersed. Upcoming research will assess the thermal properties, hyperthermic response and cytotoxicity of the hybrids for exploiting the magnetic hyperthermia effect for future controlled and localized drug release applications.

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Synthesis and application of Metal-Organic Frameworks to promote photopolymerization reactions

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Metal-Organic Frameworks (MOFs) are a class of highly porous crystalline materials and consist of a coordination compound between a metal ion and an organic ligand, presenting a 3D structure. They are a growing class of materials that have been studied over the past years due to their remarkable characteristics and varied applications [1]. This work studied the application of MOFs, with a quinoline derivative as the ligand and different metal ions, as a photoinitiator to promote the photopolymerization reaction of UDMA, considering the structural characteristics of the material, such as its high crystallinity, which can be passed on to the polymer, generating more resistant materials [1]. The choice to use a quinoline derivative comes from previous studies in our research group on the use of these compounds as photoinitiators, where good results were obtained [2]. The photopolymerization reaction is an advantageous method for obtaining polymers due to its short reaction time, lower energy consumption, dispensability in the use of toxic organic solvents, etc. [3]. Therefore, the objective of this work is to apply the results to the improvement of dental resins and for 3D printing.

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Synthesis, characterization and application of quinoline derivatives as photoinitiators in photopolymerization reactions for application in 3D printing

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In this work we related ours results about the synthesis, characterization and application of new quinoline derivative for actuation as Type II photoinitiator in the photopolymerization reaction of the urethane dimethacrylate (UDMA) [1], widely used in resin formulations for dental restoration and 3D printing.[2] The quinoline derivative (1) was obtained in three reaction steps with good yield, starting by the multicomponent reaction among 4-nitroaniline, 4-methylthiobenzaldehyde and phenylacetylene, followed by reduction of nitro group (Quinoline derivate 2) and methacrylation of amino group (Quinoline derivate 3). Analysis of the photolysis of the three quinoline derivatives shows that the formation of reactive species occurs within the first second of exposure to light, providing clear evidence of the photosensitivity of these molecules. All synthetized quinoline derivatives were tested as photoinitiators in the UDMA photopolymerization reaction using a lamp under 420 nm irradiation, and the polymers were obtained with a conversion rate of up to 77% in approximately 30 seconds [2], these results present a higher degree of conversion than that presented by camphorquinone, a commercial photoinitiator. It is worth mentioning that all polymers obtained have fluorescent characteristics, factor that may be relevant for applications such as the dental field and 3D printing. [3]

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Theoretical analysis of the vibrational and electronic properties of allicin: study of chemical reactivity via dft

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Allicin is an organosulfur compound that is considered one of the main responsible for the biological properties of garlic. It has been widely studied due to its diverse pharmacological properties and potential beneficial effects in the prevention of cardiovascular diseases [1], certain types of cancer [2] and anti-pathogenic activity against fungi and bacteria. However, the mechanisms of interaction with biological systems are not yet completely understood, requiring studies at the molecular level. This work aims to analyze the vibrational and electronic properties of allicin, to evaluate its chemical reactivity sites. The study was carried out using Density Functional Theory (DFT), using the ORCA software. The initial 3-D geometry of the allicin was obtained on the PubChem platform, under ID 65036. The molecule was optimized and calculations were performed using a hybrid functional (B3LYP), def2-TZVPP basis and def2/J auxiliary base. The total energy of the molecule was calculated as -2209.46 Eh, while the Gibbs energy was determined to be -1105.94 Eh. The energies for the HOMO and LUMO molecular orbitals were respectively -6.3259 eV and -1.0056 eV, observing a band gap energy of 5.3203 eV. The value of the magnitude of the dipole moment found was 2.6719 Debye, indicating a polar characteristic and asymmetric distribution of charges in the molecule. Absorption peaks were observed at 1210 cm^{-1}, 1085 cm^{-1}, 931 cm^{-1}. The first two peaks are associated with stretching vibrations of the double bond between sulfur and oxygen. The last peak is associated with deformation vibrations of double bonds between carbons. In summary, our study provides insights crucial for understanding allicin pharmacological effects and applications.

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theoretical study of ajoene's chemical reactivity via dft

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Garlic is widely recognized for its medicinal properties and the variety of health benefits attributed to its organosulfur compounds, which include anticancer, antithrombotic, antiviral, and antioxidant activities [1]. Among these compounds, ajoene (C9H14OS3) stands out for its stability and biological activity [2]. However, the interaction mechanisms between this molecule and biological systems are not yet fully understood. In this work, the vibrational and electronic properties of the 3D structure of ajoene are studied using Density Functional Theory (DFT). Molecular coordinates were obtained from the PubChem database, CID 5386591, and optimized via DFT. The calculations were performed using the B3LYP functional, the def2-TZVPP basis set, and the auxiliary basis set def2/J. No negative frequencies were observed. In energy calculations, the total system energy was observed to be -1620.885 Eh, Gibbs free energy -1620.723 Eh, HOMO -6.216 eV, LUMO -1.260 eV, and a band gap of 4.956 eV. In vibrational frequencies, predominant absorption peaks were observed at 1112.28 cm-1, 984.2 cm-1, and 962.76 cm-1. Furthermore, adjustments to the absorption spectrum and comparison with experimental data are necessary, because harmonic vibrations were considered. Through analysis of the HOMO, an asymmetric distribution of charges in the molecule was identified. Initial analyses indicate the presence of sites favorable for chemical reactivity. Further calculations are needed to determine whether the molecule is susceptible to electrophilic, nucleophilic, and radical attacks.

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Three-point bending tests of single hygroscopic nanofibers and emergent mechanical properties on scaffolds.

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In this work we will study interaction of water molecules with polymeric nanofibers made from hygroscopic polymers and contrast them with the electrospun scaffold.
For this, we will suspend single nanofibers over micropatterns etched on silicon. In this suspended configuration, we shall perform three-point bending tests utilizing the environmental Atomic Force Microscope (AFM) and detect bending forces of the nanofiber [1]. Bending forces will be taken at different relative humidities to quantify the effect of water on nanofibers.
In the same line, we should study bending forces of the scaffold (deposited in a silicon wafer) under variable humidities, to accomplish this the environmental AFM will be used, replacing the standard tip with a colloidal probe setting, letting us measure the effect of multiple nanofibers at once and their joint answer to mechanical stress and different humidities. Finally comparing the properties of a single nanofiber and a 3D scaffold.

Tunning the rheology of cellulose functional inks

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The rapid development of flexible electronics has achieved versatile smart platforms well suited for day life applications such as lifestyle, sports, medical-health care, defense, human-machine interface units, among others. However, the main challenges for the next-generation wearables electronics refers to portability, flexibility, biocompatibility, plus reducing the cost and environmental impact. Since nonrecyclable plastic-based are widely used on smart flexible electronics, there is a need to find green and sustainable solutions, without affecting the technological development, while promoting a circular economy model. With that aim, natural biopolymers, such as cellulose have been studied for application in a variety of flexible devices (e.g., flexible sensors and portable energy storage systems). Cellulose is a promising candidate, due to its recyclable and biodegradable nature, it is the most abundant natural biopolymer, unique chemical structure, flexibility, ease to process, mechanical strength, among other properties, which make the cellulose a material that can be applied to the circular economy model. In this sense, different cellulose-based inks were formulated with a conducting polymer, polypyrolle, and rheological fundamental studies were conducted with the aim to tune the viscoelastic properties for appropriate direct ink writing (DIW), an extrusion-based 3D printing technology.

3D printed graphene-based PEEK composites

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Polyetheretherketone (PEEK) is a high-performance thermoplastic polymer employed in aeronautics, biomedicine, and aerospace, due to its excellent mechanical properties, dimensional and thermal stability, as well as its biocompatibility [1]. In 3D printing, PEEK is employed for structural applications, allowing the development of components in complex and detailed geometries [2]. However, implementing PEEK for 3D printing faces challenges, as printed filaments do not possess the original tensile strength and rigidity of the polymer. To mitigate the loads in mechanical properties, nanoparticles can be incorporated into the polymer matrix. Particularly, graphene proves to be attractive for such an application. The addition of graphene, a high-rigidity nanomaterial, allows for the enhancement of PEEK's mechanical properties [3], making the composites suitable for filament manufacturing. Thus, this study aims to evaluate the influence of graphene incorporation at different concentrations from 1% to 5% in the PEEK polymer matrix. The morphology and distribution of graphene structures were visualized by SEM while the chemical structure was assessed by FTIR. Thermal events and degradation profiles were investigated by DSC and TGA.

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3D-printed graphene/polylactic acid electrode for electrochemical determination of venlafaxine

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3D printing technology is attractive, once that enable the manufacturing of electrodes on a large scale at a low relative cost [1]. In this work, 3D printed-electrode based on graphene and polylactic acid (GR-PLA) was built for determination of the antidepressant venlafaxine (VEN), a antidepressant classfied as concern emerging contaminant (CEC). The printing of GR-PLA electrode was carried out with GR-PLA conductive filament, using an Ender-3, Creality FDM 3D printer with a extruder nozzle at 210ºC and a bed temperature of 70ºC, in vertical orientation, with a printing speed of 30 mm s^{-1}. Previously to analysis, the GR-PLA was polished, following of a cleaning by sonication in ethanol/water 50:50 (v/v) for 8 minutes. Next, the electrode was immerged in NaOH 1.0 mol L^{-1} solution for 30 minutes. Finally, GR-PLA was subjected to electrochemical pretreatment, using amperometry, applying a potential of 1.8 V for 900 s, following of cyclic voltammetry under a potential range of 0.0 to -1.8V. Electrochemical behavior of VEN was evaluated using linear voltametry. Voltamogramms were obtained with 3.0 mmol L^{-1} VEN in BR buffer 0.04 mol L^{-1} pH 7,0 solution in a range of 1.0 to 1.8V, being possible to observe two anodic peaks around 1.0V (I_p = 2.895 µA) and 1.3V (I_p = 0.664 µA). Electrochemical studies were performed using batch injection analysis system with amperometric detection (BIA-AD). The amperogram was obtained with 200 µmol L-1 VEN in BR buffer 0.04 mol L^{-1} pH 7,0 solution, applying a potential of 1.3V, in which were presented current value of 28.268 ± 0.815 µA. It was possible to observe a high current value for oxidation of VEN using the GR-PLA coupled to BIA-AD, compared to studies in linear voltammetry, indicating the development of sensitive analytical method.

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3D-Printing of 45S5 Bioglass® PEEK Composites

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Polyetheretherketone (PEEK) is a high-performance thermoplastic polymer employed in biomedicine due to its excellent mechanical properties, dimensional and thermal stability, in addition to similar properties compared to natural bone tissues, high radiographic penetrability, as well as its biocompatibility [1]. However, bionertia makes it difficult to create a good surface between the ingrowing tissues, once PEEK lacks surface roughness - causing inflammation or even implant rejection. Searching other ways than superficial treatment to boost desired properties, one of the best solutions is to combine the polymer matrix with a ceramic - in this case, Bioglass 45S5 (BG) - due to osteoconductive, anti-bacterial, anti-inflammatory and potential angiogenic properties [3]. Beyond that point, the added load of BG increases the bioactivity, stimulating cellular process [2]. In this study, different compositions of PEEK-BG composites were obtained via twin screw extrusion, and filaments for 3D printing were produced. Test specimens were 3D printed for chemical and mechanical testing. Preliminary bioactivity tests were also carried out.

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3D printing of a new biomaterial scaffold developed from a marine compound: biological evaluation in vitro and in vivo

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Tissue engineering offers promising solutions to deal with the increasing prevalence of bone fractures and their treatment complexities [1]. The rich biodiversity of marine ecosystems provides an abundance of bioactive compounds conducive to the development of biotechnological products. This work aimed to develop and characterize scaffolds via 3D printing of a biomaterial of marine origin (Biomaterial M - BM), evaluating its biological effects in vitro and in vivo in comparison with the generic Bioglass® 45S5 (Traditional Biomaterial - BT). Scanning electron microscopy revealed a rough surface morphology for both groups. In the porosity analysis, BM had larger pores than BT. In the biomechanical analysis, BM showed greater resistance to compression. The pH was alkaline in both groups. The change in mass showed a gain for both groups, with a reduction over time. In vitro tests with MC3T3-E1 cells indicated cell adhesion and proliferation for both groups. The in vivo analyses, after implantation of the scaffolds in critical calvarial defects of male Wistar rats, after 15 and 45 days, showed in the histology, in all groups, the absence of inflammatory infiltrate or fibrotic tissue and increased bone formation between the periods. The histomorphometric analyses indicated greater bone volume for BM 45 days, greater volume and osteoid surface for BT 15 days and greater presence of biomaterial for BT and BM in the 15-day period. With regard to cellular parameters, there was a greater osteoblastic surface for BT 15 days, a greater number of osteoblasts for all groups in the 15-day period and a greater osteoclastic surface for BT 15 days. These findings indicate that BM is promising in terms of mechanical resistance and pre-clinical osteogenic potential.

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3D Printing of Biomimetic Functional Nanocomposites based on dimethacrylated PCL and ZnO nanoparticles via Vat Photopolymerization for Tissue Engineering Scaffolds

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Biomimetic design and manufacturing have long garnered extensive attention in the biomedical field. However, progress has been hindered by the limitations of conventional techniques to reproduce microscopically complex structures and the lack of functional materials [1]. This study aims to develop photopolymerizable nanocomposites based on dimethacrylated Polycaprolactone (PCLDMA) and Zinc Oxide nanoparticles (ZnO-NPs) to produce tissue engineering scaffolds via vat photopolymerization 3D printing. PCLDMA synthesis involved the functionalizing PCLdiol with methacrylate groups, while ZnO-NPs were synthed using the Pechini method and further functionalized with 3-aminopropyltrimethoxysilane (APTES) to enhance nanoparticles dispersion and interaction within the polymer matrix. Moreover, the ZnO-NPs act as additives substituting photoabsorbers to control overexposure that causes loss in dimensional accuracy. The influence of ZnO-NPs addition was evaluated by developing nanocomposites with different concentrations of modified ZnO-NPs (1.0, 2.5, and 5.0 wt.%). The photopolymerizable nanocomposites were characterized using UV-vis, FTIR, DRX, and SEM, and the mechanical properties were evaluated. Scaffolds with biomimetic designs were fabricated by optimizing printing parameters, resulting in scaffolds with good dimensional accuracy reproducibility, and printability. These findings offer significant implications for the development of promising biomaterials for the creation of patient-specific scaffolds adapted to individual needs using an advanced 3D-printing technique.

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3D Printing of Hyaluronic Ácid/Pluronic And Gelatin/Pluronic Hydrogels: ZnO vs GSNO Effects on Cicatrization and Printability

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3D printing of hydrogels is a topic that has generated considerable interest due to its ability to allow controlled material deposition. Various formulations have been developed with the purpose of increasing biocompatibility and enhancing processability. Hydrogels based on Pluronic F127® have been widely used in 3D printing due to their temperature-controlled gelation capacity (reversible). This facilitates gel manipulation before printing and ensures fidelity of the deposited filament shape (but not yet crosslinked). Hyaluronic acid and gelatin have also been used in hydrogel formulations to improve biocompatibility and/or biodegradability of the produced scaffold. Other elements that have received attention are ZnO (for its antimicrobial action) and GSNO (which in this study aims to enhance healing). Here, we evaluated the performance of cellular scaffolds obtained by 3D printing, formulated with Pluronic F127, biopolymer (hyaluronic acid or gelatin), and particle (ZnO or GSNO). The biopolymers were chemically modified (addition of methacrylate groups), allowing crosslinking (via UV light) after deposition in the printer. Rheological characterization (flow curves) was performed to evaluate processability for 3D printing. Simultaneously, FTIR was performed to assess the degree of methacrylation obtained in synthesis, but there was no success in identifying the peaks of interest. It was confirmed that the modification was successfully carried out by NMR. Compression tests of printed samples were then conducted to measure the impact of UV exposure time on the mechanical strength of the gel. Finally, the cytotoxicity of the material was evaluated using fibroblasts and the impact of NO on the healing process.

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Additive manufacturing of PLA/TPU/SEP nanocomposites: Influence of mixing protocol on rheological behavior and printing quality

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In recent years, there has been a notable rise in using additive manufacturing (AM) for tissue engineering scaffolds due to the demand for precise control over materials, structures, and geometries [1]. Poly(lactic acid)/thermoplastic polyurethane (PLA/TPU) blends have great potential, as they can present a good balance of mechanical, thermal and biodegradation performance, combined with good processability and biocompatibility [2]. PLA/TPU blends are immiscible and the use of nanoparticles as compatibilizing agents and reinforcement fillers is an alternative that has been explored. In this work, the selective dispersion of sepiolite (SEP) and its effect as compatibilizing agent in PLA/TPU blends were evaluated. PLA/TPU blend (75/25 w/w) nanocomposites were obtained by 4 different routes, at a constant SEP content of 5 phr, in the molten state using an internal mixer. The mixing protocols analyzed were: i) direct mixing of all components; ii) obtaining the PLA/TPU blend and subsequent incorporation of SEP; iii) obtaining masterbatches of one of the polymeric phases with SEP and subsequent mixing with the other polymeric phase. The influence of SEP presence and dispersion on the blend was analyzed using small amplitude oscillatory shear rheology. Porous scaffolds with a cylindrical shape were fabricated using a 3D printer based on syringe pump extrusion, and their print quality was assessed via dimensional accuracy measurements and scanning electron microscopy (SEM). Overall, the presence of SEP significantly enhanced both G' and G'' in the nanocomposites, with the highest values observed for the PLA/SEP masterbatch route. All nanocomposites exhibited excellent dimensional accuracy, suggesting that SEP positively influenced printability compared to the PLA/TPU blend, regardless of the mixing protocol.

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Advancements in 3D Printing: Incorporating Coconut Fiber into Mortar

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The construction industry aims to modernize over the years, improving technologies, methods, and techniques to enhance the efficiency and productivity of the sector. A technique that exemplifies this approach is the 3D printing of mortar, which aims to make the construction field safer, cost-effective, and reduce waste [1]. The mortar, combined with the physical characteristics of coconut fiber, such as its ability to enhance flexion, deformation, and traction resistance, can render structures more resilient to dynamic loads and capable of withstanding tensile traction. The ability to control printing direction, when combined with fibers, enhances the resistance, tenacity, and integrity of printed structures [1,2]. In this context, it is crucial to comprehend the impact of the fiber on the mechanical properties of the mortar samples produced via robocasting. The products will be developed using the DIW ceramic material technique, resulting in block specimens. The printing of specimens will follow the horizontal route, adding 2.5% coconut fiber by weight of cement. The morphological characteristics of the material will be assessed using SEM and the mechanical properties of the material will be determined using three-point bending tests. In this manner, the study aims to investigate the behavior of parts manufactured through DIW concerning the incorporation of coconut fiber and its influence on the final properties of the material.

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Alternative homogeneous panels produced with corn straw and polyurethane resin derived from castor oil

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Since the beginnings of humanity, the use of wood was present in the daily lives on the most diverse communities and still plays a significant role in modern society. However, the excessive exploitation of this resource causes worrying environmental consequences due to the deforestation of native forests. The irregular deforestation has devastating impacts on the environment, including the loss of biodiversity and the release of CO2 previously sequestered by trees. Looking for an alternative to reduce the use of wood, this work proposed the utilization of corn straw – abundant agro-industrial waste in or country – for the production of medium density particleboards. Aiming at the use of these panels and their physical-mechanical properties, used as a binder the polyurethane biopolymeric resin derived from castor oil (CPUR) to 10% in relation to dry mass of corn straw. Panels with dimensions of 35x35cm were pressed with 570 N/mm² and temperature of 150ºC for a period of 6 min in tow cycles of pressing, initially 3 minutes each with interval f 30 seconds between them. The physics and mechanics property of the panels produced, were evaluated according to the parameters of the normative document ABNT NBR 14810-2[1]. The most relevant results were in relation to MOR and MOE, as can be seen, the result of MOR reached values proportional to the 30,98 MPa, while the value of MOE was in proportion to 2123,74 MPa. The results indicate that the panels produced present potential use for civil construction and furniture industry, representing an ecologically correct alternative for protecting the environment.

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Applications of electrospinning to functional polymer membranes modified with Graphene Oxide (GO)

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The electrospinning technique is capable of producing polymeric fibers of a wide range in scale - from nanoscopic (below 100nm), to mesoscopic (between 100nm and 1µm) to microscopic (1µm and above). This study will be focusing on how mesoscopic poly(ether sulfone) (PES)fibers were spun to create a polymeric membrane for use in micro- and ultra-filtration. These membranes were also modified using graphene oxide for reduction of hydrophobicity and eventual application in separation of liquids [1]. First, the polymer solution was synthed using PES and N,N dimethylformamide (DMF). During the synthesis of the polymer solution, samples contained 0.5% to 1.5% of graphene oxide based on the (wt/wt)% of the polymer in the solution. The electrospinning parameters - applied electric voltage (15 and 20kV), work distance (fixed at 10cm), polymer flow rate (fixed at 1 mL/h), speed of the dynamic collector (315 and 740 RPM) - were modified slightly on a sample-by-sample basis. The fibers were characterized using Scanning Electron Microscopy, and their contact angle with water. The results obtained revealed that the addition of GO along with the application of an electrical potential of 20 kV resulted in membranes with uniform fibers and smaller average diameters varying from 200nm to 300nm. Unmodified, pure PES membranes had an average contact angle of 84.3°. However, the addition of GO led to a reduction in the contact angle, ranging from 77.5° for a mass fraction of 0.5% of GO, to 68.6° for a mass fraction of 1.5% of GO, indicating, overall, an increase in the hydrophilic character of the membranes and a decrease in the average diameter of the fibers obtained. These results will be discussed in more detail in the presentation.

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Bioprinted Alginate/Starch/Montmorillonite Scaffolds for Bone Regeneration

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Alginate is one of the most used materials in 3D bioprinting. It is a natural and biocompatible polymer that cross-links in contact with calcium ions. However, scaffolds manufactured using inks composed only of alginate present poor cell adhesion, impaired cell proliferation, and poor mechanical strength [1]. Starch is a natural biocompatible polymer with a long history of application in bone tissue engineering [2]. Montmorillonite is nanoclay and due to its naturally large specific area, it can significantly improve the mechanical properties of scaffolds, making them interesting materials for use in bone tissue engineering [3]. In this study, solutions containing different proportions of alginate/starch with the addition of montmorillonite (Mt) were developed to produce scaffolds through extrusion bioprinting. The viscosity suitable for printing was analyzed qualitatively by turning the solutions upside down for 10 minutes. Those solutions that did not flow were considered suitable for the formation of scaffolds. To analyze the chemical interaction of the materials, films were prepared by solution casting at room temperature and subsequently analyzed by FTIR (Fourier Transform Infrared Spectroscopy). To choose the ideal cross-linking time, the films were subjected to treatment with the cross-linking agent (CaCl2) for varying durations and analyzed by FTIR. The scaffold was designed and sliced using the software BioScaffolds V2.0 and printed using a modified 3D printer provided by the company BioEdTech. The resulting scaffolds were evaluated according to their morphology and shape fidelity.

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Bromoperoxidase activity of polynuclear oxidovanadium compounds containing oxalate as ligand and DFT studies

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Abstract

Mononuclear oxidovanadium complexes have been used as functional and structural models for the active sites of vanadium-dependent haloperoxidases.[1] However, the use of polynuclear compounds remains barely explored. Herein, oxidovanadium compounds of different nuclearities, containing oxalate (ox^{2-}) as ligand, $(Et_3NH)_2[\{V^{IV}(O)(OH_2)(ox)]_2(\mu–ox)]$ (**V_2**), $(Et_3NH)_6[(V^{V}O)_2(V^{IV}O)_2(ox)_4(\mu–ox)_2(\mu–O)_2]\cdot 2H_2O$ (**V_4**) and the polyoxovanadate $(Et_3NH)_4[ox@V^{V}_{10}V^{IV}_4O_{32}(C_6H_{12}O_2)_2]$ (**ox@V_{14}**) were evaluated as mimetic of the bromoperoxidase. The cyclic structure of **V_4** is formed by two units of **V_2** and **ox@V_{14}** is an open cage mixed-valence polyoxovanadate ($4V^{IV}/10V^{V}$). The single-crystal structures showed a supramolecular 3D network formed by hydrogen bonding. The activity of the pre-catalysts at $1,0 \times 10^{-4}$ mol L^{-1} was evaluated through the oxidative bromination of phenol red to bromophenol blue at pH 5.8 at 30 ± 0.5 ºC in the presence of H_2O_2 and KBr in dmf/H_2O and dmso/H_2O (1:4). Under these conditions the **ox@V_{14}** was the most promising pre-catalyst, while **V_4** was inactive. Kinetic studies for **ox@V_{14}** in dmso/H_2O indicate a first-order dependence on vanadium content with a reaction rate constant (k) of 460 mol^{-2} L^2 s^{-1} and an activation energy (A_E) of 29.1 ± 0.2 kcal mol^{-1}. Density Functional Theory (DFT) calculations at ω97X-D/def2TZVP level for **V_2** and **V_4** and B3LYP/LANL2DZ level for **ox@V_{14}** were used to correlate the structural and electronic properties. Moreover, the NCI, IGM and IBSI methodologies were applied to distinguish between $V\cdots O$ covalent and non-covalent interactions. Stability studies were carried out by EPR, ^{51}V NMR, ESI-MS and UV/vis/NIR in dmso and dmf for all compounds, which indicate partial breakage of the polynuclear species. The better performance of **ox@V_{14}** may be due to a higher formation rate for the active oxidoperoxidovanadium(V) species.

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Characterization of comercial zeolite and its application in adsorption of Mn2+ and Zn2+ in aqueous solution

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The pollution of water resources by metallic ions is an environmental problem that deserves attention. In this context, treatment methods that promote the removal of these contaminants from the aqueous environment have been developed. Adsorption is a promising alternative for the decontamination of effluents containing, and zeolites in turn have demonstrated good performance in this role [1]. Therefore, the present work aimed to use commercial zeolite to apply in the adsorption of Mn2+ and Zn2+ ions. The zeolite was characterized by XRD, FTIR, SEM-FEG, N2 physisorption and zeta potential. By XRD, the presence of high crystallinity was verified, corresponding to the LTA type zeolite crystal structure. By FTIR, the presence of asymmetric stretching bands of Si-O bonds (Si) and Si-O bonds (Al) was verified, corresponding to connection bridges in TO4 tetrahedra belonging to aluminosilicates with a zeolite structure. Furthermore, the material has a micrometric scale and cubic morphology, with particle s with 5µm, surface area of 0.90 m2/g and zeta potential of - 45 mV. The kinetic study of adsorption of Mn2+ and Zn2+ ions was carried out. For this, the concentration of zeolite particles was established at 1 g·L-1, and Mn2+ and Zn2+ ions at 10 mg·L-1. The contact time between the particles and the solutions was fixed in 1, 3, 5, 10, 20, 30, 45, 60 min. The suspensions were shaken and, after the determined time, they were centrifuged. The supernatants were analyzed by atomic absorption spectrometry. The results show that the equilibrium time occurred right at the beginning of the process, in 1 minute. The maximum percentage of adsorption was 69% for Mn2+ and 92% for Zn2+. The kinetic model adjusted corresponding at pseudo-second order model, which indicates that the control of the speed mechanism is chemisorption [2].

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Characterization of sands for metal casting

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Additive manufacturing by 3D sand printing is a significant innovation for the manufacture of cores and molds used in the casting of metal parts, as it allows for the production of cast components with highly complex geometry and super-thin walls and, consequently, lighter. This technology can be a great ally in overcoming the current challenges of the casting process, making it possible to produce cast components with improved dimensional accuracy, fewer defects and greater structural efficiency. In addition, it offers a reduction in post-processing costs and also stands out for being advantageous in the production of small quantities, even for less complex parts. Despite its success in Europe and the USA, in Brazil the high-cost binder jetting equipment and the lack of certificated raw materials has limited its adoption by local foundries. The large-scale implementation of this technology requires its adaptation of the technology in order to enable using different types of sands from local supplies. In this first study sands from different Brazilian mines were investigated in order to determine the most suitable for sand binder jetting. The sands were characterized regarding their particle distribution, pH, lost ignition and compared to sands already validated for 3D printing. Sands from two mines were selected as the most promising sand for 3D printing. As ongoing these sands will be validated in the 3D printer using a conventional binder jetting system. Thus, this study aims to contribute to introduce the additive manufacturing of sand molds and cores, by binder jetting technology, in Brazil.

Chemical modification of the culture medium by incorporating NanoHydroxyapatite for enhanced osteodifferentiation of hBMSCs for bioink production.

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Tissue engineering, aiming to regenerate or repair non-healing diseased tissue like bone, is a promising field relying on cells, growth factors, and scaffolds. These scaffolds, interact with cells and growth factors, providing crucial support for tissue regeneration. Nanometric hydroxyapatite, due to its properties including rapid cell proliferation and bone regeneration, is used in scaffold preparation[1].

In this work, the preparation of nano-hydroxyapatite (nHAp) was carried out using the precipitation method and based on two solutions: a phosphorus source (1) ammonium hydrogen phosphate ($(NH_4)_2HPO_4$), a calcium source, (2) hemihydrate calcium sulfate ($CaSO_4.½ H_2O$)[2]. Subsequently, the material was calcined at 3 different temperatures: 500, 700, and 900 °C, resulting in 3 different granulometries of nHAp, 32:39:113nm.

With the nHAp synthed, several studies were conducted, including verification of the material's cytotoxicity at different concentrations and its ability to promote better osteodifferentiation in human bone marrow-derived stem cells (hBMSCs). After studies of up to 14 days, no toxicity to hBMSCs was observed. In cell culture assays with modified media containing nHAp, it was also observed that the presence in the culture medium promoted increased cell proliferation and osteoinduction. After that, the production of bioink using alginate and hydroxyapatite as a base for subsequent incorporation of stem cells was produced in order to make it possible to use the material for 3D printing.

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Comparative study of electrochemical sensors fabricated through 3D printing employing graphene/PLA and carbon black/PLA filaments

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3D printing is a technique used in the manufacture of electrochemical cells and sensors. The conductive filaments used for 3D electrochemical sensor are compounds of poly(lactic acid) (PLA) and carbonaceous materials[1]. In this work, electrochemical sensors were fabricated, using 3D printing with two different filaments: graphene/PLA and carbon black/PLA and compare their performance through chemical and electrochemical studies. Structural characterization of the filaments was carried out through attenuated total reflectance infrared spectroscopy (ATR-FTIR) and Raman spectroscopy. In the ATR-FTIR, it was observed for both materials, bands at approximately 2939 (stretching of C-H bonds) and 1750 cm^{-1} (stretching of C=O bonds), which are present in the PLA structure. In the Raman spectrum, two main bands were located at 1578 and 1347 cm-1 for the GR/PLA and at 1594 and 1350 cm^{-1} for the CB/PLA, associated with the G (1600 cm^{-1}) and D (1350 cm^{-1}) vibration bands of the carbon materials. The GR/PLA and CB/PLA electrodes were printed on a Creality Ender-3 printer, polished and inserted in a NaOH 1.0 mol L^{-1} solution for 30 minutes. Then, two electrochemical pretreatments were realized, sequentially, using amperometry, applying +1.8 V by 900s in 0.1 mol L^{-1} phosphate buffer pH=7.4 solution. After this, was used the cyclic voltammetry in a range from 0.0 to -1.8 V, by 20 cycles. Contact angle measurements for the GR/PLA were reduced, indicating a higher hydrophilicity of surface electrode, after chemical and electrochemical pretreatment. As an electrochemical probe, it was used 2.0 mmol L^{-1} dopamine in a solution of KCl 0.1 mol L^{-1}. The obtained voltammograms presented oxidation and reduction peak currents for the GR/PLA five and six times larger, respectively, than those for the CB/PLA electrode.

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Effect of adding recycled PP from brewing industry components on the mechanical properties of PP compounds

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The continuous quest for cost reduction and improvement in the manufacturing sector has driven the reuse of production waste. Thermoplastic polymers are notable for their recyclability and ability to be reprocessed, thus generating significant interest across various sectors. In the beverage industry, polypropylene (PP) is utilized in components known as cups, which are specifically designed to accommodate returnable glass bottles during the cleaning process in a solution of sodium hydroxide (NaOH) at 80 °C. This practice aims to eliminate residue present in the bottles, such as labels or impurities, making it possible to reuse these bottles when packaging drinks. However, the PP cups have a limited lifespan due to the harsh working conditions. With a substantial volume of discarded PP cups in the process, there exists an opportunity to invest in their recycling. In this work, the influence of adding recycled PP to neat PP in proportions of 1, 5, and 10 wt% was evaluated. Initially, the PP cups were received, cleaned, and ground using a RONE knife mill. Neat PP and PP compounds were processed using a twin-screw extruder (AX Plásticos, model AX16:40DR), with the temperature profile ranging from 170°C to 200°C. Tensile and impact samples were inject-molded at 210 °C and 6 bar. Tensile tests (ASTM D 638) and Izod impact strength tests (ASTM D 256) were evaluated. To simulate material service conditions, the impact test was also conducted for samples after immersion in NaOH for 1, 30, 60, and 90 days at 80 °C. The mechanical results indicated that incorporating small amounts of recycled material into neat PP does not induce changes in the assessed properties. This suggests the feasibility of utilizing this material for manufacturing new PP cups, thereby fostering a circular economy.

Electrospun mats of PLA with tri-epoxidized ionic liquid with insect-repellent activity

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In this work, insect repellent electrospun mats incorporated with epoxide ionic liquids (ILs) were developed. imidazolium ILs were synthed and incorporated in different weight fractions into a poly(lactic acid) (PLA) solution and electrospun to produce non-woven mats. The effect of IL against the pea aphid Acyrthosiphon pisum (Harris) as evaluated. Moreover, the microstructure, hydrophobicity, and mechanical and thermal properties were also determined. The incorporation of ILs tends to reduce the fiber diameters but does not have a significant effect on mechanical properties and hydrophobic behavior. All mats display a three-dimensional fibrous porous structure highly flexible. Tri-epoxide ILs demonstrated a repellent effect on the A. pisum model aphid, and this effect was more visible at 10 wt. % of IL with a Repellency Index (RI) of 48.44%. The results demonstrated that electrospun mats of PLA with tri-epoxide ILs can be an eco-friendly alternative to be used as an insect repellent.

exploratory study on the vibrational and electronic properties of l-histidine, n-beta-alanyl.

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L-Histidine, N-beta-alanyl (HbA) is a compound known for its potential role in metabolism regulation and may have applications in various fields, including health and nutrition [1,2]. In this study, we conducted an exploratory investigation into the vibrational and electronic properties of HbA using Density Functional Theory (DFT). The initial molecular coordinates were obtained from the PubChem database, under ID 9369. The HbA 3-D geometry was optimized via DFT. Calculations were performed using a hybrid functional (B3LYP), def2-TZVPP base, and def2/J auxiliary base, with no negative frequencies observed. The total energy was -795.96220277 Eh, and the Gibbs energy was -795.77069559 Eh. Dipole moment 6.46233 Debye. Molecular orbitals included HOMO at -6.0290 eV, HOMO (-1) at -6.8914 eV, HOMO (-2) at -7.1243 eV, LUMO at -0.6725 eV, LUMO (+1) at -0.1562 eV, and LUMO+2 at 0.1022 eV, with a band gap of 5.3565 eV. Pronounced absorption peaks were observed around 3509, 1820, 1707, 1537, 1166 and 835 cm-1. Further data adjustments are necessary due to harmonic vibrations considerations. Through HOMO analysis, we identified a region of zero electronic density and, overall, an asymmetric charge distribution within the molecule. Initial analyses indicate the presence of favorable sites for chemical reactivity. Further calculations are needed to determine whether the molecule is susceptible to electrophilic, nucleophilic, and/or radical attacks, as well as to understand the distribution of charges and other parameters characterizing its chemical reactivity.

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Exploring Magnetic Anisotropy Modulation via Mechanical Deformations: Investigating Magnetoelastic Coupling

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Currently, magnetic control is achieved through a flow of current through cables [1], resulting in substantial energy losses. Therefore, easily controlling the magnetic anisotropy of a material can provide a pathway for producing magnetic materials and or/devices with high technological applicability. So, the present work aims to study the magnetoelastic coupling between Fe_3O_4 nanoparticles (NPs) in a 3D silicon matrix in order to control the magnetic anisotropy of flexible nanocomposites through their deformation. Our hypothesis is that the interaction of magnetic NPs in the 3D matrix under an external magnetic field will enable a modulation of the hardness of the nanocomposite. In this context, to conduct this study, Fe_3O_4 NPs were firstly synthed using the solvothermal methodology as described by Zu et al. [2] and fully characterized using powder X-ray diffraction (PXRD), transmission electron microscopy (TEM) and vibrating sample magnetometer. The results of PXRD and TEM pointed out a nanoprism morphology with a spinel structure. No secondary phases were found, which evidences no oxidation of the Fe_3O_4 NPs. The VSM measurements displayed superparamagnetic NPs at room temperature. Afterward, the flexible nanocomposites (FNano) were prepared using the characterized NPs and Mold Max™ 14NV silicone rubber. A total of 3 FNano (0.5, 1 and 5% m/m) were prepared. The FNano were found to show a gray color as long as the concentration of NPs increase. Also, the characterization through atomic force microscopy displays a smooth surface with no Fe_3O_4 NPs aggregates. The magnetic properties were further studied using VSM measurements at room temperature. The Fe_3O_4 NPs were observed to have a superparamagnetic behavior (no hysteresis) [3], while the FNano with 5% concentration showed an increased hysteresis. Finally, tension measurements will be performed under a magnetic field by using the NanoRack Sample stretching stage, coupled with Jupiter AFM equipment.

Fabrication and mechanical characterization of SLS auxetic structures

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Since its invention in 1989 by Deckard and Beaman, SLS has significantly evolved and gained momentum as a driver of the so-called fourth industrial revolution (industry 4.0), in parallel with other relevant Additive Manufacturing technologies [1]. This fabrication method allows the creation of complex geometries, benefiting from a wide material range, which includes several polymers (PA, PEEK, PEKK, PLA, PS, resin) and ceramics (zirconium sands, coated sands, alumina ceramics) [2]. On the other hand, auxetic materials are complex cellular structures presenting negative Poisson ratio, an important feature that enhances resistance to compressive loads and impact absorption [3].

In this study, PET-CF, PETG and TPU auxetic structures produced using the Fuse 1 SLS printer are tested under static compression both in FEM simulation and in physical tests. Moreover, the influence of geometric parameters and materials properties in the mechanical behavior of the auxetic structures is thoroughly discussed.

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Impregnation of Arginine in Mesoporous Silica for CO2 Capture

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In 2030, it is predicted that the release of CO2 will be approximately 46 Gt, which could cause significant global effects on living organisms and ecosystems. In order to try to reduce CO2 emissions, one of the most promising methods is the use of adsorbents with basic properties [1]. Materials such as MCM-41, SBA-15 and KIT-6 have a several advantages for use as adsorbents: MCM-41 and SBA-15 have uniform hexagonal pore structure, high surface area and thermal stability. SBA-15 and KIT-6 have micropores interconnecting the mesopores, enabling the diffusion of large molecules. In addition, the three-dimensional structure of KIT-6 and its resistance to blocking of its poros results in support wide applicability in the area of adsorption [2,3].

An alternative to increase the adsorption capacity of mesoporous supports consists of the insertion of amino groups, for example, arginine. It is amino acid with basic characteristics and non-toxic. The presente work reports on the synthesis ans characterization of adsorbent materials make up of diferent supports (MCM-41, SBA-15, KIT-6) impregnated with arginine and evaluated in CO2 capture. The weight relation of arginine/support impregnated was equal to 5, 10, 20, 30, 40 and 50% w. The presence of arginine in those supports was confirmed in the FTIR which was possible verify bands correspondents to amino groups. Besides, the insertion of arginine into the supports bring on a reduction in the textural properties such as superficial area and pore volume. The superficial area of pure support SBA-15 was reduced from 838 m^2/g to 369, 269, 114, 50, 68 and 32 m^2/g for the species with impregnation rate equal to 5, 10, 20, 30, 40 and 50% w respectively. This result is according with literature e indicate that porous of supports was fully by arginine. The adsorption experiments were performed at 1 bar and 25 °C. CO2 capture values were greater than 3.5 mmol/g for some materials, revealing promising, high-performance materials.

Influence of the calcination temperature on the formation of polaron-oxygen vacancy complexes and their role in the charge transport process in CeO_2

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This work presents initial results on an experimental study of the influence of atomic-scale defects on the morphological characteristics and charge transfer processes in CeO_2 nanoparticles. The results were obtained using the techniques of Positron Annihilation Lifetime Spectroscopy (PALS), Electron Paramagnetic Resonance Spectroscopy (EPR), and Complex Impedance Spectroscopy (IC). The study was conducted on samples of pure nanostructured ceria thermally treated in air at 600, 700, 800, 900, and 1100°C.

We have previously reported a reduction in specific surface area as a consequence of increasing the calcination temperature of the samples, along with changes in the morphology of the ceria nanograins.

PALS results revealed the presence of two types of defects: clusters of oxygen vacancies located on the surface of the nanograins and complexes with neutral total charge, located inside the nanograins, consisting of an oxygen vacancy bound to two polarons (Ce^{+3} ions). Meanwhile, EPR spectrum results highlight the presence of a signal attributed to the presence of complexes with a positive total charge formed by an oxygen vacancy bound to a polaron (Ce^{+3} ion) and a Ce^{+4} ion.

From the combined analysis of PALS and EPR results, it can be concluded that the increase in the thermal treatment temperature leads to a progressive decrease in the concentration of neutral complexes and a slight increase in positive complexes. From the IE spectra results, a correlation was established between the different thermal treatments and the position of the Fermi level in each treated sample; this behavior is directly related to a decrease in the number of carriers and, consequently, a lower electrical conductivity observed as the calcination temperature of the samples increases.

Investigation of the filling effect on metamaterial geometries applied to structures manufactured by additive manufacturing.

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In the last decade, mechanical metamaterials have attracted considerable interest due to their unique structural properties. This type of structure has diverse applications in various industrial sectors, such as: aerospace, automotive and biomedical engineering. Furthermore, metamaterials are explored through the additive manufacturing process where the internal porosity of the structural element can influence the resistance, density, stiffness and conductivity characteristics of the material. Therefore, changing filling patterns are explored by researchers to optimize the performance of these materials in specific applications, such as vibration damping, energy absorption, thermal insulation, or even to create materials with negative properties (auxetic materials). The objective of this study is to investigate the effect of filling on the mechanical properties of the re-entrant geometry, with filling variations of 30%, 60%, 90% and 100% filled. The PLA material was used as the basis of the research for both the standard material and the re-entrant geometries. Mechanical characterization was conducted using uniaxial tensile tests and deformation analysis. The results showed that samples with 60% and 90% filling exhibit very similar mechanical properties as a function of absorbed load and deformation. This observation challenges conventional expectations and suggests that, within the investigated filling range, the mechanical performance of metamaterials is not significantly affected by the filling degree. These findings have important implications for the design and optimization of mechanical metamaterials, highlighting the need to consider factors beyond simple fill volume to achieve desired mechanical properties.

Low specific mass and excellent mechanical properties of reduced graphene oxide aerogels

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Carbon aerogel is a special class of porous materials with excellent properties, including low specific mass, large specific surface area and environmental compatibility. The primary route studied for preparing reduced graphene oxide aerogel (GA) is the hydrothermal method, whose control of reaction parameters allows the production of a material with a low concentration of defects and with the possibility of industrial scale production [1]. The aim of our work is to develop GA with low specific mass and high surface area by hydrothermal synthesis, evaluating the synthesis parameters. Through implementing a hydrothermal technique that incorporates freezing and thawing, along with preheating the sample, we could achieve a specific mass of approximately 3 mg/cm^3 and favorable mechanical properties. The samples were dried by freeze-drying for 48 hours as the last step in the GA manufacturing process [2].

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Manufacturing and validation of a new generation of particleboards: a solution for irregular plastic disposal

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The growing concern about plastic waste management and the search for eco-friendly alternatives in the wood, furniture and construction industries motivated this research. This study produces pine wood particleboards with polyethylene terephthalate (PET) waste as a binder and evaluated their technical and environmental feasibility. Four different proportions of PET particles were experimented in the painels production, starting at a content of 5% with gradual variations of 5% for each new proposed treatment. The panel manufacturing process – with a density of 0.65g/cm³ – initially involved the characterization of the particles in terms of particle and density, followed by homogenization between the particles and pressing at a temperature of 180°C and pressure of 5MPa. The materials were subjected to physical-mechanical tests for tensile and flexural strength, modulus of elasticity, moisture content, thickness swelling and water absorption. Furthermore, characterization analyses, including scanning electron microscopy (SEM) and thermogravimetry (TG), were performed to understand the interactions between the PET particles and the wood matrix of the particleboards. The results demonstrated that the inclusion of PET waste as a binder made it possible to consolidate the panels, meeting the minimum criteria established by regulatory standards. Furthermore, microscopic analyzes revealed good adhesion between the PET particles and the wood matrix. Finally, the reuse of this material, as an alternative to conventional binders, reduced the dependence on virgin wood, which suggests a potential reduction in the environmental impact associated with the production process of wood particles and the management of plastic waste.

Manufacturing of transparent Fresnel lens using the 3D stereolithography printing process with a photopolymerized resin of the aluminosilicate sol-gel solution

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objects by layering material based on a digital model. This method enables the manufacturing of objects with complex designs at constant processing time and minimized project planning, making it ideal for creating custom-made, small-scale products [1]. In this work, we prepared photopolymerizable aluminum–silicate resins obtained from the hybrid sol–gel route for Vat photopolymerization (VPP) process, using a procedure described in detail elsewhere [2]. The Fresnel lenses were printed using the stereolithography process (SLA) in the "bottom-up" printing process, using the VPP mask projection (MP) process, with a commercial printer called Prusa SL1S. The quality of the pieces obtained and the curing and drying process were analyzed using Scanning Electronic Microscopy and Profilometry. The condensation of Si-O-Si species and the photopolymerization process were analyzed using FTIR and solid-state NMR. After the drying process, Fresnel lenses experience a shrinkage of 11.5% in the distance between the rings and 55% in height. The condensation of the hybrid resin occurs for both the organic and inorganic fractions, as observed from the FTIR and solid-state NMR analysis of the 29Si and 13C nuclei.

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Mechanical Analysis of Immobilizing Splints in 3D Printing by the FDM Method

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The widespread adoption of 3d printing technology, particularly Fused Deposition Modeling (FDM), has been driven by the decreasing costs of thermoplastic materials and the technology's ability to efficiently produce complex structures without extensive manual labor. This advancement has transformed various sectors, with its application becoming increasingly prevalent, especially in healthcare, where it facilitates the development of products with superior characteristics. Specifically, when it comes to immobilization splints, FDM technology makes traditional methods obsolete due to its advantages in terms of ventilation, weight distribution, and aesthetics. Therefore, it is essential to establish parameters for assessing this technology's applicability in these domains. To achieve this goal, the present study focused on characterizing the mechanical properties, such as impact resistance, bending, and tensile strength, of common thermoplastic materials including PLA, carbon fiber-reinforced PLA, ABS, PETG, and carbon fiber-reinforced Nylon, through tests on sample specimens and computer simulations of static loads. ABS and PLA demonstrated the highest mechanical performance, with tensile strengths of 15.06 MPa and 11.90 MPa, respectively. This facilitated the successful production of immobilization splints. However, when designing splints for body parts that bear greater loads, caution is warranted. Such applications may necessitate increased thickness to maintain structural integrity. For example, wrist splints manufactured using PLA material were observed to have thicknesses reaching up to 6.00 mm, indicating the need for careful consideration in their design and use.

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Microwave-assisted solvothermal synthesis of NiO microspikes-based sensor for methanol detection

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Semiconducting metal oxides (SMOs) are extensively utilized as sensor materials for detection of volatile organic compounds (VOCs) [1]. Methanol is an example of a VOC that can cause adverse health effects with long-term exposure [2]. Therefore, there is a need to develop sensors capable of detecting VOCs that can cause human health problems. In this context, this work demonstrates the synthesis and characterization of a NiO micro-spikes (MS)-based sensor utilizing metal-organic frameworks (MOFs) as a template. MOFs are a class of functional porous materials exhibiting distinctive physicochemical properties and acting as an important precursor in the production of SMOs-based hollow sensors [1]. First, the Ni-MOF was synthed using the microwave-assisted solvothermal method from nickel (II) nitrate hexahydrate, terephthalic acid, N,N'-dimethylformamide, and sodium hydroxide. The mixture was agitated for 30 min. and transferred to a microwave processing at 150 °C for 90 min. The green precipitate was washed and centrifuged with ethanol and water several times, and then dried at 60 °C for 12 h. The Ni-MOF was calcined at 500 °C for 120 min to produce NiO-MS [3]. The NiO-MS and Ni-MOF were characterized by X-ray diffraction and scanning electron microscopy. Sensing measurements were performed for 100 ppm of acetone, methanol, ethanol, benzene, toluene, m-xylene, 3-methyl-1-butanol, and 2-nonanone at 150 – 400 °C. The NiO-MS sensor showed good sensitivity and selectivity for methanol at 250 °C (response of 2.01) and good stability (0 to 45% relative humidity). Acknowledgements: CAPES, CNPq (311453/2021-0), and Fapesp (2020/06421-1). References: [1] Yi, S.; Shi, W.; Yang, X.; Yao, Z., Talanta, 258, 124442 (2023); [2] Maqbool, Q.; Yigit, N.; Stöger-Pollach, M.; Ruello, M. L.; Tittarelli, F.; Rupprechter, G., Catal. Sci. Technol., 13, 624-636 (2023); [3] Pang, H.; Guan, B.; Sun, W.; Wang, Y., Electrochim. Acta, 213, 351-357 (2016).

Photocatalytic degradation of rhodamine B by a covalent triazine framework modified with different types of niobium

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Covalent triazine frameworks (CTF) are organic materials with triazine heterocycles, with strong potential as catalysts, specially when doped with metal. This way, niobium-based materials have attracted the attention due to the photocatalytic activity. The presence of niobium species at the CTF would enhance the catalytic activity and might be explored. The aim of this work was the obtention of niobium based CTF and your evaluation for the removal of rhodamine B (RhB) from aqueous solution. The chosen CTF was obtained from the condensation of melamine with terephthaldehyde under solvothermal conditions and named **SWN-1**, with a three-dimensional structure confirmed by the absence of stretching of the iminic Ar-C=N bond, and the presence of secondary amines stretching at 3387 cm^{-1} and 1161 cm^{-1} of HN-C-NH groups, with sp3 carbon.[1,2] Over the synthesis ultra-pure Nb_2O_5 (**Nb_2O_5@SWN-1**) or ammonium niobium oxalate (**Nb(ox)@SWN-1**) were added. The solutions of RhB (25 ppm), were stirred in the presence of the solids (1 g L^{-1}) at 25 °C in the dark. After 60 min the materials achieved the adsorption equilibrium: **Nb_2O_5@SWN-1** removed 90.5% with pseudo-first order kinetics and rate constant of $3.91x10^{-3}$ min^{-1}, while **SWN-1** adsorbed 39.4%. The presence of Nb_2O_5 increased the adsorption capacity, however **Nb(ox)@SWN-1** did not remove RhB by adsorption. When 100 W white LED was turned on **SWN-1** showed first order photodegradation with rate constant of $2.72x10^{-3}$ min^{-1}, showing degradation of 57.0%. Finally, **Nb(ox)@SWN-1** showed a zero-order kinetic photocatalytic activity with rate constant of $5.8x10^{-2}$ min^{-1} and 66.3% of degradation. Studies are being conducted to correlate the modifications generated by the different niobium structures with the photodegradation of the dye.

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Pre-concentration in different solvents to allow solubilization of NMP-insoluble polymers

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N-methyl-2-pyrrolidone (NMP) is a dipolar aprotic with high boiling point and non-flammable solvent. It has large chemical and thermal resistance and low toxicity. These properties make NMP useful for a variety of industries and chemical applications [1]. In this study, a set of solvents was tested for their ability to dissolve four types of different NMP-insoluble polymers: polystyrene (PS), polyethylene terephthalate (PET), cellulose acetate and Arabic gum. These polymers were chosen because they could be used as binder in paint formulation however face challenges with respect to formulation using NMP as solvent. After the solubility tests, a higher pre-concentrated solution was prepared dispersing the maximum of each polymer in minimum volume of adequate solvent: 35 mg PS/mL ethyl acetate; 0,5 g PET/mL aniline distilled; 100 mg cellulose acetate/1,2 mL acetone + 1,8 mL cyclohexanone and 1,0 g Arabic gum/mL distilled water. Thus, finally, it was possible to solubilize the pre-concentrated solutions in NMP at the desired concentrations. PS is a polymer with a myriad of applications, from packaging to construction. PET is used in fibers from textile to PET bottles. Currently PS recycling is highly challenging, in comparison PET can be relatively easily recycled, however, the composites, like in textile, that contain more than one material, a selective dissolution of components could significantly aid the development of efficient recycling technology. [2]. In this way this study allows an alternative process to a paint formulation and can also contribute to recycling technologies.

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Robocasting fabrication of TiO2-supported WO3 catalysts for the solar-driven production of ammonia

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The increasing global demand for ammonia, particularly now that it has emerged as a relevant hydrogen carrier, stresses the need for development of sustainable and energy-efficient synthesis methods. Traditional Haber-Bosch ammonia synthesis is energy-intensive, reliant on fossil fuels, and contributes significantly to CO2 emissions. One promising alternative involves the use of solar energy to activate nitrogen reduction reactions. In this work, we report the fabrication of titanium dioxide (TiO2)-supported tungsten trioxide (WO3) catalysts, as suitable catalysts to harness solar energy efficiently. The TiO2 support was prepared using a direct-ink writing (3D printing) technology [1]. WO3 was coated using a spray pyrolysis technique followed by calcination [2]. Characterization techniques, including XRD, SEM, and UV-Vis diffuse reflectance spectroscopy, confirmed the successful incorporation of WO3 on TiO2. The catalysts were used to assemble a fixed-bed photoreactor, operated under simulated sunlight. N2-saturated deionized water is recirculated through the photoreactor and the light source is turned on. Samples are collected periodically and the NH4+/NH3 contents are determined using a colorimetric method [3]. Photocatalytic tests are being carried out to compare the efficiency of the fixed-bed catalysts with their dispersed powdered equivalents and other suitable materials as reported in the literature. Preliminary results have shown that ammonia is produced, confirming the functionality of the catalyst. Detailed quantification is still under way, and will be presented and discussed at the conference.

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Structured particleboard composites made of pine residue and vulcanized natural rubber as binder

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The Search sustainable alternatives aiming at reducing the impact of human activity on the environment has been increasing in recent decades. In this context and looking for alternatives that, has been the use of waste of different sectors industrial aiming at the production of various materials, as well as adding value to this waste. One of the sectors that produces a large amount of waste is the furniture and sawmill industry, this wood residues can be used to produce panels for use in sector such as civil construction and the furniture industry itself. In that regard, the present study has as objective to obtain the panels particleboard structured with residue of pine and vulcanized natural rubber as binder. For the production of the panels, an open parallel roller mixer was used and the mass concentration of NR (was used 100 phr of NR as reference), as well as vulcanizing agents (sulphur, stearic acid, zinc oxide, and the accelerators TMTD and MBTS) were kept fixed and varied the concentration of pine in 100 and 200 phr. After vulcanization of composite panels Pine/NR at 150ºC in a termopress, physical tests were carried out, such as: density, swelling after 24h and water absorption after 24h. All these trials were carried out in accordance with the standards ABNT NBR 14810-1, 21,2 and ASTM D10373. To evaluated the morphology and interaction between the pines and NR phases in composite panels, SEM analyses were carried out on the fractured section of the samples. By SEM analyses, it was possible check a quite homogeneous distribution of pine particles, and a good interaction of wood particles with NR particles. This behaviour makes it clear that the process of obtaining composite panels using an open mixer with parallel rollers provides better mixing of the phases and improves the interaction between them. Finally, with these results of the materials show themselves very effective in the use of liners and thermal walls, and in other casual occupation.

Study of electrochemical performance of 3D-printed graphene/PLA electrodes under different electrochemical pretreatments

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3D electrochemical sensors has been highlighting by enabling building of a wide possibility of designs. In order to improve their electrical properties, electrochemical pretreatments (PTs) have been studied, provinding better electrochemical responses in development of analytical methods [1]. In this work, the electrochemical performance of 3D printed-electrode based on graphene and polylactic acid (GR-PLA) after different conditions of electrochemical PT was investigated using dopamine (DOP) as standard molecule. Different electrochemical PTs were evaluated, using chronoamperometry technique, applying a potential of 1,8 V for 900 s, following of cyclic voltammetry in phosphate buffer solution 0,1 mol L^{-1} pH 7,4, under a potential range of 0,0 to -1,8 V (1) and using chronopotentiometry in H_2SO_4 solution 0,5 mol L^{-1}, after the study of parameters as current density (100 mA cm^{-2} for anodic PT; -50 and -100 mA cm^{-2} for cathodic PT) in time intervals of 150, 200 and 300 s (2). The studies were performed using cyclic voltammetry with 1,0 mmol L-1 DOP in KCl solution 0,1 mol L^{-1}. It was possible to observe a higher peak current and a less peak-to-peak potential separation (ΔE_p) for GR-PLA after the PT 2, applying -100 mA cm^{-2} for 150 s (I_{pa} = 77,28 µA; ΔE_p= 0,304V) compared to application of 100 mA cm^{-2} for same time (I_{pa} = 39,26 µA; ΔE_p= 0,587V). Better responses were obtained with the PT 2 - cathodic, from application of -100 mA cm^{-2} for 200 s (I_{pa} = 81,51 µA; ΔE_p= 0,504V). Under the optimum conditions, PT 2 – cathodic also provided a best voltammetric behavior regarding to PT 1 (I_{pa} = 68,70 µA; ΔE_p= 0,321V). The comparative study of electrochemical PT was performed for 3D GR-PLA and the application of -100 mA cm^{-1} for 200 s provided a better electrochemical behavior for DOP.

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Synthesis and application of quinoline derivate as photoinitiator in photopolymerization reactions

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In this work we related ours results about the synthesis, characterization and application of new quinoline derivative for actuation as Type II photoinitiator in the photopolymerization reaction of the urethane dimethacrylate (UDMA) [1], widely used in resin formulations for dental restoration. The quinoline derivative (1) was obtained in three reaction steps with good yield, starting by the multicomponent reaction among 4-nitroaniline, 4-methylthiobenzaldehyde and phenylacetylene, followed by reduction of nitro group (Quinoline derivate 2) and methacrylation of amino group (Quinoline derivate 3). Analysis of the photolysis of the three quinoline derivatives shows that the formation of reactive species occurs within the first second of exposure to light, providing clear evidence of the photosensitivity of these molecules. All synthed quinoline derivatives were tested as photoinitiators in the UDMA photopolymerization reaction using a Kessyl lamp under 370 nm irradiation, and the polymers were obtained with a conversion rate of up to 40% in approximately 60 seconds [2]. These results present a higher degree of conversion than that presented by camphorquinone, a commercial photoinitiator. It is worth mentioning that the polymers obtained have fluorescent characteristics, a characteristic that may be relevant for applications such as the dental field [3].

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Synthesis and characterization of hydrogels based on graphene and single-walled carbon nanotube

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Carbon-based nanomaterials represent a diverse class of materials with varied and unique properties, which make them suitable for numerous applications. Conventional strategies for preparing this class of materials involve using large amounts of energy, toxic solvents, and many steps, making it expensive, which reinforces the search for the development of cost-effective synthesis strategies. Hydrogels based on graphene are examples of these materials and have a wide range of applications, from removing contaminants of environmental interest in analytical sensing to energy storage. To increase these multifunctionalities, this work aims nano-architect and characterize hybrid hydrogels based on graphene and carbon nanotubes. The materials were prepared using a route developed and patented by our group, and the process involves the reduction of graphene oxide (GO), in an autoclave in the presence of single-layer carbon nanotubes (SWCNT) and the reducing agent (ascorbic acid). For the formation of hydrogels, the proportions between GO and CNTs were kept fixed (1:1), and the percentage of reducer in the syntheses was varied at 0, 5, 10, and 25 mmol/L. The samples were characterized by Infrared Spectroscopy (FTIR-ATR), Raman Spectroscopy, and Scanning Electron Microscopy (SEM). Hydrogels were obtained in a single step and through a sustainable route in less than two hours. The materials presented a three-dimensional porous structure that was cohesive and self-supporting. The effect of different amounts of the reducing agent was evaluated. It was observed that small variations in the ascorbic acid content promoted significant morphological and structural changes. FTIR and Raman results indicated the effective reduction of GO to reduced graphene oxide. The presence of CNTs in the medium affects how the GO sheets are reduced and how the hydrogel is structured, forming materials with different architectures (porosities, degree of packing, functionalization). The SEM images rev

Synthesis and characterization of Nb_2O_5 for adsorption of Mn^{2+} in aqueous solution

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The increasing presence of heavy metals in waste waters poses a significant environmental challenge due to their persistence and potential for bioaccumulation [1]. To address this issue, this work explores the design and synthesis of three-dimensional (3D) Nb_2O_5 nanoparticles as a functional material for the removal of Mn^{2+} from aqueous solutions through adsorption. Nb_2O_5 nanoparticles were synthed using the peroxide oxidation method at 100 °C for varying durations (4, 12, and 24 hours). Structural characterization by XRD confirmed the orthorhombic phase, while TG/DSC analysis revealed substantial mass loss below 500 °C, attributed to the removal of adsorbed and coordinated water. The 3D structure of the nanoparticles, confirmed by Field emission electron scanning microscopy, is evidenced by the presence of grains on the order of 10 nm, which are aligned forming rods on the order of 1 µm. High surface areas were confirmed by nitrogen physisorption analysis, measuring 174 m^2/g for the 4-hour synthesis, 163 m^2/g for the 12-hour synthesis, and 174 m^2/g for the 24-hour synthesis, facilitating efficient adsorption. Adsorption capacities for Mn^{2+} reached 69%, 67%, and 79% for the 4-hour, 12-hour, and 24-hour samples, respectively. The Langmuir model provided a good fit for the isotherms, suggesting chemical monolayer adsorption with a maximum capacity of 1.472 mg/g. This study demonstrates the potential of Nb_2O_5 nanoparticles as an effective adsorbent for Mn^{2+} removal, offering a promising strategy for remediating heavy metal contamination in industrial and environmental settings.

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Synthesis and characterization of Niobium (V) oxide (Nb2O5) powders

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Niobium (V) oxide (Nb2O5), an excellent metal oxide with unique characteristics, exhibits great potential and properties such as stability in aqueous media, photo-catalytic activity, and redox properties. Nb2O5 has significant applications in electrochromic displays, gas sensing, biosensing, photoelectrodes, and water decontamination. The properties of Nb2O5 strongly depend on its synthesis procedure and the thermal treatment conditions[1,2]. Consequently, many researchers have been trying to change Nb2O5 properties by modifying synthesis procedures. The research mainly focused on the synthesis of Nb2O5 thin films than that of Nb2O5 powders. In this study, Nb2O5 powder was synthed via the Sol-gel method. Initially, Niobium (V) ethoxide Nb(OC2H5)5 was dissolved in ethanol and gradually hydrolyzed by adding a small amount of water. The conditions for thermal treatment of amorphous Nb2O5 precursors were determined based on the basis of DSC curves. XRD patterns of Nb2O5 samples obtained via the Sol-gel method revealed that the sharpness and intensity of diffraction peaks improved progressively with increasing calcination temperature, indicating crystalline growth of Nb2O5. At 650°C, orthorhombic crystalline structures (T-Nb2O5) were observed. The synthesized Nb2O5 powder will be utilized to prepare three-dimensional (3D) niobium films for use in applications such as photocatalysis and solar cells. The authors acknowledge the CAPES, CNPq, INCT and the PPGEM – UTFPR – CP/PG for financial support.

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Synthesis and characterization of zinc oxide nanoparticles incorporated into SBA-15 matrix: exploring compatibility and potential applications

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Composite materials have garnered significant interest within the scientific community owing to their unique combination of properties. However, the selection of such materials necessitates careful evaluation of their compatibility and interaction. Mesoporous ordered silica, such as SBA-15, possesses high surface area, thermal and mechanical properties, and a bi-dimensional hexagonal porous structure with silanol groups capable of incorporating ions, molecules, antigens, and nanoparticles. Zinc oxide nanoparticles (ZnO_NPs) are renowned for their antimicrobial activity and photocatalytic properties. However, ZnO_NPs agglomeration is a concern; therefore, incorporating them into inorganic matrices can mitigate this issue. Hence, this study focuses on two different methods to obtain ZnO:SBA-15 composites and their potential applications. One method involves incorporating ZnO_NPs onto SBA-15 using previously prepared nanoparticles synthed from zinc acetate dihydrate as a precursor in a reflux system. The other method entails in situ synthesis of ZnO_NPs directly within the SBA-15 system. Various techniques were employed to study the physicochemical properties of the ZnO_NP and the ZnO:SBA-15 composites. Characterization results demonstrate the successful incorporation of ZnO species into the SBA-15 matrix. SAXS measurements for all composites revealed characteristic reflections of a bi-dimensional porous structure, indicating preservation of the SBA-15 mesostructured after ZnO-NP incorporation. UV-Vis spectroscopy confirmed the expected absorption band at approximately 367 nm, characteristic of ZnO-NPs, and XRD confirmed the hexagonal structure of ZnO for all materials. TEM images showed the presence of zinc nanoparticles in all composites. Potential applications include antimicrobial activity and cosmetic areas, leveraging the combined properties generated in the composites.

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Synthesis, characterization and Fenton-like catalytic properties of copper-modified graphitic carbon nitride

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Catalysts based on graphitic carbon nitride (g-C_3N_4) with a 3D porous struture modified by metallic ions have shown to be a promising alternative for application in environmental remediation processes [1]. Thus, the present work investigates the catalytic potential of g-C_3N_4 modified with copper in the proportions 100/0, 95/5, 85/15 and 70/30. The synthesis of the materials was carried out via thermal polycondensation of melamine at 550 °C for 2 hours in an inert atmosphere. The samples obtained were named as CN, CuCN-5, CuCN-15 and CuCN-30. Preliminary characterizations of the materials were performed by XRD, FTIR, SEM and EDS. The catalytic activity was evaluated through the degradation of indigo carmine (30 mg/L) and methylene blue (10 mg/L) dyes in the presence of 10 mg of each catalyst and 25µL of H_2O_2. XRD patterns confirmed the formation of g-C_3N_4 in all materials. A decrease in peak intensity (100) in CuCN-15 and CuCN-30 samples suggests that copper was incorporated into the g-C_3N_4 matrix, while FTIR spectra reveal greater amounts of Cu-Nx species, active sites responsible for catalytic activity, in these two samples [2,3]. The pseudo first order kinetic model was used to describe the catalytic process of degradation of MB and IC dyes. The MB degradation was 99% in the CuCN-30/H_2O_2 system after 20 min of reaction at a removal rate of 0.2 min^{-1}, while for IC, the CuCN-15/H_2O_2 system obtained 87% removal after 40 min at 0.04 min^{-1}. Finally, although the results presented here prove the potential application of copper-modified g-C_3N_4 materials, studies of chemical stability, optimization of catalyst synthesis conditions and new structural characterizations are still needed.

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Synthesis of microporous crystalline materials from low-cost silica sources.

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Zeolites are three-dimensional microporous crystalline materials formed by the arrangement of silicon and aluminum tetrahedra coordinated by oxygen atoms. The different spatial orientations of these tetrahedra generate various structures with channels and cavities on the order of molecular dimensions. Such materials are widely used as adsorbents, ion exchangers, and catalysts. In an effort to obtain zeolites through environmentally friendly methodologies, efforts have been made to employ alternative low-cost raw materials derived from waste. Rice husk is a byproduct of the rice processing industry and is rich in silica; thus, the study aimed to evaluate the use of silica from rice husk for the synthesis of beta-type zeolites (BEA). The extraction of silica from rice husk and the crystallization period (24, 48, 72, and 120 h) were evaluated. X-ray diffraction (XRD) results revealed that the characteristic reflection at $2\theta = 22.5°$, indicative of the BEA structure, appeared after 24 h of synthesis. All characteristic reflections of Beta zeolite were observed after 48 hours of synthesis, confirming the success of the synthesis and the formation of the structure with phase purity. After 72 h of crystallization, some reflections became more defined, although with intensities similar to those of the 48 h sample. The XRD pattern of the 120 h sample indicated a decrease in intensities, suggesting that prolonged crystallization time led to consumption of the zeolitic structure formed. TGA confirmed that the organic structure directing agent (OSDA) was occluded in the zeolitic structure. The DTG reveals that the increase in crystallization time led to the displacement of mass loss events between 120–550 °C to higher temperatures, indicating increase interaction of the OSDA with the inorganic structure. The mass losses between 120 and 550 °C, attributed to the elimination of molecules, were 14.5%, 15.4%, and 13.6% for the 24, 48, and 72 h samples, respectively.

Tetracycline adsorption using polymeric aerogel

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Contamination of water resources resulting from the release of pharmaceuticals can lead to the development of pathogen resistance, as well as can be harmful to the human health and the environment [1]. In this context, it becomes necessary to develop materials that are efficient in removing these antibiotics from water resources, including the tetracycline. In this context, here we developed a 3D printed aerogel by combining sodium alginate (SA), carboxymethylcellulose (CMC) and gelatin (Gel), to manufacture antibiotic adsorbents. The morphological aspects of the 3D printed structure were observed through scanning electron microscopy (SEM) analysis, and the chemical structure before and after the antibiotic adsorption process was analyzed using Fourier-transform infrared spectroscopy (FTIR). Aerogel swelling tests were conducted to evaluate the materials absorption capacity in an aqueous medium. Adsorption tests demonstrated the high efficiency of the material, with values exceeding 90%. Additionally, tests were performed at different values of pH, revealing that the optimum pH is 7 for antibiotic adsorption in aqueous media. Acknowledgments: the authors thank to CAPES, CNPq, FAPESP and Embrapa. References: [1] Luo X. et al, Environmental Science Nano, vol. 8, 2478-2491 (2021); [2] Chen G. et al, Chemical Engineering Journal, vol. 423 (2021).

theoretical characterization of vibrational and electronic properties of papain (*carica papaya*) by dft: study of chemical reactivity

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Papain (Carica Papaya) has been extensively studied experimentally for its potential wound-healing effects, yet few theoretical studies have been conducted in the literature [1,2]. In this study, we characterize the vibrational and electronic properties of papain using Density Functional Theory (DFT) to understand its chemical reactivity and bioactivity. The initial molecular coordinates were obtained from the PubChem database under ID 5249653, and the papain 3-D geometry was optimized via DFT. Calculations were performed using a hybrid functional (B3LYP), def2-TZVPP base, and def2/J auxiliary base, with no negative frequencies observed. The total energy was -913.724 Eh, and the Gibbs energy was -795.76824217 Eh. Molecular orbitals included HOMO at -4.2869 eV, HOMO (-1) at -4.6410 eV, HOMO (-2) at -4.8569 eV, LUMO at -3.0113 eV, LUMO (+1) at -1.3001 eV, and LUMO (+2) at -1.2218 eV, with a band gap of 1.2759 eV. Pronounced absorption peaks were observed around 3364, 1806-1745, and 1282 cm^{-1}. Further data adjustments are needed due to harmonic vibrations considerations. Through HOMO analysis, we identified a region of zero electronic density and, overall, an asymmetric charge distribution within the molecule. Initial analyses indicate the presence of favorable sites for chemical reactivity. Further calculations are necessary to determine whether the molecule is susceptible to electrophilic, nucleophilic, and/or radical attacks, as well as to understand the distribution of charges and other parameters characterizing its chemical reactivity.

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The use of 3D printing technology in the production of bipolar plates for direct ethanol fuel

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In this work, the feasibility of printing bipolar plates for direct ethanol fuel cells was evaluated using conductive and non-conductive polymer filament-based ABS (acrylonitrile butadiene styrene) with a diameter of 1.75 mm. Serpentine and parallel serpentine models with dimensions based on literature research were used for the fabrication of ethanol distribution channels in the bipolar plates. Bipolar plate modeling was performed using Solidworks® software, as well as Slicer3D® for visualization, processing, and segmentation of the models. The study evaluated parameters such as injection nozzle and deposition bed temperatures for each type of polymer used, as well as visual parameters for the appearance of the fabricated part.

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Three-dimensional graphene macrostructures decorated with iron nanoparticles for caffeine degradation

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Constructing three-dimensional macrostructures is one way to optimize the properties of graphene-based nanomaterials and their application possibilities. When these macrostructures are decorated with metallic nanoparticles, they can have new specific and optimized characteristics. For example, iron nanoparticles can provide the material, besides high adsorption capacity, magnetic properties, and catalytic capacity to degrade several molecules. Thus, the objective of the present work was to prepare graphene macrostructures decorated with iron nanoparticles for the removal and degradation of caffeine, a chemical indicator of contamination of aquatic environments. The 3D graphene-based macrostructures were obtained from the single-step thermochemical reduction of graphene oxide in the presence of a reducing agent (ascorbic acid) and the metal precursor (iron chloride)[1]. The materials were characterized by scanning electron microscopy (SEM), infrared spectroscopy (FTIR), and Raman spectroscopy and tested for their photocatalytic efficiency against caffeine molecules. The results showed that different three-dimensional graphene structures homogeneously decorated with iron nanoparticles were efficiently prepared in a single-step environmentally friendly synthesis. The characterization techniques were fundamental in understanding each material's structure, confirming the presence of iron nanoparticles, and evaluating the and distribution of pores and nanoparticles in the macrostructures. A direct relationship was observed between the macrostrure's compaction and the nanoparticles' , depending on the amount of reducing agent added. The degradation tests showed that the materials are promising photocatalysts, capable of eliminating up to 90% of the analyte in solution in only fifty minutes.

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Zeolitic Imidazole Frameworks (ZIFs) applied in glyphosate adsorption

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Imidazole zeolitic structures (ZIF), have a porous structure and high surface area, similar to natural zeolites, have been applied as adsorbents [1]. The herbicide glyphosate is the most used herbicide in the world and studies reveal its direct relationship with environmental contamination at various trophic levels of the aquatic environment. Furthermore, it is associated with the development of several diseases, such as respiratory, dermatological, neurological diseases and even the development of cancer. In view of this scenario, global organizations such as USEPA and WHO have limited glyphosate concentrations in aqueous effluents to 0.7 mg/L and 0.1 µg/L, respectively [2]. This made the development of research into remediation techniques for herbicides in the aqueous environment very important. Adsorption is one of the most used. The application of MOFs in the adsorption of the herbicide glyphosate can be evaluated, due to the presence of phosphonate and carboxylate functional groups in the herbicide structure, which allow it to form interactions with metal ions, electron acceptors, forming highly stable complexes [2]. Thus, the present work aimed to synthe and characterize the ZIFs of Co, Ni and Cu and subsequently apply them in adsorption tests for the herbicide glyphosate for which the adsorptive process was kinetically evaluated, determining adsorption capacities (Qe) of 28 .08, 30.03 and 21.84 mgg^{-1} for the Co, Ni and Cu ZIFs, respectively.

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FM03-High entropy Alloys: Microstructure, properties and new perspectives

Computational thermodynamic calculation of multicomponent alloys-hydrogen systems for developing hydrogen storage materials

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Hydrogen plays an important role in the transition from a fossil fuel-based to a renewable source-based energy. Hydrogen can be produced from the surplus energy generated by solar, wind, tidal, and biomass sources, acting as an energy vector, i.e., storing and transporting the surplus energy to be used whenever and wherever is needed. However, the storage of hydrogen itself is not an easy task because of its low volumetric density even under high pressure. Solid-state hydrogen storage in metal hydrides has been considered a suitable alternative for storing and transporting hydrogen for many applications. The main advantage of metal hydrides is the possibility of storing large amounts of hydrogen in low volumes under different pressure and temperature conditions. Many high-entropy alloys (HEAs) can interact with hydrogen and form high-entropy hydrides (HEHs). Since the hydrogen storage properties highly dependent on the chemical composition of the of the HEA/HEHs, exploring the vast compositional space of HEAs offer a great opportunity for the discovery/designing of new materials with hydrogen storage properties that can be tunned to meet specific application requirements. In this work, it will be presented to how computational thermodynamic calculation of multicomponent alloys-hydrogen systems can be employed to explore the vast composition field of HEAs and to design hydrogen storage materials for different applications. The thermodynamic tools employed are the CALPHAD method and thermodynamic models for calculating pressure-composition-temperature (PCT) diagrams of HEAs-H systems implemented in open-source codes. Examples of single body-cubic centered (BCC) and single C14-Laves phase HEAs designed with these tools will be presented.

Crystallographic Features and Growth Mode of a Directionally Solidified Three-phase Eutectic High Entropy Alloy

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The microstructures obtained from eutectic solidification are among the most intriguing phenomena in metallurgy. Eutectic growth enables the direct formation of multiple solid phases from the melt. In regular eutectics, the formation of solid phases relies on cooperative growth, which involves the rejection and incorporation of atoms at the solid/liquid interface, leading to atomic cross-diffusion within the interfacial liquid. Therefore, different solid phases grow side by side. While the growth of binary eutectics is well understood, there remains a gap in our comprehensive understanding of the mechanisms involved in three-phase eutectic growth. In this context, the emergence of high entropy alloys (HEAs) has offered a novel approach to producing eutectic microstructures. Recently, a three-phase eutectic high entropy alloy was found in the Al-Co-Cr-Fe-Ni-Nb system. This presentation aims to investigate the growth mode and crystallographic features of this ternary eutectic high entropy alloy using directional solidification in Bridgman equipment. Varying the eutectic growth rate induces changes in both the scale of the microstructure and the growth mode. In this regard, samples were directionally solidified at different growth rates. At growth rates as low as 1 µm/s, highly regular microstructures were observed. With increasing growth rates, a cellular eutectic microstructure was obtained. The application of transmission electron microscopy enabled accurate identification of the phases present in the eutectic microstructure, which is formed by the L ↔ Laves-B2-FCC phase transformation.

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Design of high and medium-Mn steels by different approaches and the effect of interstitial elements on phase stability and mechanical behavior

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High and medium-manganese steels have attracted attention in materials science for their exceptional combination of mechanical properties, particularly strength and ductility. The mechanical behavior of these materials resembles multiple FCC multicomponent alloys (together with High-Entropy Alloys, HEA's) with relatively low stacking fault energy (SFE) [1]. The presence of plasticity mechanisms such as Twinning Induced Plasticity (TWIP) and Transformation Induced Plasticity (TRIP) plays a critical role in their distinct behavior, which can be directly related to the chemical composition. This study explores the design and characterization of high and medium-Mn steels, with a particular focus on the influence of interstitial elements (C and N) on their phase stability and mechanical performance. By integrating various modeling approaches, this research aims to provide an understanding of the phase stability and the deformation mechanisms applicable not only to steels but also to any FCC alloy. The calculations of the critical resolved shear stress, alongside the stacking fault energy predictions and the martensite start (Ms) temperature, were evaluated across different alloys and confronted with the experimental findings [2]. The phase stability is one of the main parameters that impaired the mechanical behavior; in which the presence of nitrogen alone proved to be insufficient to fully stabilize the austenitic phase (FCC) for medium-Mn steels. Nevertheless, the concurrent presence of both interstitial elements in solid solution has shown promising results in achieving materials that unify high strength with exceptional ductility.

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High-entropy alloy nanoparticles for green hydrogen generation

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In this presentation, we explore the significant role of high entropy alloys in catalysis, particularly through the lens of nanoparticles derived from these materials. Highlighting the surge in global and Brazilian investment towards green hydrogen, generated via electrolysis of water, we delve into the use of high-entropy alloy nanoparticles as catalysts for the hydrogen evolution reaction. Our research leverages computational simulations, employing density functional theory, to examine the impact of compositional variations on both the structure and catalytic efficiency of these nanoparticles. Additionally, we will present our progress in creating a comprehensive database for high-entropy alloy nanoparticles. This database not only enhances our understanding of these materials but also facilitates the development of interpretable machine learning models. By applying various descriptors and machine learning techniques, we aim to provide deeper insights into the properties and potential of our high-entropy alloy nanoparticle collection.

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Short-range order and local lattice distortions in High-Entropy Alloys: state of the art

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Understanding the complex atomic-scale structures within High-Entropy Alloys (HEAs) is crucial for tailoring their properties to diverse applications. The present contribution aims to provide an overview of the state-of-the-art experimental techniques employed in probing local lattice distortions and short-range order in HEAs, focusing on synchrotron / neutron-based advanced characterization with X-ray absorption spectroscopy and X-ray / neutron total scattering.

The primary challenges in analyzing multi-component alloys lie in the inherent reduced scattering contrast between the five or more alloying elements, often neighbors in the periodic table, and their simple crystal structures with few or even one single Wyckoff site. These characteristics constrain the amount of information that can be obtained from the data, a statement that can apply to transmission electron microscopy, as well. On the other hand, laboratory-based thermo-physical methods such as differential scanning calorimetry and electrical resistivity showed to be valuable in corroborating and quantitatively estimating order within HEAs.

It becomes evident that only the combination of several independent experimental approaches, ideally complemented by simulations, can effectively assign the contribution of each element to the solid solution and to the alloy overall performance.

Finally, it is important to recognize and take into account that every experimental method has its own strengths and weaknesses, to be shortly addressed in the final part of the lecture.

Structure of high entropy metallic alloys

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High entropy alloy is a novel metallic medium characterized by absence of a reference metal, as for in common alloys (Fe-based, Al-Based Ti-based ... alloys). Though basically multielemnentary solid solutions, HEA are more than simple random distribution of four or five metallic elements on a Bravais lattice. They are also characterized by local lattice distortions and potential short range order which affect the ideal configuration entropy and chemical properties. Composition and structural (distortions) flexibility give potentially high tunable ability for adapting properties and future prospect. For exemple, they have revealed interesting perspectives for hydrogen storage capacity [1].

Relevant characterization of complexity is always a challenge but necessary for optimization of properties, studies and analyses. As for in the theory of information [2], the entropy or “uncertainty” provides a unique value for characterizing complexity, as far as it is properly evaluated.

Often mentionned, the ideal entopy is most likely not relevant. An approach based on structural domains distribution (probability of occurrence of given arrangement) is proposed to evaluate an entropy of complex alloys. It was used to characterize metallic glasses and demonstrated a generalized effect on the mechanical behavior and glass transition of amorphous phases. An attempt is made to use a similar approach using simulation to characterize the HEA.

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Tailoring the Deformation Mechanisms in Non-equiatomic Co-Cr-Fe-Ni-Mn Medium/High Entropy Alloys (M/HEAs) to Achieve Enhanced Mechanical Behavior

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Thermodynamic calculations (e.g. using CALPHAD) were used to identify three non-equiatomic CoCrFeMnNi M/HEAs with different deformation characteristics, namely, twinning induced plasticity (TWIP) and transformation-induced plasticity (TRIP). The three alloys - Co15Cr15Fe50Mn10Ni10, Co20Cr20Fe40Mn10Ni10, and Co25Cr25Fe30Mn10Ni10 - were produced by vacuum induction melting, cast into a copper chill mold, homogenized, thermomechanically processed, recrystallized, characterized, and tested in tension at 25 °C and -100 °C. The annealed and deformed samples were characterized by a combination of electron backscattered diffraction (EBSD), high-energy synchrotron X-ray diffraction (HE-SXRD), and transmission electron microscopy (TEM). Increasing the Co and Cr concentrations is shown to result in lower stacking fault energy (SFE), increased recrystallization rates and lower grain growth rates resulting in finer grain in the Co25Cr25 alloy, where the highest strength-toughness was observed. Due to the decrease in SFE with increasing Co and Cr, a transition in the dominant deformation mechanisms from TWIP (Co15Cr15) to TWIP/TRIP (Co20Cr20) to TRIP (Co25Cr25) was observed. This work sheds light on the development of novel FCC M/HEAs from the CoCrFeMnNi system, by identifying alloys that exhibit an optimal strength-ductility/toughness balance. Sigma formation, known to increase with increasing Cr and Co, was not observed under the conditions studied.

Comparative Analysis of the Influence of Atomic Volume Difference and Electronegativity Difference on Solid Solution Strengthening.

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Solid solution strengthening (SSS) plays a crucial role in enhancing the mechanical properties of high-entropy alloys (HEAs). The lattice friction stress influences dislocation mobility within the lattice, impacting material strength. HEAs, with their multi-principal element compositions, may exhibit relatively large lattice distortion, contributing to enhanced strength. In this context, understanding the mechanisms governing SSS in HEAs is crucial for optimizing mechanical properties. Historically, various models have been proposed, emphasizing inputs such as atomic and Young's modulus mismatch or electronegativity difference. Varvenne's model emphas atomic volume disparities, while Oh's model highlights electronegativity differences as the primary determinant of SSS in Face-Centered Cubic (FCC) systems. These models present a scientific disparity, necessitating further investigation to determine the predominant factor influencing SSS in HEAs. Hence, this study aims to reconcile the conflicting models proposed by Varvenne and Oh, which attribute SSS in HEAs. Alloying additions of Pd and V were introduced into the CrCoNi system and pure Ni to test both models. These alloys offer a diverse range of differences in electronegativity and atomic volume, providing an ideal platform for experimental exploration. The experimental results will shed light on the conflicting models, elucidating the predominant role of atomic volume against electronegativity in SSS.

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Design of Low-Cost ZrNbFeCo Medium Entropy Alloy for Hydrogen Storage at Room Temperature

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"Medium Entropy Alloys (MEAs)" are a subclass of multicomponent alloys with promising applications in developing new metal hydrides with tunable hydrogen storage (H_2S) properties. MEAs are typically a simple mixture of three or four elements, in equiatomic or non-equiatomic ratios, ranging from 5 to 35 at% [1, 2]. Recently, we showed that the ZrNbFeCo equiatomic MEA, prepared from high purity elements, exhibits excellent H_2S properties, absorbing up to 1.14 wt% of hydrogen at room temperature with fast kinetics, good reversibility and good stability due to its dominant C14-Laves phase [3]. This work investigates the effects of using a commercially available ferroniobium (FeNb) alloy, instead of pure Fe and Nb, on the crystal structure and H_2S properties of ZrNbFeCo. This substitution aims to create a more cost-effective alloy with similar performance. The alloy was obtained by arc melting under an inert argon atmosphere. Characterization techniques such as XRD with the Rietveld refinement method, SEM/EDS, and TEM will be used to stuyd the alloy’s microstructure. The H2S performance will be evaluated with absorption/desorption kinetics and PCT isotherms. Initial XRD results show the presence of a major C14-Laves phase, like the original composition, and it’s expected that the SEM/EDS also show a similar phase distribution. Initial H_2S results suggest improved absorption kinetics at room temperature, so it’s expected that the PCT curves show a similar behavior. Further analysis is necessary to fully understand the impact of the promoted substitution.

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Detection of chemical short-range ordering through thermal analysis in the equiatomic CrCoNi alloy.

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Previously, it was believed that medium/high entropy alloys were constituted in a random solid solution, meaning each element would have the probability of occupying an atomic position equal to its molar fraction[1]. Recent research has evaluated the influence of mixing enthalpy to determine phase stability, obtained at low temperatures and its influence on the formation of chemical short-range ordering (CSRO). Due to the complexity of the CSRO phenomenon, detecting and quantifying this phenomenon experimentally is a major challenge[2]. Therefore, this study aims to evaluate CSRO in the Co33Cr33Ni33 alloy aged at 748 K for different times using CrNi2 as a reference alloy, through molecular dynamics simulation predictions using Monte Carlo in conjunction with experimental analyses of specific heat, synchrotron X-ray diffraction, and transmission electron microscopy. The results obtained from specific heat analysis detected exothermic and endothermic reactions in both alloys, associated with the order/disorder reaction. Microstructural characterization analyses did not detect any formation of another phase in the ternary alloy, and only the formation of long-range ordered phase in the binary alloy. The simulations were consistent with experimental results at temperatures above 873 K.

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Effect of atmosphere control during the arc-melting production of the (TiNbV)85Cr15 alloy on its hydrogen storage properties

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Hydrogen is an energy vector that allied to renewable sources becomes a possible solution for the next generation and storage of energy. Multicomponent alloys that crystallize within the body centered cubic crystalline structure have been widely studied to storage hydrogen, such as (TiNbV)85Cr15[1,2]. The atmosphere control during the synthesis of multicomponent ingots is a challenge to the large-scale production process since oxygen might deteriorate the hydrogen absorption/desorption properties. In this work, the effect of the protective atmosphere during the synthesis by the arc-melting process of the (TiNbV)85Cr15 alloy was investigated. The alloy was produced under different protective atmospheric controls, which lead to different oxygen content in contact with the molten alloy. The alloy was characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM) and chemical analysis for oxygen quantification. The hydrogen storage properties were evaluated using volumetric tests in Sieverts-type apparatus. The results showed the effect of oxygen content from different levels of molten metal protection on the microstructure and hydrogen storage properties of the alloy. Although the higher oxygen content of about 0.66 wt% leads to the formation of oxides in the microstructure, the hydrogen storage properties of the alloy produced under a less protective atmosphere is not considerably affected, with a slightly reduction in capacity and small increase in the hydrogen absorption and desorption equilibrium pressures.

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Exploring High Entropy Alloys: Genetic Algorithm Selection and Multi-Technique Characterization

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In this study, a Genetic Algorithm (GA) [1] was developed to effectively identify high entropy alloys (HEAs) showcasing optimal mechanical properties. The GA was tailored to prioritize single-phase face-centered cubic (FCC) HEAs, assessed through empirical models [2,3], and emphasizing high values of the Hall-Petch constant (K) and critical resolved shear stress (σy) to ensure superior ductility and strength, respectively. Subsequently, the most promising alloy composition was synthed and subjected to comprehensive characterization. This included analyses through scanning electron microscopy, transmission electron microscopy, synchrotron X-ray diffraction, and Vickers microhardness testing. These characterization techniques provided detailed insights into the alloy's microstructure and mechanical properties. The results revealed an unconventional alloy composition, highlighting the efficacy of the proposed methodology in uncovering unbiased and innovative alloy compositions within a multi-objective framework. However, microstructural analysis unveiled a presence of multiple phases, indicating potential limitations in phase prediction using empirical parameters and emphasizing the GA's sensitivity to input variables. These findings contribute to advancing our understanding of HEA selection methodologies and empha the need for further refinement in predictive modeling approaches.

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How might we utilize the QUATI Beamline to elucidate the behavior of complex alloys during reaction conditions?

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The X-ray Absorption technique is highly appealing due to its atomic and specific sensitivity. However, a single technique is often insufficient for fully characterizing Complex Alloys. At the QUATI Beamline [1], a combination of techniques is planned to address the intricate challenges posed by these materials. This Beamline will enable access not only to the local structural information provided by XAFS but also to Long Range order using XRD and Raman Spectroscopy simultaneously on the sample under reaction conditions. These complementary techniques can provide a comprehensive understanding of transitions in complex alloys, allowing researchers to achieve in-depth characterization that facilitates a profound understanding of kinetic processes. These possibilities, combined with dedicated data analysis programs developed for this purpose, will be presented, showing how with this convergence of techniques and analysis is possible solve the complex puzzle given for this samples.

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Hydrogen and Small Molecules Adsorption on High-Entropy Nanoparticles: A Density Functional Theory Investigation.

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Metallic alloys, especially those formed by transition metals, have been widely used in various technological applications. Recently, a special type of metallic alloy formed by five or more elements, called high-entropy alloys, has attracted attention for exhibiting remarkable properties, ranging from catalytic processes to sensors. In this work, we conducted a theoretical analysis based on DFT to propose a special type of high-entropy nanoparticle obtained from a previously synthed decagonal quasi-crystal metallic bulk with the Al70Co10Fe5Ni10Cu5 stoichiometry [1,2].

We investigated the structural and formation properties of a sample of these nanoparticles and examined their interactions with hydrogen atoms and small molecules to determine if the nanoparticles follow the same trends as other forms of high-entropy alloys, such as their 2D counterparts.

We found that these nanoparticles exhibit a strong affinity for interacting with both hydrogen and other molecules. This suggest that these nanoparticles have great potential for use in building molecule sensor devices.

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Microstructural changes and hydrogen storage properties of High-Entropy Alloys derived from the (TiZrHfV)($Nb_{1-x}Cu_x$) system, where x = 0, 0.6, 0.8, 1.0.

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This study focused on exploring the microstructure and the hydrogen storage properties of High-Entropy Alloys (HEAs) derived from the (TiZrHfV)($Nb_{1-x}Cu_x$) system, where x = 0, 0.6, 0.8, 1.0. The TiZrHfVNb alloy (x = 0) was already reported by S. Sleiman and J. Huot (2021) and used as a reference for the other compositions in this study. The full Nb alloy was reported to have a single BCC phase in the as-cast state and absorbed 2.0 wt.% of hydrogen within an incubation time of 400 seconds. To understand the effect of the addition of a comparatively small atom on the crystalline structure of the alloy and the hydrogen storage properties, Cu was incrementally added at the expense of the atomic percentage of Nb. The alloys were produced by arc-melting and studied by detailed structural and microstructural characterizations performed by XRD and SEM/EDS. The XRD experiments followed by Rietveld Refinement for x = 0.6, 0.8, and 1.0 showed the presence of the C14 Laves phase, respectively, of 70%, 76%, and 86% in weight. It was also identified in all the alloys a minor amount of BCC phase. With the increase in the atomic percentage of Cu, the SEM images showed a change in the microstructure. For the reference alloy (x = 0), the microstructure is very homogeneous, consistent with a full BCC structure. Conversely, with the increase of Cu, it became clearly the appearance of an interdendritic bright region rich in Hf and Cu, very poor in V, and a dendritic dark region very rich in V, both consistent with the characteristics of the intermetallic ordered C14 Laves phase. Hydrogen storage properties have been also systematically investigated. The alloys went through a thermal activation procedure, which consisted of heating the samples to 450 °C for 3 hours in vacuum. After the thermal activation, the Cu-based HEAs absorbed 1.4-1.6 wt.% at room temperature and 20 bar of hydrogen, with an incubation time of 20-60 seconds. However, the alloys were not able to desorb at room temperature. To investigate this behavior, the alloys were desorbed at 100°C, 200 °C, 300°C and 400 °C. At maximum temperature, the full Cu alloy (x = 1) desorbed 28% of hydrogen, while this amount increased to 53% (x = 0.8) and 60% (x = 0.6). The calculated hydrogen enthalpy for the alloys is about -100 kJ/mol.H2, indicating that the alloys form very stable hydrides, which explains the lack of desorption at room temperature. Compared to the reference BCC-structured alloy, the absorption steps were easier for the C14 Cu-based alloys, but the amount absorbed was significantly smaller.

Microstructural, Corrosion and Mechanical Properties Characterization of Biocompatible High-entropy Alloys (Bio-HEAs) with BCC-Structure

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High-entropy alloys (HEAs) with a body-centered cubic (BCC) structure are attracting attention due to their excellent mechanical properties, corrosion resistance, and high biocompatibility, making them ideal for biomaterial applications [1,2]. These alloys tailored specifically for biomaterial use are commonly known as Bio-HEAs. In this study, Bio-HEAs derived from TiZrNbMoSnx and TiZrNbTaSnx systems (for x = 0, 3, and 5 at%) were obtained by arc melting and characterized as biomaterial. We aim to investigate the mechanical properties, corrosion resistance, and biocompatibility of the Bio-HEAs after the following microstructural alterations: i) the addition of Sn in proportions of 0, 3, and 5 at% in the TiZrNbTa and TiZrNbMo alloys; ii) the use of heat treatments at controlled temperatures; iii) the use of severe plastic deformation using the High-Pressure Torsion technique. Preliminary results reveal that the alloys in their as-cast state possess a single-phase configuration with a BCC structure. SEM images accompanied by compositional mapping reveal the existence of a microstructure predominantly composed of a BCC phase with a homogeneous distribution of elements in the as-cast samples. Vickers hardness tests revealed a significant increase in hardness with the addition of Sn; for example, in the as-cast state, for samples with 5 at% of Sn: from 476.6 HV to 544.5 HV for the TiZrNbMoSn5 alloy; from 342.0 HV to 457.2 HV for the TiZrNbTaSn5 alloy. After HT, all samples showed a slight decrease in hardness. Nanoindentation tests for measuring Young's modulus, corrosion resistance, and evaluation of the biocompatibility of the alloys, in the as-cast and HT states, are currently in progress. Selected samples will be processed by HPT, which will be carried out at Kyushu University, Japan.

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Phase equilibria at 1100 °C in the Zr-rich region of the Al-V-Zr system

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High entropy alloys containing Al and refractory metals are promising structural materials for aeronautical applications, complementary to Ni-based superalloys. Conceptually, these alloys are preferably composed of at least five metallic elements with concentrations between 5-35 at%. [1]. The knowledge about the phase relations in the Al-V-Zr system corresponds to an important contribution for the development of these alloys, especially for research projects related to the development of thermodynamic databases. Previous studies by our research group raised questions about the stability of the ternary phase $Zr_{13}V_2Al_5$, indicated as stable phase in the isothermal sections at 1100 °C reported in the literature [2,3]. If its existence is not confirmed, new phase equilibria in that region should be determined. In the present work, the experimental investigation of phase equilibria in the Zr-rich region of the Al-V-Zr system was carried out by arc-melting samples, followed by heat treatment at 1100 °C, microstructural characterization using SEM, EDS and XRD. The $Zr_{13}V_2Al_5$ ternary phase was not found in equilibrated samples at 1100 °C, corroborating the authors' previous results in the range of 1050 to 1200 °C, and diverging from the 1100 °C sections proposed so far regarding this ternary system. Thus, the (Zr)-ht phase equilibrates, at 1100 °C, only with the Zr_2Al, $ZrAl_2$ and ZrV_2 phases.

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Probing Chemical Short-Range Order in CrCoNi through a new design strategy

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The multi-principal element alloy (MPEA) design approach represents the premise of vastly expanding the possible compositions for alloys. FCC MPEAs have demonstrated their potential for multiple engineering applications, including the CrCoNi alloy, one of the toughest materials known. However, much remains elusive in understanding the structural behaviors of MPEAs. The complexity associated with multiple principal elements (absence of a clear solvent) has sparked considerable interest in MPEAs literature. For instance, studies indicate that the slight local preference between the elements can lead to chemical fluctuations and, consequently, to chemical short-range order (CSRO). Yet, the characterization of this phenomenon is proven to be highly difficult and controversial [1]. In an effort to elucidate these fundamental questions, the following design approach was proposed: Addition of alloying elements that would favor CSRO occurrence while also providing a significant contrast to facilitate detection/characterization. For this objective, different CrCoNi-X alloys (X = Ta, Mo, Nb or Al) were produced via arc-melting. The samples were homogenized into a single-phase FCC condition. After processing, a final "CSRO aging" treatment was carried out at 475 °C to minimize the tendency of random chemical distribution. For all samples, both the aged and fully recrystallized conditions were characterized via SEM, DSC, TEM (with electron diffraction and EDS), and In-situ Dilatometry with High-Energy XRD. The results show variation in the CSRO distributions, which were interpreted in terms of the chemical bonding between the different atomic pairs and Waren-Cowley parameters.

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The site blocking effect in interstitial solid solutions described by Johnson-Mehl-Avrami-Kolmogorov model

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Important materials for the society technological development present interstitial solid solutions such as carbon in steel and hydrogen in metals. Since 1963, thermodynamic models have been developed aiming to describe the behavior of the interstitial solid solutions [1]. Accurate models to describe the interstitial solid solutions is paramount to design new materials and to improve computational tools. Thus, this work focused in describing the configurational entropy of interstitial solid solutions with the site blocking effect (SBE), i.e., when the previous occupation of one interstitial site by an interstitial specie prevent some of the near neighbor sites to be occupied, thus, reducing the number of configurations possible for the interstitial solid solution. Since the occupation of interstitial atoms is random, the blocking of neighbor sites also can be assumed as random. Therefore, we proposed that the Poisson statistics can be employed to describe the blocking phenomenon and we derived a model to describe the SBE with the format of the well-known Johnson-Mehl-Avrami-Kolmogorov equation. This model was called JMAK model for SBE and describes the fraction of blocked sites as function of occupied sites, which can be used to calculate the configurational entropy of interstitial solid solution [2]. The JMAK model allows to estimate the fraction of blocked sites considering the overlapping of blocked sites in a simple and direct way. The validation of the model was carried out by comparing with the configurational entropy obtained from both numerical simulation, and experimental data for V, Nb, and Ta [3] with those calculated using the JMAK model.

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Analysis of Mechanical Resistance and Corrosion Performance in High Entropy Alloys: A Comparative Study of Al-Co-Cr-Ni-V and Al-Co-Cr-Fe-Ni-V Systems

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High entropy alloys (HEAs) constitute a class of multicomponent metallic systems characterized by a high number of principal elements, typically exhibiting equiatomic or near-equiatomic compositions, ranging between 5 and 35 at.%. These alloys that can have their properties tailored through adequate selection and variation of constituent elements are promising for advanced structural applications. Among HEAs, those based on the Al-Co-Cr-Fe-Ni system have received particular attention due to their exceptional properties. The formation of body-centered cubic (BCC) phases within these alloys contributes to high hardness and wear resistance. This study aimed to explore new alloy compositions within the Al-Co-Cr-Ni-V and Al-Co-Cr-Fe-Ni-V systems. The alloy design was guided by empirical parameters and thermodynamic calculations employing the CALPHAD method via Thermo-Calc software. The alloys were obtained by arc melting and structurally and microstructurally characterized by scanning electron microscopy and X-ray diffraction techniques. Mechanical properties were assessed through micro and nanoindentation techniques, while corrosion resistance was evaluated by potentiodynamic polarization tests. In their as-cast conditions, HEAs exhibit a biphasic microstructure consisting of BCC phases with B2 and A2 structures, alongside dendritic morphology. Hardness values for as-cast alloys ranged from 500 HV and 735 HV, while elastic moduli varied from 160 to 217 GPa. Alloys with higher amounts of V exhibited the highest levels of hardness and modulus of elasticity. Regarding corrosion behavior, alloys containing Fe showed superior performance, especially the equimolar alloy. These Fe-containing alloys demonstrated higher corrosion potentials, higher pitting potentials, and lower corrosion currents compared to alloys without Fe.

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CALPHAD Simulations of High Entropy Alloys Using Pandat Databases - A Comparison Between Experiment and Calculations

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High entropy alloys (HEAs) represent a frontier in materials science, offering intriguing combinations of mechanical properties derived from complex multi-component systems. This study focuses on applying CALPHAD (Calculation of Phase Diagrams) simulations to predict the phase equilibria of various HEAs using Pandat software and databases. The thermodynamic calculations are compared with experimental results from several HEAs developed by the research group, assessing the accuracy and predictive power of current thermodynamic models. The HEAs investigated include systems based on V-Cr-Fe-Mn-Co-Ni, with and without elements such as Al-Ti to form precipitates. Each alloy system was synthed using arc melting, followed by homogenization, and characterized by techniques such as X-ray diffraction (XRD) and scanning electron microscopy (SEM) to identify the existing phases and their distribution. The experimental phase equilibria were juxtaposed with the results from Pandat simulations, which utilized both existing database parameters and newly optimized data specific to the alloy systems. The results were also compared to other empirical criteria. The findings reveal a strong correlation between the calculated and experimentally determined phase diagrams, demonstrating the effectiveness of the Pandat databases in capturing the complex behaviors of HEAs. However, discrepancies in minor phase predictions, especially at lower temperatures, highlight the challenges in modeling the subtle thermodynamic nuances of HEAs. This study underscores the critical role of CALPHAD simulations in the design and optimization of HEAs and suggests pathways for refining these computational tools to enhance their application in materials discovery and development.

Characterization of a Duplex CrCoNiAl High-Entropy Alloy Produced by Directional Solidification with Different Cooling Rates

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High-Entropy Alloys (HEAs) represent an innovative class of materials distinguished by the absence of a primary alloying element. Comprising of concentrated solid solutions of various alloying elements, the CrCoNi system stands out within this class [1]. While the focus of developing these alloys has been on compositions favoring the formation of face-centered cubic (FCC) structures, studies suggest that duplex alloys in this system, containing both bodycentered cubic (BCC) and FCC phases, may display exceptional mechanical properties [2]. This study aims to assess the influence of the presence of the BCC phase in the Cr44Co35Ni16Al5 MPEA and evaluate the impact of cooling rates on microstructure morphology. The alloy was manufactured using directional solidification techniques with low and various cooling rates. This approach emerges as a promising method to stabilize the BCC phase and prevent the formation of the sigma phase [3]. Optical microscopy, scanning electron microscopy (SEM), and transmission electron microscopy (TEM) showed that the increase of cooling rate had an effect in reducing dentritic spacing and lamellar spacing in the eutectic regions of the as cast samples. Vickers microhardness and tensile tests revealed that the reducing of those spacings, as well as the presence of the second phase BCC, increased the resistance of the material when compared to a similar alloy with a pure FCC microstructure.

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Characterization of different carbide distributions for a Cr-Co-Ni alloy

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Multi-principal element alloys (MPEAs) or high/medium-entropy alloys are characterized by not having a well-defined solvent. More than a new class of materials, they represent a new conception of alloy design. Among the face-centered cubic (FCC) MPEAs, the Cr-Co-Ni system stands out for having toughness values among the highest ever observed for any engineering material. Additionally, alloying with small amounts of carbon can further elevate this property [1,2]. As such, this study aimed to investigate the effect of carbon addition to a Cr-Co-Ni alloy and better understand the effect of carbide distribution on the material's hardness and microstructure. To achieve this, the alloys were produced and processed by two different routes: without and with a precipitate dissolution step. In the first case, a heterogeneous dispersion of second-phase particles was obtained, while for the second route, the distribution was homogeneous and more efficient in increasing the final hardness. Characterization was carried out via optical microscopy, scanning electron microscopy (with energy dispersive X-ray spectroscopy), X-ray diffraction, transmission electron microscopy, Vickers micro-hardness and tensile testing. Alongside with Hall-Petch (HP) analysis, microstructural characterization revealed almost no precipitation hardening effect for the carbides but a strong HP strengthening effect. In summary, a comprehensive investigation of carbide precipitation (considering different fractions, particle s and distributions) within a Cr-Co-Ni FCC matrix was studied. The findings are anticipated to significantly contribute to the understanding and guidance of future processing strategies for high-performance MPEAs.

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Characterization of Eco-Friendly Refractory Ceramics with Complex Compositions: Microstructural Analysis and Comparison

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Electrofused magnesia-chromite aggregate (EMCA) is renowned in the realm of refractory ceramics, particularly for its mechanical properties such as resistance to corrosion and thermal shock damage. However, its high toxicity, stemming from the release of hexavalent chromium (known to be allergenic and carcinogenic to humans) under working conditions, necessitates its replacement in industrial settings with a product free from chromium or other toxic compounds in its composition. In a prior study conducted by our group[1], it was confirmed that the microstructure of EMCA comprises a periclase matrix with spinel precipitates and oriented microcracks. Utilizing complex ceramics design principles, two environmentally friendly compositions were developed as potential alternatives to EMCA. This study aims to delve deeper into the analysis and comparison of the microstructures of two of these compositions, to identify the most suitable conditions, through various heat treatments, to replicate the microstructure of the commercially utilized product. The selected compositions, which exhibit thermodynamically predicted complex spinel formation, were fabricated via solid-state sintering and subjected to heat treatments at 1200°C, 1300°C, and 1400°C for 24 hours. Techniques such as scanning electron microscopy and synchrotron X-ray diffraction were employed to characterize the microstructures. The anticipated outcomes of this investigation are expected to provide valuable insights for the controlled replication of the microstructure of electrofused magnesia-chromite aggregate.

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Computation Materials Design of High Alloys for Strength and Toughness

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Designing strong single-pahse high entropy alloys with the potential for precipitation hardening presents a significant challenge across various alloy systems, owing to the intricate interplay of composition and heat treatment parameters. In this overview talk, we will explore the utilization of artificial intelligence (AI) alongside thermodynamic calculations based on the CALPHAD method to analyze diverse datasets encompassing multiple alloy compositions. Through the application of filtering criteria, we aim to identify general trends and predict the capabilities of these alloys for both solid solution hardening and maximum precipitation hardening, thereby enhancing their yield strength. We will discuss previous results from our research group and broader implications of these methodologies in the field, highlighting their potential for efficiently identifying and developing novel precipitation-hardenable alloys with good combinations of mechanical properties. This approach offers insights into the overarching challenges and opportunities in alloy design, paving the way for advancements in materials science and engineering.

Electrodeposition of high entropy FeCoCrNiMn coating on SAE 1020

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High entropy alloys (HEA) represent a relatively new class of metallic materials. They are composed of multiple components, without a predominance of elements, in an equiatomic form of five or more elements, with atomic concentrations between 5 and 35%. They present a distorted crystal structure and a combination of characteristics that affect their structure and functionality. These alloys exhibit excellent mechanical properties, such as high strength, hardness, wear and compression resistance, and chemical properties, including corrosion resistance. From the point of view of practical engineering applications, the and cost of components manufactured with HEA and produced by conventional casting methods are still considered a barrier. In this sense, coatings based on high entropy alloys have been gaining prominence in the scientific scenario to improve surface characteristics of conventional metallic alloys in a variety of applications, as resistance to corrosion and wear, when applied to low-cost metallic substrates, such as carbon steels and aluminum alloys. The electrodeposition process is considered advantageous in relation to the cost of equipment necessary for its execution and a more precise adjustment of the deposition conditions. In this study FeCoCrNiMn HEA coatings were electrodeposited on SAE 1020 steel. Process parameters as concentration of elements in the electrolyte, current-voltage values and process time of 15 and 30 minutes as well as substrate surface finish, were evaluated. The coatings obtained were characterized by X-ray diffraction, scanning electron microscopy and spectroscopy of dispersive energy. The electrochemical behavior in a 3.5 wt% NaCl aqueous solution was evaluated by the techniques of impedance spectroscopy and linear polarization. The results show the formation of a homogeneous coating on the steel surface and good corrosion resistance.

Evaluation by Thermal and Mechanical Analyses of the Short-Range Ordering Effect on $Cr_{33}Co_{17}Ni_{50}$ Alloy

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In the last 20 years, a new class of alloys called multi-principal element alloys (MPEAs) has emerged. This new class consists of three or more elements in equimolar or nearly equimolar proportions, that is, without the presence of a primary element. Recent research on these alloys seeks to understand the interactions governing short-range chemical ordering, aiming to pave the way for improvements in mechanical properties. Therefore, this study evaluates the influence of aging heat treatments at 350°C for different durations on the $Cr_{33}Co_{17}Ni_{50}$ alloy, aiming to induce short-range order (SRO) phenomenon and to observe possible relationships with alloy properties. The objective of this work is to analyze the influence of SRO on the $Cr_{33}Co_{17}Ni_{50}$ alloy through microstructural characterization (XRD and SEM), analysis of mechanical property (microhardness), and physical property (specific heat). Comparing the microhardness of the samples, it was possible to observe that the increase in aging time may result in a slight increase in microhardness and grain . It was also observed through microstructural characterizations that aging did not cause the presence of a second phase in the sample.

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Heat Treatment and Thermomechanical processing for Modifying the As Cast Microstructure of High Entropy Alloys of the TiVNbCrMn System

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Multicomponent alloys containing five or more elements in compositions ranging from 5 to 35 at. % are called as high-entropy alloys (HEAs). HEAs have shown potential for technological applications, such as solid-state hydrogen storage. Alloys from the TiVNbCrMn system have exhibited high hydrogen capacities of the order of 3.3 wt%. Despite the good results, these alloys have been studied in their as-cast condition, characterized by dendritic morphology, large grains, and interdendritic segregation. Modifications of the as-cast microstructure and improvement in chemical homogeneity can be achieved by heat treatments and thermomechanical processing. These modifications can potentially affect hydrogen absorption and desorption properties. Hence, this work aimed to evaluate the effect of heat treatments and thermomechanical processing on the microstructure of $Ti_{35}V_{35}Nb_{20}Cr_5Mn_5$ and $Ti_{32}V_{32}Nb_{18}Cr_9Mn_9$ alloys. The alloy design was carried out using Thermo-Calc and the ingots were produced by electric arc melting technique. Homogenization heat treatment and hot deformation were performed at temperatures above 950°C. Structural and microstructural characterizations were performed by X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM) and Electron Dispersive Spectroscopy (EDS) techniques. Samples in the as-cast condition exhibited a single solid solution with cubic crystal structure (BCC-A2) with dendritic microstructure. After the heat treatment, dendritic morphology was still present, but there was segregation of Ti at grain boundaries and precipitation of Laves phase. Hot rolling processing successfully modified the as-cast microstructure, eliminating dendrites, and samples exhibited dynamic recrystallization necklace structure. It also resulted in significant grain refinement and enhanced alloys' homogeneity.

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High corrosion resistance of nanograined and nanotwinned Al0.1CoCrFeNi high-entropy alloy processed by high-pressure torsion

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Corrosion is responsible for the failure and the reduction of the lifetime of many metallic materials. For load-bearing components, there is a high demand to produce alloys with good strength and high corrosion resistance in corrosive environments. This study investigates the corrosion resistance of Al0.1CoCrFeNi high-entropy alloy following high-pressure torsion (HPT) [1,2], focusing on the influence of stored energy, diffusion coefficient, and the high-entropy effect. HPT was conducted with varying turns to induce shear strain. Microstructural analysis revealed a single-phase FCC structure with increased crystal defects and reduced crystallite post-HPT. Samples with higher HPT turns formed high-angle grain boundaries, equiaxed nanograins, and numerous nanotwins, contributing to a notable increase in Vickers microhardness from 159 Hv for the initial sample to 550 Hv after 5 turns of HPT. The uniform and pitting corrosion resistance of Al0.1CoCrFeNi alloy decreased after 1/16 and 1/4 turns and increased after 5 turns. Increasing the density of dislocations after 1/16 and 1/4 turns enhanced the surface reactivity and corrosion, while the formation of non-equilibrium grain boundaries after 5 turns made the diffusion of chromium feasible to the surface to form passive films for protection against corrosion. A comparison of Al0.1CoCrFeNi and CrMnFeCoNi Cantor alloy suggested that the passivation mechanism by the protective element depends on the high-entropy and sluggish diffusion effects in HEAs [3]. Local enrichment of the sample with the protective element will occur only if the mixing entropy of the sample is low enough to allow segregation of passivating elements with less influence of sluggish diffusion.

High throughput manufacturing of high entropy alloys

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High entropy alloys (HEA) consist of multiple elements at high concentrations, offering a vast array of potential compositions. Consequently, employing a high throughput experimental setup becomes imperative to optimize the most promising compositions that yield the desired properties. Samples featuring compositional gradients offer a convenient means to study multiple compositions within a single specimen. Various methods exist to generate a compositional gradient within a sample, such as diffusion couples or coating techniques. However, beyond the manufacturing setup of samples with multiple compositions, their mechanical characterization poses a significant challenge. Traditional experiments like tensile tests can be exceedingly time-consuming, requiring a specimen for each composition. Here, nanoindentation emerges as a rapid solution for characterizing a single sample with a compositional gradient, enabling the extraction of mechanical properties such as hardness and elastic modulus for each composition. This work explores different approaches and strategies for creating a compositional gradient in HEAs using diffusion couples, while also delving into the nanoindentation technique for their characterization. The results point to a good convergence between the techniques and the simulations, as well as other classical experimental approaches.

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Influence of Al addition on the microstructure and the oxidation resistance of the WMoNbTiCrAlx (x = 0, 0.25, 0.5, 0.75, and 1) RHEAs

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A new class of materials was discovered in 2004, known as high-entropy alloys (HEAs) and is described as alloys with multiple elements containing at least 5 main elements with an atomic percent between 5 and 35 At. %. In these alloys, the high configurational entropy can stabilize solid solution phases with simple structures, compared to potentially fragile intermetallic phases[1]. In this context, high-entropy alloys (HEAs) based on refractory metals were first documented by Senkov et al. (2010)[2], and the results showed their superior melting temperatures and promising high-temperature properties. Nevertheless, a significant drawback of refractory metal-based alloys lies in their low oxidation resistance at high temperatures, along with their high density. To mitigate these issues, certain refractory metals have been substituted with lighter elements such as Al, Cr, and Ti. Addressing this concern, a novel refractory system with Al addition, WMoNbTiCrAlx (x = 0, 0.25, 0.5, 0.75, and 1), was developed via arc melting, followed by analysis of the microstructure and mechanical properties in the as-cast alloy condition, and revealed formatin of only the solid solution phase with the BCC structure, with a typical dendritic structure and elemental segregation. Oxidation resistance was assessed by analyzing the mass gain of the samples at 1000 °C for 12 hours. The results indicated that the Al addition enhanced oxidation resistance. Other results indicate that the Al addition also increases hardness and decreases density.

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Magnetic properties of high-entropy compounds (Y0.2La0.2Gd0.2Pr0.2Er0.2)Al2 and (Y0.2La0.2Nd0.2Pr0.2Er0.2)Al2

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In recent years, configurational high-entropy alloys have surfaced as an innovative approach in the realm of metallic alloy development. Alongside alloys, high-entropy compounds have also gained attention. Systematic inquiries into the magnetic properties of these materials remain limited. Consequently, high-entropy magnetic materials represent a relatively unexplored category with substantial potential for applications, while also offering an enticing platform for experimental and theoretical exploration. In this study, we developed a theoretical model for configurational high-entropy compounds based on rare earth elements of the type (R1,R2,R3,R4,R5)Al_2, which was satisfactorily applied to the ferromagnetic compound (Gd,Tb,Dy,Ho,Er)Al_2 using experimental data on magnetization, specific heat, and magnetocaloric effect reported in the literature. We prepared and characterized two new compounds: $(Y_{0.2}La_{0.2}Gd_{0.2}Pr_{0.2}Er_{0.2})Al_2$ and $(Y_{0.2}La_{0.2}Nd_{0.2}Pr_{0.2}Er_{0.2})Al_2$. The first exhibits a magnetic transition temperature around 34 K and a magnetization of 2.07 μB/f.u. at 70 kOe, which is significantly lower than the expected value of 3.84 μB/f.u., considering all magnetic moments aligned in the direction of the applied magnetic field. The second compound shows a transition temperature around 19 K and a magnetization of 1.24 μB/f.u. at 70 kOe, which is also much lower than the expected value (3.09 μB/f.u.), considering the same alignment of the magnetic moments. Soon, we will apply the theoretical model to the experimental data of these new configurational high-entropy compounds.

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Microstructure and Mechanical characterization of SiC-reinforced CrMnFeCoNi high entropy alloy

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The CrMnFeCoNi alloy is the most studied and well-known among the high entropy alloys, with the first works being published in the early 2000s. These alloys, due to their compositional versatility, have potential applications in the aerospace, automotive, among other industries. Recent studies indicate to possibility of synergistic combination between a high-entropy phase and a ceramic reinforcement. This study synthed the alloy with different SiC contents (0%wt, 5%wt, and 10%wt) by vacuum arc melting, starting from high-purity metal powders. Characterization involved X-ray diffraction, optical microscopy and Vickers microhardness. The diffractograms indicated the formation of an FCC phase, typical of this alloy under all SiC contents. However, with the addition of SiC, new phases, different from those expected, were observed. This fact was intensified with the increase from 5%wt to 10%wt. The sample without SiC addition presented a uniform microstructure with the presence of some pores and an average hardness of 183 HV. For the sample with 5%wt of SiC, a biphasic microstructure was observed with an average hardness of 363 HV, with a bright dendritic region surrounded by a darker phase rich in carbides. The sample with 10%wt of SiC has a refined microstructure, consisting of a matrix with a hardness of 640 HV and thin dispersed plates (possibly carbides) with a hardness around 1000 HV. Two mechanisms can be attributed to this change. The first is attributed to more intense heterogeneous nucleation during solidification promoted by the increase in SiC concentration. The second mechanism indicates the decomposition of SiC followed by the in situ formation of chromium carbides. The chromium present in the alloy has a greater affinity for carbon than the other components, promoting the formation of chromium carbides and other intermetallic phases.

Production and Characterization of High Entropy Alloy for Validation of Artificial Intelligence Method

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Artificial intelligence (AI) algorithms play a crucial role in analyzing and training models to forecast material properties based on data. The quality and diversity of the data used in training are determining factors for the predictive capability of the model. The more comprehensive and varied the dataset, the higher the accuracy and flexibility of the algorithm [1]. In the current project, we aim to use CALPHAD parallel high-throughput calculations to generate data to train an artificial intelligence model. This model will subsequently be employed in conjunction with a genetic algorithm for alloy selection [2]. The objective is the attainment of a single-phase face centered cubic alloy, with expressive hardening by solid solution and TWIP/TRIP effects. Different configurations of both algorithms will be explored to select the most 3 prominent compositions. The differences and accuracy of both models will be discussed as well as potential candidates for future production and characterization will be shown. Through this analysis, we aim to gain a holistic understanding of the alloys' properties, enabling the assessment of the algorithm's potential for future applications.

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Production and Characterization of High-Entropy Alloy Ni-Co-Fe-Cr-Al-Ti Precipitation Hardenable by High-Efficiency CALPHAD

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High-Entropy Alloys (HEAs) has been gaining prominence in materials Science due to their unique compositions and premise of addressing some currently existing properties gaps. One design strategies for HEAs is controlling precipitation hardening to achieve enhanced mechanical properties. For this purpose, an alloy of the Ni-Nb-Fe-Cr-Al-Ti system, Ni56.8Fe23.4Cr10.6Ti5Al2.6Nb1.6 (at.%), studied in this work, was designed via the computational method of high-efficiency CALPHAD. Equilibrium solidification calculations were performed through HTC module of Pandat software, PanHEA2021 database was used to carry out the thermodynamics calculations, the module automatically conducts calculations based on user-defined compositional limits, concentration steps and temperature range. These calculations provided imput for solid solution strengthening calculation and precipitation, leading to final composition. The alloy consists of a FCC matrix and can be precipitation hardened forming ordered precipitates that provide anchoring mechanisms, hindering dislocation movement, significantly increasing the material's strength It was manufactured in electric arc furnace under argon atmosphere and subjected to heat treatments. Processed under different initial conditions, the alloy was homogenized for 8 hours at 1200 ºC, resulting in cracking during cold rolling. Fine Nb-rich precipitates presence in the matrix and on the crack surfaces was investigated via Scanning Electron Microscopy (SEM) with Energy Dispersive Spectroscopy (EDS) analyses. To better understand the precipitates effects, the alloy was subjected to aging treatments at different times (from 15 min up to 48 h) and characterized via Vickers microhardness, SEM-EDS, High-Energy X-ray Diffraction and Differential Scanning Calorimetry (DSC).

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Production and Characterization of High Entropy Alloy with Optimized Toughness by Genetic Algorithm

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In the quest for novel materials, Multi-Principal Element Alloys (MPEAs) stand out for their ability to offer unique properties, optimized for each application [1]. Genetic algorithms (GAs) play a key role in alloy composition. By adapting to various variables, GAs can be tailored to create alloy families that achieve desired objectives through iterative mutations and crossovers.[2].In this study, a GA was created to search and select families of single-phase FCC MPEAs with expressive hardening by grain refinement and solid solution. Previous studies from our group reinforce the importance of the input parameters. In this scenario, the shear modulus (G) was particularly selected to be studied in further depth in the present study, by selecting different input sets considering values for both pure metals and elements in its FCC state. Variation of G values led to the selection of distinct prominent compositions. From these compositions, computational simulations were conducted using thermodynamic calculations via the CALPHAD method to confirm the expected structure. Subsequently, the alloys were produced with high-purity elements via arc melting and homogenized at a temperature above the solvus predicted by the CALPHAD. Samples underwent cold rolling, in order to get various grain s for obtaining a Hall-Petch curve. Then, they were analyzed via SEM/EDS and x-ray diffraction to verify the formation of predicted phases. The potential of GAs as a predictive tool in discovering and optimizing new MPEAs with enhanced properties is discussed.

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Synthesis and characterization of WMoCrTiAlSi refractory high-entropy coating designed by high-throughput methods

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Abstract:
In this work, a methodology was proposed for the synthesis of a high entropy alloy (HEA) thin film with refractory properties. The aim was to deposit a film with microstructural characteristics of HEA, with the presence of a disordered solid solution matrix. To design the alloy, a minimum set of target properties of interest was defined for the alloy: yield strength, oxidation resistance and cost of raw materials. Based on these properties, six constituent elements were chosen, and an artificial intelligence model trained with data mined from public literature [1] was then developed to determine the optimal chemical composition of W22,5Ti22,5Mo14,5Si14,5Al13Cr13. Then, a film deposition process was proposed based on the magnetron sputtering technique with three targets, using a balance of powers to achieve the ideal stoichiometry. Two samples were deposited, one with a rotating sample holder to enhance homogeneity and uniformity, and the other with a static configuration, aiming for a film with a compositional gradient. Characterization of the samples revealed a morphologically uniform, chemically homogeneous single-phase BCC microstructure and the presence of the effects of high entropy and severe distortion of the HEA network [2].

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Synthesis by arc melting of MgZnSnSbBi high entropy alloy and characterization of their properties.

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Electronic soldering is a crucial process in the manufacturing of electronic devices, and the choice of solder alloys plays a fundamental role in their effectiveness and durability. In the material science field are crescent the interest of development of new solder alloys Pb free, with comparable characteristics of the soldering traditional materials [1]. In recent years, the field of high entropy alloys (HEAs) has emerged as a vibrant and promising area of materials science research. The combination of multiple elements at equimolar concentrations in high entropy alloys offers the opportunity to adjust a variety of properties, including melting point, mechanical strength, electrical conductivity, and corrosion resistance. Research and development of low melting point high entropy alloys (LMHEAs) stand out as a potential alternative for replacing these materials [2,3]. The objective of this work was the synthesis and characterization of a nearly equiatomic MgZnSnSbBi alloy. The synthesis of this alloy was carried out using Mg, Zn, Sn, and Bi pellets (commercial purity) and Sb powder (high purity). The elements were melted and homogenized in a arc melting furnace, under an argon atmosphere, in a cooled copper crucible. Characterization of this alloy included microscopy, X-ray diffraction, density determination and exploratory differential scanning calorimetry. LMHEAs, in particular, have attracted interest due to their ability to melt at substantially lower temperatures compared to conventional alloys [2,3]. This unique characteristic not only expands the range of potential applications but can also offer significant advantages in terms of processability and energy savings.

The partial isothermal section at 1000°C in the Ti-rich region of the Al-Hf-Ti system

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A new concept of metallic alloys has been developed by the scientific community in recent years. These are alloys of multiprincipal elements, also known as High Entropy Alloys (HEAs), which combine five or more elements in equiatomic or semi-equiatomic proportions. HEAs with refractory metals and aluminum as constituents are potential alloys for structural applications in the aerospace industry at high temperatures [1]. To contribute to their development, the Al-Hf-Ti system has been experimentally investigated in this work since little information is available in the literature: one complete isothermal section at 1100°C [3] and one partial isothermal section at 1000°C in the Al-rich corner. For the present work, a partial isothermal section at 1000°C in the Ti-rich (45-95 at.%) region of the Al-Hf-Ti system is proposed. Twelve samples were produced by arc-melting mixtures of pure elements under Ti-gettered argon, followed by annealing at 1000°C for 10 days. Their microstructures were characterized by Scanning Electron Microscopy, Energy Dispersive Spectroscopy, and X-Ray Diffractometry. The results show the stability of two solid solutions related to the terminal elements, a bcc (Hf,Ti)ht and a hcp (Hf,Ti)rt, the first equilibrating with TiAl3 and TiAl phases, in agreement with the results reported by [3].

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Unraveling the abnormal hardness increase effect for MPEAs after incomplete annealing

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With its exceptional mechanical strength, particularly at high temperatures, CrCoNi alloy has garnered increasing research interest over the past decade as one of the toughest materials ever made [1]. However, a characteristic of CrCoNi and other FCC multi-principal element alloys (MPEAs) is their modest yield strength and hardness. Nonetheless, an abnormal increase in these properties was observed in literature for a cold rolled Cantor (CrMnFeCoNi) alloy annealed at 773 K, for which almost no recrystallization occurred [2]. This not fully understood phenomenon could pave the way forward into designing processing routes for even better mechanical properties for MPEAs. As such, for this work, a high-purity Cr-Co-Ni alloy was fabricated through arc-melting, homogenized and cold rolled up to 76 % reduction followed by annealing at temperatures of 673 K, 773 K, and 873 K for 1 h each. The hardness analysis, carried out with a Vickers microindenter, indicated that the sample annealed at 773 K showed the highest value, with a 30% increase compared to the cold rolled sample. Electron backscatter diffraction (EBSD), Transmission electron microscopy (TEM) and ASTAR (Automatic Crystal Orientation/Phase Mapping for TEM) characterizations confirmed that the abnormal increase effect is not caused by precipitation (akin to what is reported in the literature). What was found was an intricate deformation substructure. The dislocation distribution was further characterized via data processing of the EBSD and ASTAR results, and the findings are believed to be highly promising for better understanding and future design of processing strategies for high-performing MPEAs.

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Use of Density Functional Theory (DFT) in Study of electrical properties and Short-Range Ordering in High Entropy Alloys

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High Entropy Alloys (HEAs) are metallic materials characterized by the absence of a principal element, instead comprising concentrated solid solutions with concentrations of each element ranging between 5% and 35% [1]. The diverse definitions of HEAs result in a vast array of compositions, necessitating the use of computational tools for their analysis. Density Functional Theory (DFT), a simulation method rooted in quantum mechanics, has been successfully applied to study HEAs [2]. DFT enables the prediction of material properties such as energy gaps, elastic constants, and interface energies. In this study, the LSMS-DFT code was employed to forecast electronic properties such as the density of occupied states (DOS). The input data for DFT calculations consisted of supercells of HEAs with various compositions and conditions generated using Monte Carlo Molecular Dynamics (MDMC). The results of DFT simulations were compared with experimental data on electrical conductivity obtained from samples produced in an arc furnace, aiming to assess the reliability of predictions and gain insights into short-range ordering (SRO) within these alloys. This involved examining how the electronic properties of the material change relative to the degree of SRO.

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Wear behavior of AlCoCrFeNi HEA with Nb and Ti additions

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In the past two decades the concept and applications of metallic alloys with multiple main elements in equal or almost equal atomic percentages, known as high entropy alloys (HEA), have been widely studied. This alloy concept presents an innovative perspective of high performance alloys. The AlCoCrFeNi system is one of the most studied and its properties can be optimized with the addition of a sixth element, among which Nb and Ti can be highlighted, which are of strategic interest in technological advancement. The objective of this work was to study the effect of the addition of Nb and Ti on the wear behavior of AlCoCrFeNi system. The design of HEA was carried out using the CALPHAD method. Ingots of AlCoCrFeNiNb0.6, AlCoCrFeNiTi0.5 and AlCoCrFeNiTi1.2 were obtained by arc-melting furnace. The formed phases were analyzed by X-ray diffraction (XRD) and scanning electron microscopy associated with energy dispersive X-ray spectroscopy (SEM-EDS). The hardness and elastic modulus were estimated by nanoindentation and the wear behavior by the wear test using the linear reciprocal method. The profile and morphology of the worn surfaces were analyzed by optical profilometry and SEM. The addition of 0.6 mol of Nb led to the formation of homogenous B2/Laves hypoeutectic microstructure, while increasing Ti concentration led to the formation of Cr-rich BCC-A2 and Fe-Ti rich Laves phase. The average hardness values obtained were 790 HV, 597 HV and 731 HV for AlCoCrFeNiNb0.6, AlCoCrFeNiTi0.5 and AlCoCrFeNiTi1.2 HEAs, respectively. While the three compositions exhibited comparable friction coefficient, the alloy with Nb addition showed superior wear behavior. This was evidenced by the lower volume of material loss and the lower wear rate, which can be attributed to the fine and homogeneous hypoeutectic microstructure. The detailed examination of the worn surfaces showed features of abrasion, adhesion and oxidation wear were observed.

FM04-2D Materials: Fundamentals and Applications

Amplification of interlayer exciton emission in twisted transition metal dichalcogenides heterostructures

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Transition metal dichalcogenides (TMDC) heterostructures (HS) are obtained by stacking two or more different monolayers (ML). These structures host spatially indirect interlayer excitons (IX) with unique properties that depend on the twist angle and stacking order of two or more MLs [1]. However, the practical applications of IXs are limited by their weak oscillator strength, which leads to a significant reduction in emission. Therefore, innovative solutions to substantially improve the emission of interlayer excitons are desirable. Here, we present two concepts to enhance the emission of interlayer excitons in twisted TMDC HSs for future use in nanophotonic devices. One concept is based on advanced WSe2/WSe2/MoSe2 heterotrilayer (HTL) systems. In this system, the interlayer exciton formed in the HTL region exhibits up to a 10-fold increase in photoluminescence yield compared to the heterobilayer (HBL) region on the same sample. Detailed optical and numerical investigations show that the interactions between the three layers significantly contribute to the formation and relaxation mechanisms of interlayer excitons, resulting in the observed luminescence enhancement [2]. The second concept utilizes light-matter interaction of TMDC HSs integrated into chirped distributed Bragg reflectors, which feature energetically separated cavity resonances. This configuration enables cavity-coupled emission of intra and interlayer excitons that are energetically separated in a WSe2/MoSe2 HSs. The chirped microcavity, in combination with TMDC HSs, shows potential for studying moiré physics and enhancing light-matter interactions in TMDC-based devices [3]. Overall, our approaches offer versatile tools for future studies and applications of TMDC HS using innovative layer and cavity designs.

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Atomically-Thin Novel 2D Materials: Science, Technology and Applications

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The detection of toxic or harmful gases is mainly essential for the monitoring environment, human safety and industrial products manufacturing/monitoring. Recently, atomically thin two-dimensional (2D) inorganic semiconductor materials provided a unique opportunity for the nano/optoelectronics devices due to their atomic thickness, layered structure, extraordinary electronic and optical properties. Moreover, most of the topical research work on layered chalcogenides is understandably focused on single atomic layers. However, it is uncertain if the single atomic layer units are most ideal structures for enhanced gas-solid interactions. To probe this concern, we have synthed single layer and few layer thick nanosheets of various graphene like 2D materials including MoS_2, WS_2, $MoSe_2$, SnS_2, $SnSe_2$, $PtSe_2$, black phosphorus etc. using various methods such as micromechanical exfoliation, liquid exfoliation, electrochemical exfoliation, chemical vapor deposition method etc. and tested for gas sensing applications. The morphology, thickness/layering and elemental analysis of the sheets were characterized by using SEM, TEM, AFM, Raman spectroscopy and XPS etc. techniques. It is noteworthy that the 2D few layer MoS_2 nanosheets are better suited for superior NO_2 and NH_3 gas sensing applications, whereas SnS_2 nanosheets are highly suitable for alcohol sensing application. The 2D semiconductors in the form of electronic grade ink of $SnSe_2$ nanosheets based sensor device with different thicknesses was assessed for the humidity and NH_3 gas sensing performances showing high sensitivity and faster recover time. The results also show that compared to the thicker counterpart, sensor device of few layers exhibit excellent sensitivity, recovery and ability to be tune the sensing performance with thickness and can be used in lab on chip devices. The advantage of the 2D nano materials based sensor devices are the high sensitivity, faster recover time and devices are operated at room temperature. Electronic grade ink of 2D semiconductor materials might provide new direction for realizing ultrathin, flexible sensor devices with applications ranging from conventional sensor devices to portable and ultra-light devices.

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Covalent versus non-covalent linked 2D-Co_3O_4/GO heterostructures: catalytic and electrochemical properties

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The vertical stacking of 2D materials has led to the now well-known van der Waals heterostructures (vdW-Hs), which have fascinating synergetic properties. A whole new approach for obtaining these structures is through the covalent bond of the stacked layers, leading to cross-linked heterostructures (CL-Hs). This is a ground-breaking strategy for the design of 3D structures with controlled connections among 2D homo/hetero structures. In this work, we are interested in producing self-standing CL-Hs composed of graphene oxide (GO) and 2D-Co_3O_4. In this sense, 2D-Co_3O_4 was functionalized with APTES [1], leaving -NH2 groups available to connect to GO through amide bonds, leading to the Co_3O_4/GO CL-Hs. For this to be possible, the carboxylic groups of GO surface were previously activated through the EDC/NHS cross-linkers [2]. After the synthesis, the materials that were highly hydrophilic, turned into a self-standing hydrophobic platform. Co_3O_4/GO structures without covalent linkages presented high hydrophilicity. Contact angle measurements attested these behaviors. Infrared spectroscopy (FTIR) and X-ray photoelectron spectroscopy (XPS) certified the presence of all functional groups, especially the amide bonds, referred to C=O stretching at around 1640 cm^{-1} in the FTIR spectrum and the peak at 399.7 eV in the XPS. Scanning electron microscopy revealed the layered structure of the produced platform. Finally, the investigation of catalytic and electrochemical properties showed superior performance of the covalently bonded material. Indeed, the intriguing confined and controlled spaces between neighboring 2D layers in CL-Hs possibly favor new chemical processes that are worth investigating.

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Electronic and optical properties of phosphorene nanoribbons

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Phosphorene is a recently developed two-dimensional (2D) material that has attracted tremendous attention because of its unique anisotropic optical properties and quasi-one-dimensional (1D) excitons. We use first-principles calculations combined with the maximally localized Wannier function tight binding Hamiltonian (MLWF-TB) and Bethe-Salpeter equation (BSE) formalism to investigate quasiparticle effects of 2D and quasi-1D blue and black phosphorene nanoribbons. Our electronic structure calculations shows that both blue and black monolayered phases are semiconductors. On the other hand black phosphorene zigzag nanoribbons are metallic. Similar behavior is found for very thin blue phosphorene zig-zag and armchair nanoribbon. As a general behavior, the exciton binding energy decreases as the ribbon width increases, which highlights the importance of quantum confinement effects. The solution of the BSE shows that the blue phosphorene monolayer has an exciton binding energy four times higher than that of the black phosphorene counterpart. Furthermore, both monolayers show a different linear optical response with respect to light polarization, as black phosphorene is highly anisotropic. We find a similar, but less pronounced, optical anisotropy for blue phosphorene monolayer, caused exclusively by the quasi-particle effects. Finally, we discuss the role of hydrogen passivation on the electronic and optical properties of phosphorene nanoribbons and the advances in the understanding of quasi-one dimensional phosphorus-based materials.

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Engineering of single-photon emitters based on 2D materials

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Two-dimensional (2D) van der Waals materials have arisen as a novel platform to explore the characteristics of non-classical light throughout the fabrication of single-photon emitters (SPEs)[1-3]. Their large range of emission wavelengths, site-controllability, and the accessible properties tuning by engineered strain and defects, turning them into potential candidates for several applications, however, high-quality 2D-SPEs are still challenging to achieve, requesting the development of further fabrication techniques to accomplish the metric required in photonic quantum information technology. Here, we investigate the quantum-optical properties of WSe_2 SPEs generated on different substrates. A systematic study was conducted on dielectric site-controlled nanopillars and doped-substrates. Interestingly, by conducting off- and quasi-resonant optical excitation, we observe a substrate dependence on the number of quantum emitters and their extracted linewidths, and lifetimes, in which the doped surfaces command the properties of defect-states created in WSe_2 SPEs. In addition, we perform magneto-photoluminescence studies, where extracted g-factors for the systems above show a substrate-dependent response. Our findings unveil important characteristics of 2D materials SPEs, which may shed light on their weakly known nature and boost their applicability in quantum technology and optoelectronic semiconducting devices.

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From Forrest To Electronics: A Sustainable Perspective

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According to the United Nations University’s Global e-waste monitor, a record of 62 Mt of electronic waste was generated worldwide in 2022, which represents a record in human history, up 21% in only five years. The report also predicts that global e-waste will reach 82 Mt by 2030. This makes e-waste the world’s fastest-growing domestic waste stream, powered mainly by higher consumption rates of electric and electronic equipment, short lifecycles, and few options for repair. Sometimes it is mentioned that “e-waste is a toxic waste stream where valuable finite resources are lost”. The global consumption of electronics is forecast to double by 2050. In this context, printed electronics and 3D printing are an interesting alternative to conventional manufacturing methods and materials, reducing the weight of electronic components and offering more energy-efficient and sustainable solutions. Therefore, electronics, including flexible printed circuits are facing a critical challenge: How to balance, decreasing supplies with growing volumes of e-waste? In part: by using new sustainable approaches, either in terms of materials and technological processes! Here We propose the use of a new manufacturing technology supporting flexible and organic/inorganics electronics by exploring single laser processes for direct generation of conductive structures on biodegradable substrates. By means of different kinds of laser sources, conductive carbon nanostructures can be generated on carbon-based precursor materials and substrates via thermo-photo pyrolysis: the so-called Laser-Induced Graphene (LIG).

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Giant Enhancement of Photoluminescence and Valley Polarization of Multilayer MoS_2 by Ion Intercalation

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The optical characteristics of van der Waals (vdW) layered semiconductors exhibit significant sensitivity to the layer number, offering a means to tune their optical properties through the manipulation of interlayer coupling. We demonstrate the active control of interlayer coupling strength in multilayer MoS_2 through electrochemical ion intercalation. Specifically, we show that direct band multilayer MoS_2 can be achieved with giant enhancement of photoluminescence and valley polarization.

Graphene derivatives and its applications in biomedicine

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Graphene and its derivatives, has shown an easy functionalization with biological molecules such as DNA, enzymes, antibodies, RNA, c-DNA, viruses and bacteria among other biological systems generating a wide range of applications in order to develop new disease biosensing devices due to the low cost and speed to obtain results compared to conventional techniques. In this study we report a novel electrochemical portable biosensor for viruses detection and quantification based on reduced graphene oxide films. The working electrode was built following the synthesis of lysozyme-reduced graphene oxide (rGO) films proposed by Graphene oxide is synthed using modified Hummer's method and chemically reduced using hydrazine and lysozyme. Thin-films were produced by dip-coating deposition using rGO solution onto a gold substrate pre-treated with cysteine. We report the successfully application for RNA virus detection using cDNA functionalization on the working electrode surface and quantification of RNA concentration with a linearly dependency of chronoamperometric current. Also, it shows selectivity against an RNA different from the one used for electrode functionalization. The novel biosensor was applicated for RABV and Sars Cov-2 in-situ detection in nasopharyngeal swab samples of bat and humans showing a difference in response of positive samples from negative samples. This new biosensor proved to be an innovative electrochemical method for in-situ virus diagnosis including machine learning to improve efficiency.

Nano-bio-eco interactions of Graphene-based Materials: Toward Safe and Sustainable Innovation

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Graphene-based materials (GBMs) represent highly promising advanced materials for innovative applications. Consequently, they have garnered significant attention owing to their distinctive physicochemical properties, which hold potential for the development of novel products and technologies. However, this interest poses a pertinent challenge, as these materials can potentially be released into the environment, interacting with living systems. Thus, comprehending the nano-bio-eco interactions of GBMs is imperative for ensuring safe and sustainable innovation. Experimental research employing an integrated material characterization approach, coupled with in vitro and in vivo testing, stands as a crucial strategy for elucidating the interactions of GBMs with biological and environmental systems. In this context, we present findings from a decade of investigation into graphene oxide-based materials conducted at the Brazilian Nanotechnology National Laboratory at CNPEM in Campinas. This research encompasses aspects such as purification and functionalization, physicochemical characterization, and the study of interactions with biomolecules and pollutants linked to their toxicological and environmental effects. Finally, this presentation seeks to broaden the discourse to encompass other 2D materials; drawing upon the insights gained from graphene oxide research toward safe and sustainable innovation.

Nanocarbon-Antitumoral Aptamer Platforms with Potential for Diagnosis of Colorectal Cancer

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The possibility of manipulating matter and controlling processes at the nanoscale, which overlaps the scale of biological structures and processes, has brought unprecedented advances in nanobiotechnologies. An example is the construction of multifunctional nanoplatforms, with special attention to those based on carbon nanostructures (nanotubes and graphenes) containing biomolecules (proteins, peptides, nucleic acids) or drugs anchored on their surface. They can outperform conventional molecular compounds due to their high reactivity and ability to undergo multiple functionalizations, generating technological solutions with high sensitivity, specificity, and selectivity. In this talk, we will describe our group's efforts to 1) carefully obtain nanocarbon-protein/aptamer platforms for biosensors with diagnostic potential for colorectal cancer; and 2) understand nanomaterial-biomolecule interactions.

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Nano-optics of two-dimensional materials studied by nanospectroscopy and nano-imaging techniques

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Light-matter interactions in the far-field electromagnetic zone, defined by the spatial region wherein light propagates, are typically studied by conventional methods which scrutinize light signal directly scattered from matter. Nevertheless, by principle such techniques cannot access the optical near-field corresponding to the non-propagating and evanescent radiation field confined near surfaces under illumination. In the near-field zone, the nano-optics of two-dimensional materials (2DMs) express fundamental concepts whose full experimental description can only properly be attained from nanoscopy techniques. In this context, the scattering-scanning near-field optical microscope (s-SNOM) and synchrotron infrared nanospectroscopy (SINS) rise as powerful nanoscopies able to retrieve unique information from the optical near-field using a nanoprobe to mediate light-matter interactions. Here, it will be shown the use of these nanoscopies to provide for the full characterization of nano-optical phenomena in 2DMs. It will be reviewed a case employing SINS to probe the dynamic properties of polaritons[1] held by 2DMs. The polariton group velocity was modulated by engineered functional substrates leading to acceleration of the polaritonic pulse and revealing its wave-particle characteristics[2]. In sequence, it will be presented the use SINS and s-SNOM to fully describe the near-field thermal radiation emitted by anisotropic 2DMs. This phenomenon intrinsically manifests itself in the near-field zone giving rise to coherent, directional and temperature-dependent radiation located in narrow bands around the material’s resonances of the local density of photonic states[3]. Therefore, it will be demonstrated that s-SNOM and SINS are instrumental in studying state-of-the-art aspects of the nano-optics of 2DMs.

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Sustainable and multifunctional 2D-based nanomaterials as an alternative in the search for solutions to global challenges

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2D nanomaterials represent a diverse class of materials, mostly with an exceptional variety of properties, which makes them suitable for applications in solving humanity's global challenges. However, there is an incisive need to seek new strategies for obtaining multifunctional nanostructures through sustainable and low-cost methods, fulfilling their role in energy, environmental, and agricultural applications. However, most conventional strategies for preparing this material and its composites involve energy-intensive conditions and high production costs. In this sense, the environmentally friendly synthesis of nanomaterials through cost-effective strategies and the provision of waste recovery are of great relevance. This presentation will present our advances in the green synthesis of different 2D-based nanomaterials designed for sustainable applications such as energy storage and generation, water purification, sensing molecules of biological and environmental interest, and sustainable agriculture, without leaving aside the toxicity assessment of the materials developed.

Anchoring Lithium Polysulfides by Defects and Phase Engineering in MoS_2

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Li-S batteries have been considered as a promising technology due to their high theoretical performance and the lower cost of the sulfur raw material, in addition to using a cathodic material of low relative toxicity and easy recycling. The efficiency of Li-S batteries is still unfeasible due to critical issues affecting cyclic reversibility and discharge rate. Materials and additives have recently been studied in the solution of these problems, in the anchoring of polysulfides with materials that induce strong chemical interactions with electrochemical intermediates as one of the main approaches of studies focused on the enabling of such materials in Li-S batteries. Of these, transition metal dichalcogenides have shown promising results in remediating some of the problems. Therefore, a study of the modulation of electronic and chemical properties of molybdenum disulfide (MoS2) monolayer with first-principles calculations is presented. The binding and anchoring of polysulfides to their surface were studied by means of binding energy analysis, both in the 2H and 1T' phases. The results indicate that 2H-MoS2 has a higher binding energy with short-chain lithium polysulfides and sulfur, a trend that continued with the introduction of point defects, while the 1T'-MoS2 phase demonstrated a maximum binding energy with intermediary polysulfides and with S8, especially with sulfur vacancy defects, which are also the type of defect with the lowest formation energy. It was also found that in sulfur vacancy defects, for both crystalline phases, there is an incorporation of sulfur from short chain polysulfides to the sulfur vacancy. This ability to incorporate, and retain, S could be useful in incorporating the material into composites that aim to trap lithium polysulfides on their surface and keep them in the cathode compartment, to maintain the integrity of the exterior cathode, and perhaps could also play a catalytic role in the lithium polysulfides reduction process.

Assessment of repeatability and reproducibility in graphene oxide synthesis: metrological approach towards certification as reference material

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This study focuses on evaluating the repeatability and reproducibility of the graphene oxide (GO) synthesis process, employing a rigorous metrological approach required to produce a candidate for a certified reference material of GO [1]. Seven samples of GO were synthed following a well-established protocol [2] and subjected to a series of analyses, including optical and structural characterization in addition to determination of BET surface area (the targeted property of a certification) and thermogravimetry (TG). Throughout the experimental procedure, meticulous measurements were implemented to quantify and mitigate sources of uncertainty, thereby ensuring the reliability and accuracy of the obtained results.

A comprehensive statistical analysis of the collected data was carried out to determine key parameters such as standard deviation, degrees of freedom, and confidence intervals. Notably, the GO's evaluated average surface area, resulting from seven different syntheses, was (235.0 ± 4.2) m² g-1, indicating significant consistency among the produced samples. The low standard deviation observed in BET analysis underscores the robustness of the adopted protocol of measurements and suggests reliable replicability of the graphene oxide synthesis process.

This metrological approach to GO synthesis provides insights into its properties, benefiting scientific and industrial communities, and aims to refine synthesis procedures and BET measurement protocols.

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Biodegradable nanographite polymer composites with modular electrical conductivity for flexible devices

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Carbon allotropes with 2D structures possess a unique combination of excellent tribological properties, high electrical conductivity, and extraordinary thermal conductivity. Integrating carbon nanomaterials with polymers is an effective approach to enhance the composite performance; however, in many cases, the actual performances of the resulting composites are noticeably lower than theoretical predictions. These properties are closely related to composite architectures; therefore, the structural design of composites is a key factor in improving various properties [1]. Thus, development of nanostructured composite materials with a complex internal structure and nanostructural management based on controlling the dispersion and distribution of charges in the polymeric matrix has a crucial impact on the final electrical conductivity values of the composites. A cutting-edge niche in the future clothing industry is the integration of smart devices with garments. The growing demand for these devices has increased academic and industrial interest in developing flexible and low-cost heaters with low energy consumption. Importantly, these devices should be thin and able to adapt to the curves of the human body, not restricting user mobility, allowing for complete activity performance [2]. In this work, a biocompatible and biodegradable composite material based on polymers and various carbonaceous precursors was developed, exhibiting characteristics of electrical conductivity and resistance that can be modulated. This material can be utilized in applications that demand high electrical conductivity (1000 S/cm), such as flexible conductors, or high resistance for use as flexible devices, with potential applications across various fields.

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$BiVO_4$/NiO heterojunction produced by RF magnetron sputtering for application in hydrogen evolution reaction

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Green hydrogen production has been widely studied to attain sustainability, considering the global fuel crisis. Since hydrogen is a high-energy, zero-carbon alternative fuel, its use as a clean energy source is beneficial [1]. A low-cost, low-energy pathway reported in the literature is the catalytic water splitting via photoelectrocatalysis, in which semiconductor oxides are used in photocatalytic hydrogen conversion cells [1]. By combining semiconductors in a heterojunction, charge carriers can migrate between semiconductors, delaying the recombination of the electron-hole pair. As a strategy to mitigate these effects, p-n heterojunction using thin films of bismuth vanadate ($BiVO_4$) and nickel oxide (NiO) were deposited by RF magnetron sputtering and analyzed by different characterization techniques, including XRD and photoelectrochemistry. The main goal of this work was to increase the lifetime of the electron-hole pair by promoting electronic transitions through conduction bands in both semiconductors. Our investigation was based on the optimization of properties guided by a factorial experimental design. Chronoamperometry trials with visible light excitation showed that the heterojunctions exhibit higher photocurrent than single-layer films, a likely indication that charge separation and a decrease in their recombination were favorable. This behavior is promising for continuous improvement in the electro-photocatalytic performance of the devices.

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Chemical strategies for doping, anchoring, and perforation of graphene derivatives

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Here, we present a critical analysis of different chemical strategies that can be used to doping graphenic materials with nitrogen, boron, phosphorus and sulfur. The experimental proofs that assert the inclusion of heteroatoms into the basal plane of graphene have been evaluated. The preparation and investigation of hybrids with single metal atoms, metal clusters and metal nanoparticles anchored on graphene derivatives will be presented. It was demonstrated that anchoring Ag-nanoparticles on graphenic nanosheets can stabilize them. Chemical methods for preparing doped zero-dimensional (0D) nanomaterials from 2D graphene nanosheets will be discussed. It has been observed that the perforation of graphene can enhance the specific surface area of the nanosheet, ensuring effective wetting and penetration of electrolytes to the electrode surface, facilitating rapid charge transfer, and boosting the electrocatalytic efficacy of the transducers [1]. This study reports the first example of nitrogen-doped holey-reduced graphene oxide (N-MHG) with a mesoporous morphology of the graphene basal plane. It is shown that such material can be synthed through a one-step hydrothermal treatment of graphene oxide. A straightforward procedure for the purification of N-MHG has also been developed. AFM, TEM, and Raman analyses have revealed that N-MHG possesses a highly mesoporous network structure with a pore ranging from 10-50 nm [2]. X-ray photoelectron spectroscopy (XPS) data have indicated a partial reduction of the graphene oxide sheets during the etching process but also show a 3-5 times higher content of C=O and O–C=O fragments compared to rGO. This could account for the remarkable stability of the N-MHG aqueous suspension.

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Deep Ultraviolet emission from monolayer h-BN studied by Cathodoluminescence performed in a Scanning Tunneling Microscope

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Hexagonal boron nitride (h-BN) is a layered material with a wide electronic band gap. Like other 2D materials, it has different optical properties when in monolayer form.[1] In particular, photoluminescence and optical reflectance spectroscopy measurements confirmed the direct band gap emission at ~6.1 eV h-BN monolayers grown on HOPG by high-temperature molecular beam epitaxy.[2] Supporting this result, recent cathodoluminescence (CL) measurements carried out on h-BN/HOPG reported the presence of a weak emission peak attributed to phonon-assisted recombination of direct excitons.[3] As well as not having a limit on the excitation energy, the use of CL avoids the presence of Raman signals close to the luminescence simplifying data interpretation. Despite the high surface coverage of monolayer hBN, these samples have regions both with thicker layers and disordered growth. Therefore, it is mandatory to have high resolution images of the region probed by CL. Here, we studied the deep ultraviolet (DUV) emissions of h-BN using low energy CL performed in a scanning tunneling microscope (STM-CL). In this setup, for instance, it is possible to excite regions as small as tens of nm with free electrons of 100 to 300 eV. In this way it will be possible to locally excite the sample in previously characterized regions.

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Development of a gas sensor based on carbon nanomaterials for CO_2 monitoring in natural gas

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In the pre-salt layer wells, monitoring variable levels of CO_2 remains a challenge, as it often requires sensors to operate in highly complex environments [1-3]. This work aimed at developing a gas sensor for CO_2 monitoring in natural gas. It was found that a sensitive element, based on nanomaterials, can distinguish contaminations ranging from 0 to 100% of CO_2 in compressed natural gas (CNG). Several tests demonstrated a lifetime of over 8 months, rapid response and return times, stability, compactness, low cost, and operation at room temperature. The project is currently in the laboratory preparation phase to be applied at the Cacimbas Gas Treatment Unit (CGTU), a Petrobras facility located in Espírito Santo - Brazil. Therefore, this paper will present the entire development and operation of the gas sensor for monitoring CO_2 in natural gas.

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Development of PETG/graphene nanocomposite by 3D-Printing: Effect of graphene concentration on mechanical and morphological properties

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The highlighted benefits of graphene have increasingly attracted the interest of different industrial sectors. Graphene is a 2D nanomaterial that presents outstanding mechanical, chemical, electrical, and thermal properties, being those advantages mainly attributed to the C–C sp^2 hybridized bonds. Due to that, distinguished enhancements in mechanical properties are achieved when small amounts of graphene are incorporated into polymeric matrices. Polyethylene Terephthalate Glycol (PETG) is a thermoplastic polymer that presents higher printability when compared to acrylonitrile butadiene styrene (ABS) and greater ductility than polylactic acid (PLA), being a good alternative to produce parts by 3D-printing. In this work, we produced nanocomposites of PETG/graphene with different graphene concentrations (0.1 wt.%, 0.5 wt.%, and 1.0 wt.%) by the solvent intercalation method, followed by extrusion. Nanocomposite filaments with a diameter of 1.75 mm were obtained by extrusion and used in a 3D printer to produce specimens for tensile and impact tests. In addition, the surface, and transversal sections of specimens were analyzed by scanning electron microscopy. As main results, the presence of graphene increased the melt flow index of PETG, attributed to the lubricating effect provided by graphene to the polymeric matrix. Furthermore, the nanocomposite with 1.0 wt.% of graphene presented superior Young modulus and tensile strength, and greater tenacity when compared to neat PETG. The morphological analysis of the printed specimens revealed that graphene is well dispersed in the polymeric matrix, contributing to improving the composite performance. In addition, this work allowed for optimizing parameters for processing nanocomposites using 3D printing.

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Development of sustainable water-based multifunctional nanofluid with xanthan gum (XG) and graphene oxide (GO)

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The exploration of oil in ultra-deep waters (offshore) is crucial due to the high demand for this resource. However, challenges, like the complex task of drilling through salt layers and stringent environmental concerns persist. Drilling fluid plays a fundamental role in the well drilling process, aiding in drill cooling, gravel transportation, and other functions. Although water-based fluids are preferable environmentally, they tend to be less efficient and degrade under high pressures and temperatures.

To tackle this challenge, companies are turning to nanotechnology-based solutions to develop fluids capable of operating efficiently under extreme conditions. One of the primary materials used for this purpose is graphene oxide (GO), known for its exceptional mechanical strength, lubricating properties, and compatibility with water-based fluids. Additionally, GO is chemically stable and can enhance the rheological properties of the fluid. The study focuses on developing and characterizing water-based drilling fluids with GO and xanthan gum (XG), a common biopolymer in the oil industry. A simplified production method was devised, utilizing GO as a filler and XG as a matrix. This method yielded a concentrated dispersion, which was subsequently diluted in the matrix at varying concentrations, facilitating scalable manufacturing.

The light of this approach lies in its focus on water-based fluids as an environmentally sustainable alternative for offshore operations. Implementing these fluids reduces both environmental impact and operational risks.

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Diamond-like C_4X_2 (X = B or N) nanosheets: properties and potential application in hydrogen evolution reaction

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Graphene stands out as the foremost two-dimensional (2D) material, distinguished by its structure as a zero-gap semimetal comprising carbon atoms arranged in a honeycomb pattern with sp^2 hybridization. It represents the foundational unit for various other nanomaterials such as fullerenes, nanotubes, graphite, and single-layer diamond (2D diamond). Moreover, we can change its properties through doping and functionalization with diverse types of atoms and integrating with other 2D systems [1, 2]. Recent advancements in synthesizing and characterizing 2D materials have brought substantial attention to 2D diamonds, showcasing promising applications across various fields, including batteries, quantum computing, nano-optics, and nanoelectronics. In this context, we investigated the structural, thermodynamic, dynamic, elastic, and electronic properties of diamond-like C_4X_2 (X = B or N) systems [2]. Notably, our current results underscore the potential of these systems as efficient catalysts for the hydrogen evolution reaction.

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Double-layer stacking in the commensurate CDW phase of 1T-TaS2 observed by resonance and polarized Raman Spectroscopy

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The layered transition-metal dichalcogenide material 1T-TaS2 possesses successive phase transitions upon cooling, resulting in the formation of charge density waves (CDWs) and a commensurate CDW structure below 160 K. Recently, a double-layer stacking configuration was shown to form a Peierls-like instability in the electronic structure of the commensurate phase. In this work, we employ a multiple excitation and polarized Raman spectroscopy to resolve the behavior of phonons and electron−phonon interactions in the commensurate CDW phase of 1T-TaS2 [1]. We observe a distinct behavior from what is predicted for a single layer, and a richer number of phonon modes that are compatible with the formation of double-layer units. The multiple-excitation results show a selective coupling of each Raman-active phonon with specific electronic transitions hidden in the optical spectra of 1T-TaS2, suggesting that selectivity in the electron−phonon coupling must also play a role in the CDW order of 1T-TaS2 [1].

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Electrical Characterization of Transition-metal dichalcogenides using Scanning Microwave Impedance Microscopy (sMIM)

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In this study, we investigated the local effects of gating voltage on monolayer, bilayer, and few-layer Transition-metal Dichalcogenides (TMDs) using Scanning Microwave Impedance Microscopy (sMIM). Specifically, we focused on MoS_2 (molybdenum disulfide), $MoTe_2$ (molybdenum ditelluride), and WTe_2 (tungsten ditelluride). sMIM enables the utilization of microwave reflections from the tip-sample nanometric interaction to measure the local electrical properties of the samples such as dielectric constant, electric resistivity and dopant concentration at a nanoscale range. We examined how the conductivity and permittivity of the fabricated samples change locally on the surface of the TMDs when source-drain and gate voltages are applied, linking the results to the semiconductor or semimetal characteristics of the TMDs under investigation. Finally, KPFM (Kelvin Probe Force Microscope) results on the nanoscale imaging of the surface potential on each TMD is discussed.

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Evaluation of Eco-Friendly Anticorrosive Polyurethane Coating Using Graphene Oxide

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Graphene oxide (GO) has attracted attention as an additive in coatings due to its impermeable properties, offering corrosion protection [1], while remaining compatible with water borne formulations, thereby aligning Green Chemistry principles (GCP). Water-borne polyurethane (WPU) resins exemplify GCP, boasting low volatile organic compound content, contributing to decrease emissions and air pollution [2]. Additionally, WPU resins exhibit excellent resistance to abrasion, chemicals, and UV radiation, ensuring durable, high-quality protective coatings. The incorporation of GO into resins is a stablished strategy for enhancing the corrosion resistance of coatings. However, achieving uniform dispersion of GO within the polymeric matrix is a common challenge highlighted in the literature, which can compromise the anticorrosive performance of the coating. In this context, the goal of this work is to evaluate the anticorrosive performance of a WPU containing different concentrations of GO, from 0.01% to 1.0% (w/w). The dispersion of GO within the resin was assessed using 2D mapping via Raman spectroscopy. The barrier properties were evaluated by potentiodynamic polarization in 3.5% NaCl solution. The results presented herein demonstrate that PU resin containing GO concentration lower than 0,05% (w/w) exhibited excellent dispersibility in the polymeric matrix and optimal corrosion resistance behavior, with very low current density values, lower than 10-9 A/cm2.The favorable electrochemical response for corrosion protection is achieved through a combination of optimal graphene sheet and excellent dispersibility within the polymer matrix.

Evidence of Thickness-dependent Surface Induced Ferroelectricity in Few-layer Germanium Sulfide obtained via Scanning Tunneling Spectroscopy

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The discovery of ferroelectricity in two-dimensional van der Waals materials has sparked an enormous interest in the scientific community, due to its possible applications in next-generation nanoelectronic devices, such as random-access memories, digital signal processors, solar cells, among others. In the present study, we used vapor-phase deposition to synthe ultrathin germanium sulfide nano-flakes on a highly oriented pyrolytic graphite substrate. Nanostructures of variable thicknesses were characterized using scanning tunneling microscopy and spectroscopy. Tunneling currents under forward and backward biases were measured as a function of the nano-flake thickness. Remarkably, we clearly observe a hysteresis pattern, which we attribute to surface ferroelectric behavior, consistent with screening conditions of polarization charges. The effect increases as the number of layers is reduced. This experimental result may be directly applicable to miniaturized memory devices, given the two-dimensional nature of this effect [1].

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Exploring Theoretical Aspects of 2D Silicate Exfoliation from Rhodonite Mineral via Mn Doping

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Advancements in technology are driving a increased demand for natural resources, prompting the exploration of novel materials across various fields such as environmental protection, energy harvesting, and electronics. Silicates, abundant in the Earth's crust, are emerging as promising alternatives due to their varied chemical compositions, environmental resilience, and manipulability through processes like doping and defect engineering. Particularly, piroxenoid silicates possess numerous octahedral sites, housing bivalent cations like Ca2+ or Mg2+ between silicate chains, offering anisotropic bonding potential exploitable in the exfoliation process. Additionally, these materials naturally incorporate transition metals (e.g., Fe, Mn), imparting unique properties such as magnetic ordering, distinct from pristine silicates. With the advent of scalable exfoliation methods for natural silicates, these materials can be thinned into layers where confinement effects profoundly alter their properties. Here, employing state-of-the-art ab-initio simulations based on density functional theory (DFT), we investigate the characteristics of 2D R-silicate experimentally exfoliated from natural Rhodonite ($CaMn_4Si_5O_{15}$). Our findings reveal that exfoliated Rhodonite exhibits potential as a selective gas sensor for H_2S. The presence of naturally occurring Mn dopants introduces a magnetic moment originating from the Mn d and O p states near the valence band edges, which amplifies upon exfoliation into ultrathin 2D layers. This study contributes theoretical insights into the utilization of exfoliated natural silicates in various technological applications. We thank CCM/Propes/UFABC for all the computational resources provided.

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Flexible gas sensor based on rGO-ZnO for NO2 detection at room temperature

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The increase in air pollution due to industrialization and urbanization requires more versatile gas sensors with low energy consumption and low cost, which can monitor environmental conditions in real-time. With the advancement of technology, flexible gas sensors have been studied to meet this demand. This work aims to develop flexible rGO-ZnO gas sensors on PET substrate for NO_2 detection. Zinc oxide (ZnO) was synthed using the Pechini method and commercial rGO. The rGO and rGO-ZnO solutions with different ZnO concentrations (1, 2 and 5% volume) were prepared in distilled water and deposited on interdigitated Cr/Au electrodes by drop-casting. XRD measurement confirms the formation of ZnO NPs with a wurtzite structure. SEM images show that the rGO-ZnO composites have ZnO NPs anchored and wrapped in the rGO sheets. Gas detection measurements show that all sensors were sensitive to NO_2 at room temperature (RT) and that the sensor that obtained the best sensing properties was the rGO-5%ZnO sensor. Furthermore, compared to the response with other gases, the rGO-5%ZnO sensor exhibits higher selectivity to NO_2. Automated bending tests demonstrated that the sensors can be reliably used as flexible gas sensors.

From graphyne monolayers to roll-up structures: exploring the thermal transport in nanoscrolls

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Graphynes are 2D carbon allotropes composed of benzenoid-like hexagonal rings connected by acetylenic groups, presenting both *sp* and sp^2 hybridized carbon atoms. Theoretically predicted in 1987 [1], only recently have some structures been experimentally realized. Nanoscrolls are structures obtained by rolling up nanosheets into a papyrus-like topology [2]. In this work, Equilibrium Molecular Dynamics simulations [3], with the reactive force field AIREBO, were carried out on graphene (as benchmark) and α,β,γ-graphyne to explore their thermal conductivity (κ) in different topologies: flat and rolled up nanosheets. The Green-Kubo relations for transport properties were used to calculate κ through integration of the heat flux autocorrelation function. Our results show that graphynes exhibit κ approximately one to two orders of magnitude lower than graphene. The presence of the acetylenic groups is found to degrade the thermal conductivity, which is strongly reduced from graphene (highest density) to α-graphyne (lowest density). Among the various graphynes, the γ type has the highest κ value. Our findings suggest that scrolling and periodicity affect thermal transport, with nanoscrolls showing lower performance in thermal transport along their axial axis, compared to the nanosheets from which they were originated. Additionally, thermal conductivity decreases as temperature increases (up to 500 K), following a power law ($\kappa \sim T^{-n}$). These findings may have applications in the thermal and thermoelectric management of nanodevices based on these materials.

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Graphene as transparent conductive electrode in silicon heterojunction solar cells

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In the photovoltaic market, silicon solar cells occupy a major share (~94%) due to their high efficiency. Among them, silicon heterojunction (SHJ) approach provides higher open-circuit voltages (VOC) than the wafer-based technology due to better contact passivation. However, most common materials used as conductive spreading electrodes (CSE), like Indium Tin Oxide (ITO), are too scarce for mass production.
Graphene is a carbon nanomaterial with interesting structural, electrical and optical properties and an attractive potential for applications in solar photovoltaics. In this work we characterized the structural, electrical, and optical properties of ~1 cm2 graphene sheets by changing the numbers of layers, to evaluate its performance as CSE on silicon heterojunction solar cells.

Graphene is transferred through a polymer free process onto SiO2 and glass substrates. With scanning electron microscopy, we observe that graphene covers almost the entire surface and some wrinkles are formed, so the mean thickness of the graphene film is in the order of 6 nm.

Through spectroscopic ellipsometry we determined the refractive index as a function of wavelength. Between 400 and 800 nm, our graphene samples on glass have n values in the order of ~1.7, which is similar to commercial ITO; while, optical transmittance measurements, show larger transparency for graphene than ITO. Regarding electrical properties, graphene on Si substrates presents a lower sheet resistance compared to ITO, which decays further with the addition of a second film.

Our results show that graphene is a promising material to be used as conductive spreading electrode in silicon heterojunction solar cells. Thus, in this work the performance of SHJ cells with graphene instead of ITO is evaluated through current-voltage measurements.

Investigating Oxidation Mechanisms in 2D Materials: Ab Initio Study of Mono-elemental Layers

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This study explores the intricate dynamics of oxidation in 2D materials, particularly focusing on mono-elemental layers of arsenic, antimony, and bismuth both freestanding and supported by silicon carbide substrate. Employing ab initio calculations, we analyze the oxidation process through a comprehensive examination of O2 spin-state transitions within Landau–Zener methodology. Our investigation reveals distinct oxidation behaviors influenced by spin–orbit coupling and substrate interactions. Energy barrier analyses elucidate contrasting trends across the pnictogen family for with freestanding and SiC-supported. Moreover, we demonstrate the role of spin–orbit coupling in oxidation mechanisms, particularly in SiC-supported setups. Our findings indicates the enhanced oxidation resistance of SiC-supported bismuth, showcasing its potential for robust performance under atmospheric conditions. This research provides valuable insights into optimizing 2D material-substrate dynamics for practical applications in realistic environments.

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Investigation of doping effects on the local electrochemical activity of transition metal dichalcogenides 2D materials

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Strategies to enhance a catalysts' electrochemical activity are based on precise material design. This study presents a comprehensive analysis of doping 2D materials with transition metals (TMs)1, combining theoretical predictions with experimental investigation to elucidate the impact of doping on electronic and electrochemical activity. Focusing on a MoS2 monolayer, we investigated the coordination of some 3d TM atoms using a combination of Density Functional Theory (DFT) simulations and scanning probe microscopies, notably Scanning Electrochemical Cell Microscopy (SECCM)2. Our systematic exploration, particularly on Ti- and Ni-doped MoS2 monolayers, centered on hydrogen evolution as probe reaction. SECCM measurements revealed heterogeneous changes in MoS2 basal plane electrochemical activity upon Ti doping, contrasting with homogeneous decreases observed for Ni doping. Local point of zero charge (PZC)3 by SECCM measurements and Kelvin Probe Microscopy (KPM) images supported these findings, indicating a decrease in MoS2 work function upon Ti doping, consistent with DFT simulations. KPM surface potential images suggested that Ti coordination on MoS2 is more favorable in regions with higher surface potential, elucidating the observed heterogeneity in Ti-MoS2 SECCM mapping and implying a more ionic interaction between Ti and the MoS2 surface. Conversely, Ni coordination occurred across the entire flake surface, regardless of the initial surface potential. These findings underscore TM coordination as an effective, minimally invasive method for doping 2D materials, augmenting their electrochemical activity at the basal plane. Variations in electrochemical behavior offer avenues for tailored design and optimization of 2D materials, promising advancements in various electrocatalytic processes.

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Luminescence enhancement and Raman spectroscopy study of *in-situ* Vanadium doped WSe_2 monolayers

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Monolayer Tungsten diselenide (WSe_2) is a direct band gap semiconductor that has excellent luminescence properties which are of great interest for optoelectronics applications [1, 2]. In this study, we investigated the effect of vanadium (V) incorporation in WSe_2 monolayers grown by CVD. Our results indicate that lightly V-doped WSe_2 exhibits up to a threefold photoluminescence (PL) intensity enhancement as compared to pristine WSe_2 monolayers and a strongly quenched PL signal for highly doped samples. Resonance Raman spectroscopy measurements were performed to study the disorder effects as well as to observe a frequency shift in the main vibrational modes of WSe_2 in off-resonance Raman spectroscopy due to the presence of V in the lattice. X-Ray photoelectron spectroscopy measurements were also performed to study the chemical changes of the samples. These results are of great interest in the field of defect engineering of 2D materials.

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Magneto Dependence of Excitonic States of Twisted WSe2

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Monolayer transition metal dichalcogenides (TMDs) exhibit rich physics related to their excitonic complexes. In these materials, the reduction of the dielectric screening collaborates with the intensification of Coulomb interaction and, consequently, the formation of exciton with high binding energy and other complexes involving more carriers. In particular, TMDs present spin-orbit coupling, promoting valence and conduction band splitting, and valley structure can be verified with circularly polarized light. In a slightly different system, the band structure and the excitonic properties can be tuned if two layers of TMDs are placed, one on top of the other with a twist angle, producing a twisted WSe2 material (t-WSe2). In our work, we investigate the excitonic states of high-quality t-WSe2 encapsulated in hBN crystals. We investigate the photoluminescence's polarization and magneto dependency at low temperatures. Comparing with the monolayer case, we observe a similar valley polarization and magnetic behavior. Also was observed emissions from the non active hBN ZO phonon mode and its sum with A1g WSe2 phonon mode caused by coupling in the interface between the materials. Finally, we observe a new emission that rises for high magnetic fields (B > 7 T) is verified whose identification is still under progress. Our results may reveal a electron-phonon coupling owing to the quantum confinement effects of Moiré pattern in twisted semiconducting 2D heterostructures.

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Magnification of Plasmon Resonances in Monolayer MoS_2 via Conjugated Molecular Adsorbates

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The adsorption of carbon-conjugated molecules represents an established route to tune the electronic and optical properties of transition metal dichalcogenide (TMDC) monolayers. Here, we demonstrate from the first principles that such a functionalization with the prototypical compounds pyrene and tetracene enhances the magnitude of selected plasmon resonances in the MoS2 monolayer, without significantly altering their energy and dispersion [1]. Our results indicate that this magnification can be achieved by properly aligning the molecules with respect to the direction of the transferred momentum. The distinct signatures in the loss function of the interface compared to those of its constituents suggest the presence of non-negligible interactions between them and the possibility of using electron energy loss spectroscopy to detect the presence and the orientation of molecular adsorbates on TMDCs.

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Optical and magneto-optical investigation of defects in WS_2 and WSe_2 monolayers

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The increasing interest in 2D transition metal dichalcogenides (TMDs) for the next generation of ultrathin devices led to a natural concern about defects in these materials. The spatial inhomogeneity of TMDs properties caused by several possible defects can deeply affect their applicability. On the other hand, there is also a great effort in the defect engineering of 2D TMDs to controllably tune their properties. In this context, there is a significant demand for the characterization of distinct defects in TMDs to understand their impact on electronic, optical, mechanical, magnetic, and physicochemical properties of these materials. Here, we performed optical and magneto-optical experiments such as photoluminescence, magneto-photoluminescence, resonant Raman spectroscopy and resonant nonlinear optical spectroscopies to study vanadium-doped and aged WS_2 and WSe_2 monolayers. We investigated the electronic band structure and optical transitions dependence on vanadium doping in WS_2 monolayers through a broadband optical characterization [1]. In addition, our magneto-photoluminescence measurments revealed a giant g-factor related to a defect peak in vanadium-doped WSe_2 monolayers and an assymetric valley Zeeman shifting in vanadium-doped WS_2 monolayers. Finally, magneto-optical experiments showed a strong magnetic response in aged WS_2 and WSe_2 monolayers associated with a spin-flip transition between mid-gap states [2]. Our results unveil novel and tunable properties of vanadium-doped TMD monolayers and shed light on the potential of the defect engineering of these 2D materials for spintronic applications.

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Patterning defect arrays on the basal plane of ultra-large MoS_2 monolayers using electron beam lithography

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The transition metal dichalcogenides (TMDs) stand out among the most studied materials in recent years to produce green hydrogen from water, for their high performance in the hydrogen evolution reaction (HER). Among the TMDs, MoS_2 has shown promising catalytic properties [1]. The catalytic sites of MoS_2 monolayers towards hydrogen evolution are well known to be vacancies and edge-like defects. However, it is still very challenging to control the position, and defective areas on the basal plane of MoS_2 monolayers by most of the defect-engineering routes. In this work, the fabrication of defect arrays with resolution of approximately 200 nm on high aspect ratio MoS_2 monolayers using nanolithography and O_2 plasma is reported for the first time. By adjusting the and distance of the patterns, it is possible to establish a quantitative relationship between the number of defects, i.e. edges created in the basal plane, and their electrocatalytic performance. The electrocatalytic activity of the arrays toward the HER was measured by fabricating microelectrodes using a recently reported method that preserves the catalytic sites [2]. This catalyst showed outstanding activity, with an onset overpotential of 437 mV. Characterization analyzes by Raman, AFM, KPFM, SEM and EDS revealed that the exposed regions underwent effective corrosion, resulting in only the substrate remaining in those areas.

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Plasmon phonon-polaritons in minimally twisted bilayer graphene and talc heterostructures observed by s-SNOM

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Twisted bilayer graphene (TBG) shows remarkable electronic properties, including superconductivity and correlated insulating states[1]. On electrostatically gated TBG devices with high doping, scattering scanning near field optical microscopy (s-SNOM) reveals triangular domains due to the different optical conductivity of each of the stacking arrangements of the TBG superlattice[2]. In this work, we present a study of plasmon phonon-polaritons in minimally twisted bilayer graphene and talc heterostructures using s-SNOM in the mid-infrared (IR) range without any electrostatic gating. Our experiments were carried out with a mid-IR laser source ranging from 920 cm^{-1} up to 1140 cm^{-1} and allowed us to image highly confined plasmon polaritons. In some laser frequencies, we have also observed sixfold domain wall arrays with the same period as the TBG superlattice within the talc reststrahlen band. This work provides new insights into TBG and talc heterostructures electronic and polaritonic properties. We believe our findings will stimulate further research on designing and characterizing novel heterostructures for electronic and optoelectronic applications.

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Probing rigid-layer modes in a van der Waals mineral by terahertz time-domain spectroscopy

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Since the discovery of graphene, great attention has been attracted to naturally occurring van der Waals materials [1], which can be exfoliated down to a few layers, thus being a low-cost source for two-dimensional materials. As interesting quantum phenomena can emerge from low-dimensionality, these systems have become the promising building blocks for novel electronic, optoelectronic, and mechanical nanodevices. Among the candidate materials one can highlight the mineral clinochlore [$Mg_5Al(AlSi_3)O_{10}(OH)_8$], one of the most abundant phyllosilicates in nature [2]. In this work, we have studied low-frequency rigid-layer modes as a path to shed light on the strength of the inter-layer coupling. We have employed our terahertz time-domain spectroscopy (THz-TDS) experimental setup [3] to analyze bulk samples of clinochlore. This powerful technique is known to enable direct determination of the complex refractive index of materials. From our measurements, we have found a very distinctive sharp resonance centered in 1.13 THz, which exhibited a small temperature dependence. Further polarization-dependent measurements have also demonstrated a birefringent behavior of clinochlore, which was observed through the detection of Faraday rotation and ellipticity on and off resonance. Moreover, THz-TDS measurements were also conducted on the related mineral talc, helping us to discuss the possible origins of the resonance in clinochlore. Finally, density function theory simulations were made considering the existence of iron impurities on the mineral and its effect on the frequency of the rigid-layer modes and refractive index.

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PRODUCTION OF ULTRATHIN HETEROSTRUCTURES AND DEVICES FOR NANOELECTRONICS

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Isolated two-dimensional materials (2DMs) have been widely studied due to their intrinsic electrical, mechanical, and optical properties [1]. Recently, the combination of two or more 2DMs in the so-called van der Waals heterostructures (vdWHs) has allowed improvements in the optoelectronic quality of multifunctional devices and in the observation of new quantum phenomena that do not exist in isolated forms [2]. Consequently, this has boosted the use of these 2DMs, as well as technological applications of these ultrathin and hybrid vdWHs, mainly in areas related to nanoelectronics [3]. In this project, we manufactured and characterized samples of graphene encapsulated in biotite natural crystals from a Brazilian mine and compared the results with the 2D crystal most used in the literature, hexagonal boron nitride (hBN). We demonstrated that natural 2DMs can be easily incorporated into ultrathin vdWHs with graphene. Our Raman spectroscopy analysis showed that biotite crystals induce a spontaneous charge transfer to the graphene, inducing doping without applying external gate bias. The results were then compared to the electrical characterization of field effect transistor (FETs) nanodevices, thus corroborating the total charge density transferred to graphene, as well as the type of charge carrier. Therefore, our study seeks to contribute to the area of electronic devices with low production costs using natural 2DMs from Brazilian soil.

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Quantum confinement emissions on strained monolayer WSe2 : A Tip Enhancement Photoluminescence Spectroscopy (TEPL) approach on single photon emitters

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Transition-Metal Dichalcogenides (TMDCs) exhibits exceptional photoluminescence when cleaved down to a monolayer, even in a low power regime [1]. Its spectrum is dominated by the complex excitonic behavior, including dynamics from both bright and dark excítons. When placed on top of a substrate with nanopillars, the 2D material becomes host of quantum single photon emitters with sharp lines in cryogenic environment [2]. However, although the emission is localized, its origins are still not well understood and the relations between strain, stress, curvature and the role of band defects is not clear. In this work, we develop an alternative way of producing these nanopillars, reducing the steps needed and obtaining a cleaner stable organic structure that are also transparent, enabling back illuminated spectrography. We also perform cryogenic photoluminescence, obtaining a single photon emitter spectra with less than 1 nm linewidth that becomes absent when the temperature increases. Despite that, we carry out a Tip Enhanced Photoluminescence Spectroscopy in room temperature, which enabled us to navigate through out our 150 nm nanopillar and map the emissions with a 9 nm resolution, much beyond the diffraction limits of standard optical measurements. Surprisingly, an arising peak was observed on top of the pillar confined in a small region (~40nm) which we believe are associated with the hybridization of dark excítons with the bound excítons (defects level). This new emission are probably correlated to the single photons and could help understand its origins. Because of the amplified signal and nanometer resolution, our study presents a new way of approaching quantum confined excitons that are not observed in normal room temperature photoluminescence experiments and suggest that the arising single photon emitter on TMDCs are more related to a resonance process provoked by inducing strain than the curvature itself.

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Ramam Spectroscopy Studies of $PtSe_2$ and The Formation of Selenium Vacancies Using Temperature

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Platinum diselenide (PtSe2) is a transition metal dichalcogenide (TMD) material with relatively weak van der Waals interaction between the interlayers, which creates a pathway to exfoliate these materials into two-dimensional (2D) nanosheets. 2D TMD materials have the potential for applications in hydrogen evolution, optoelectronic devices and photocatalytic applications. Raman spectroscopy is an essential characterization tool for 2D materials with the potential to understand defects due to the sensitivity of the Raman technique with the breaking of the rule of conservation of momentum, breaking of the local symmetry, i.e., Raman peaks can shift, broaden, alter their relative intensity, or additional peaks occur with the presence of defects. The main defects studied for Raman are vacancies, isolated functional groups, substitutional atoms, dislocations and grain boundaries. In this work, a thin PtSe2 film was sinthed via the selenization (closed quartz ampole) of a thin Platinum film prevously deposite by sputtering on a Si-SiO2 substrate. Raman spectroscopy was used to study its structure and stability over a range of temperatures (RT- 300°C). Transmission Electron Microscopy (TEM), X-ray Diffraction (XRD), Scanning Transmission Electron Microscopy (STEM) and X-ray Photoelectron Spectroscopy (XPS) characterizations were performed before and after in-situ Raman studies. It was possible to observe the the generation of selenium vacancy defects in the material with the shift of Raman peaks to lower energies, possibly due to the local atomic change in the structure and the appearance of the LA band (Longitudinal Acoustic Mode), considered a defect band in Raman spectroscopy.

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Raman and Photoluminescence Spectroscopies of in-plane $MoSe_2$-MoS_2 Heterostructures grown by chemical vapor deposition

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Transition metal dichalcogenides (TMDs, such as MoS_2 and WSe_2) and the van der Waals (HS) heterostructures formed by them, either by vertical stacking or in-plane joining, have been widely studied in the last decade due to their physical and chemical characteristics, including strong excitonic effects and the possibility of understanding new phenomena and properties. Lateral heterostructures present a question of scientific interest due to the atomic meeting of the crystal lattices of different TMDs [1], enabling the study of grain boundaries, for example, and also leading to applications in diodes for use in photoelectronics [2]. The heterostructures can be obtained using the chemical vapor deposition (CVD) method, since HS samples obtained by transfer methods present limitations for engineering applications, and the CVD method allows the control of several key parameters for growth, enabling certain changes in synthesis depending on the application required [3]. This work aims to study samples of lateral (in-plane) $MoSe_2$-MoS_2 heterostructures synthed by CVD using salt in a two-step process. These heterostructures were analyzed with Raman spectroscopy at different energies, including laser in the resonant range, and by photoluminescence, in order to understand what happens at the interface of the HS.

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STUDY OF ONE-DIMENSIONAL DEFECTS IN WS_2 MONOLAYERS BY RAMAN AND PHOTOLUMINESCENCE SPECTROSCOPIES

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Over the past few years, there has been extensive research on transition metal dichalcogenides (TMDs) owing to their unique optoelectronic characteristics. The exploration of defects in these materials has emerged as a promising avenue for their utilization in semiconductor devices. To illustrate, punctual defects serve as sources for single-photon emission, playing a crucial role in the quantum information devices sector [1]. Meanwhile, highly ordered defects, as line defects, can act as spin polarizers [2] and have demonstrated their capacity to host quantum phases, such as charge density waves [3]. In this context, the use of Raman and photoluminescence spectroscopies has proven to be a robust method for investigating defects in 2D materials, as demonstrated in previous studies published by our research group. In this particular work, we employed chemical vapor deposition (CVD) to synthe monolayers of tungsten disulfide (WS_2) and produced linear defects through lithography using a helium ion beam. The obtained data reveals promising results, such as the anisotropy of certain Raman modes and alterations in the photoluminescence spectra. These observations suggest the emergence of new optical properties in WS_2. Hence, this study aids in the understanding of one-dimensional defects in W-based TMDs, which find extensive use in the semiconductor technology industry.

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Temperature- and pressure-dependent vibrational properties of GaSeTe

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In this work, we present a temperature- and pressure-dependent Raman study of bulk GaSe0.5Te0.5 in order to access its thermal and mechanical properties. By combin-ing density functional theory (DFT) calculations and temperature-dependent Raman measurements, we calculate the anharmonic constants relative to three- and four-phonon decay processes, the mode-Grüneisen parameters, Debye temperature, and the thermal expansion coefficient. From the high-pressure experiments and DFT calculations, we show that A1g and E2g Raman modes present a nonlinear pressure dependence, with A1g modes being more compressible higher ∂ω/∂P values than E2g mode. Furthermore, a comparison with the GaSe system shows that the alloy is more compressible, thus presenting higher pressure coefficients and smaller bulk modulus. [1].

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The interplay between magnetic proximity effects and charge transfer in monolayer WSe_2 on CrSBr

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Magnetic proximity interactions and spin dependent charge transfer between transition metal dichalcogenides (TMD) semiconductors and two-dimensional semiconductor magnets are interesting tools to manipulate spin and valley degrees of freedom in non-magnetic TMD monolayers [1]. Here, we have investigated the impact of CrSBr, a direct gap semiconductor with A-type antiferromagnetic (AFM), on optical and magneto-optical properties of WSe_2/CrSBr heterostructures. The photoluminescence (PL) of WSe_2/CrSBr reveals different emission peaks such as exciton and trion peaks, several localized dark exciton (LDE) peaks and a broad defect band (D). Remarkably, these emission peaks show different behaviours with increasing magnetic field and a clear influence of the magnetic order of CrSBr. Under paralell magnetic field an increase of LDE emission intensities accompanied by a decrease of bright emission and D intensities are observed after the magnetic field induced ferromagnetic (FM) transition of CrSBr. Under perpendicular magnetic fields, unusual magnetic field dependence of PL intensity and valley exciton g-factor values are observed and suggests an asymmetric magnetic proximity exchange interaction. Furthermore, the WSe_2/CrSBr heterostructure has a broken-gap (type-III) band alignment resulting in an efficient charge transfer process which is sensitive to the magnetic order of CrSBr. In general, our results are explained by the interplay between the asymmetric magnetic proximity interactions and magnetic field dependence of charge transfer in WSe_2/CrSBr. Finally, our work suggests that vdW heterostructures with antiferromagnetic-nonmagnetic interfaces such as MoSe2/CrSBr or WSe_2/CrsBr are atractive platforms to modify the valley and exciton properties of TMDs for possible applications in spintronics and quantum technology [2].

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Thermal Properties and Morphological Features of PET Nanocomposites Reinforced with Graphene Oxide

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The production of polymer composites with graphene oxide (GO) has been intensely studied in recent years in the efforts to obtain new innovative materials with properties suitable for industrial applications [1]. The current work investigates the improvements of thermal properties and characterizes the morphological modifications for polyethylene terephthalate (PET) nanocomposites that contain GO as the nanofiller in different weight contents, comparing these properties with those of neat PET. GO was synthesized through the chemical route with subsequent sonication, following a modified Hummers' method [2], and transferred to an organic solution using rapeseed oil as the solvent. The composite specimens were manufactured using a double-screw extruder followed by injection molding. FTIR confirmed the presence of oxygen functional groups covalently bonded to the basal plane, while SEM imaging showed a good dispersion of the nanofiller in the bulk of the polymer; moreover, it allowed the identification of the corrugated structure of the GO layers. The glass transition and melting temperatures of PET increased along with the increase in GO content, indicating improvements in dimensional and thermal stability. A similar behavior was observed for thermal conductivity, which makes GO a promising candidate for the processing of PET in the plastics industry. Finally, crystallinity was observed to decrease for specimens with higher GO content, which may be attributed to the lower mobility of the polymer chains due to the presence of the nanofiller platelets dispersed in the glassy medium.

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Unveiling the electronic properties of BiP_3 triphosphide from bulk to heterostructures by first principles calculations

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In this work, we conducted a detailed study on the structural and electronic properties of bismuth triphosphide (BiP3) in bulk, few-layers, and monolayer forms. Our results show that the BiP3 bulk presents a stable layered structure with metallic characteristics. The exfoliation energy of 1.07 J/m2, comparable to other triphosphides, suggests that the material can be easily exfoliated. The band gap is thickness-dependent, with a semiconductor-to-metal transition between four and five layers. It occurs due to significant interlayer coupling and quantum confinement effects. We also analysed the heterostructure formed by the deposition of graphene (G) on few-layer BiP3. For both monolayer (G/m-BiP3) and bilayer (G/2L-BiP3) BiP3, we observed the formation of a metal-semiconductor junction characterized by weak vdW interactions along the interface. Both structures present a p-type Schottky contact. Our study reveals that the Schottky barrier height (SBH) can be modulated by adjusting the interlayer distance between G and BiP3. This modulation results in a transition from n-type to p-type Schottky contact for G/m-BiP3 and the establishment of an ohmic contact in G/2L-BiP3. Furthermore, the SBH is also modulated by applying a transverse electric field across the vdW heterostructure, leading to a transition from n-type to p-type Schottky contact and the formation of an ohmic contact. Additionally, we demonstrate that the n-doping of graphene can be tuned by increasing the number of BiP3 layers onto which it is deposited, as well as by applying an external electric field. All these findings indicate that few-layers BiP3 is a promising candidate for developing nanoelectronic, optoelectronic, and graphene-based contact devices.

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Visible light absorption in large-area WS_2 monolayer samples grown by CVD

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In recent years, Tungsten disulfide (WS_2), a two-dimensional material, has garnered significant attention from scientists due to its exceptional optoelectronic properties. However, the investigation of its visible light absorption has been relatively limited, primarily constrained by the of synthed WS_2 samples [1]. In this study, we successfully synthed centimeter-scale monolayer WS_2 samples on fused silica via chemical vapor deposition (CVD). During the growth process, precursor materials including WO_3 and sulfur were strategically positioned within the central region of a 1-inch quartz tube, while a fused silica substrate was situated above the WO_3 powder. This configuration enabled controlled growth of WS_2 layers on the substrate surface. The quartz tube assembly was placed within a two-stage furnace for precise thermal treatment. Resonance Raman spectroscopy was employed for comprehensive analysis, revealing that the edges of the synthed samples predominantly exhibit bilayer or multilayer structures, whereas the central region predominantly comprises monolayer WS_2. Absorption measurements of visible light were conducted via both transmission and reflection. The absorption spectra obtained via reflection and transmission exhibit similar structures. The both spectra feature three prominent peaks accompanied by broad bands, centered around 410 nm, 520 nm and 650 nm, respectively. The consistency in the observed structures is further supported by theoretical calculations utilizing a spread of valence band Wannier functions [2], which is elaborated upon in subsequent discussions.

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Adsorption of norfloxacin from aqueous solution by a bidimensional covalent organic framework

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Norfloxacin (NFX) is an antibiotic commonly used to a large spectra of bacteria, such as Escherichia coli, Klebsiella sp. and Proteus sp. Due to the low biodegradation in water NFX is considered a pollutant with strong effects to aquatic food chain.1 A strategy to remove NFX from water is the use of covalent organic frameworks (COF) as adsorbents. These organic and crystalline nanomaterials have high surface area and possesses functional groups which can interact with pollutant and adsorb them. The aim of this work was evaluating the NFX adsorption capacity of a bidimensional COF from aqueous solutions. The material was obtained from the reaction of 2,4,6-triformylphenol and p-phenylenediamine in water and HOAc in sealed ampules at 120 °C for 3 days. The surface area of the obtained material was 557 m^2/g. The adsorption tests were carried out in 15 ppm solutions, at pH = 5.0 and 8.0, added from the COF in the concentration of 1 mg/mL. The COF was capable of removing the NFX in a range between 17.14 to 26.06%. The equilibrium concentration (q_e) was achieved after 60 min and decreased from 1.77 to 0.51 as the pH increased from 5,0 to 8,0, respectively. The adsorption kinetics was evaluated as a pseudo-first order with rate constant of $2{,}2x10^{-4}$ min^{-1}. Actually, studies are carried out to understand the interaction between the COF and NFX and how can the adsorption be increased.

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Adsorption process on sulfur vacancies of MoS_2

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Within nanotechnology and materials science' fields, two-dimensional materials (2D), such as molybdenum disulfide (MoS_2), have been the focus of intense research [1,2]. Thanks to its unique 2D layered structure composed of one molybdenum atom between two sulfur atoms, MoS_2 exhibits distinct properties and has broad applications. The structure of any material is subject to defects, and MoS_2 is no exception to this reality. These defects can have both beneficial and detrimental effects. In optoelectronic devices, these defects can negatively impact device performance as they facilitate carrier recombination, reducing the average free path of photoinduced carriers.[1] The primary source of defects in MoS_2 is sulfur (S) vacancies.[1] They are active centers for molecular adsorption and chemical functionalization.[3] They are also responsible for trapping and non-radiative decay, making them the main defects of MoS_2.[1] Aiming to reduce the electronic effects induced by S vacancies, passivation emerges as an option.[1,2] It is believed that water (H_2O) or oxygen gas (O_2) may play a role in passivating S vacancies, ideally removing the intermediate states created by defects without causing significant changes in carrier density, due to the isovalence between oxygen (O) and sulfur (S).[1,3] MoS_2 were synthed by sulfurization of sodium molybdate. After obtaining the material, samples will be exposed to different gases (O_2, H_2O, and N_2), both with and without an excitation source (green laser) for varying periods of time and temperatures. Results obtained using an excitation source in room ambient suggest a passivation effect. Further investigations and results are underway.

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A new synthesis route to obtain heterostructures based on g-C3N4 derivatives and graphene

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With the isolation of graphene in 2004, physical phenomena that had been predicted for years for truly two-dimensional (2D) structures could be experimentally tested and their properties measured [1]. At the same time, these properties were shown to be influenced or tuned by derivatization and chemical functionalization and various graphene materials began to be obtained, characterized and exploited as nanotechnology enablers in strategic industrial sectors. Currently, the major challenge has been the architectural combination of the different 2D structures, with a view to obtaining increasingly multifunctional, low-cost, sustainable and innovative materials. One example is obtaining hybrids between graphene and its derivatives and graphitic carbon nitrides (g-C_3N_4). This work proposes a new synthesis route for the construction of heterostructures based on g-C_3N_4 fragments functionalized with cyamelurate-type groups and graphene. The synthesis was divided into three stages: i) obtaining the g-C3N4 synthed by the polycondensation of melamine; ii) obtaining the fragments functionalized with cyamelurate-type groups iii) obtaining the heterostructures by dispersing g-C_3N_4 fragments functionalized with cyamelurate-type groups in graphene aqueous solution. The material obtained was called F-C_3N_4@G. All the samples were characterized using different techniques, including XRD, FTIR, SEM and Raman, confirming the formation of the heterostructures.

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Caloric Effect Due to the Aharonov–Bohm Flux in an Antidot

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In this work [1], we report the caloric effect for an electronic system of the antidot type, modeled by combining a repulsive and attractive potential (parabolic confinement). In this system, we consider the action of a perpendicular external magnetic field and the possibility of having an Aharonov–Bohm flux (AB-flux) generated by a current passing through a solenoid placed inside the forbidden zone for the electron. The energy levels are obtained analytically, and the model is known as the Bogachek and Landman model. We propose to control the caloric response of the system by varying only the AB-flux, finding that, in the absence of an external magnetic field, the maximization of the effect always occurs at the same AB-flux intensity, independently of the temperature while fixing the external magnetic field at a non-zero value breaks this symmetry and changes the point where the caloric phenomenon is maximized and is different depending on the temperature to which the process is carried. Our calculations indicate that using an effective electron mass of GaAs heterostructures and a trap intensity of the order of 2.896 meV, the modification of the AB-flux achieves a variation in temperature of the order of 1 K. Our analysis suggests that increasing the parabolic confinement twofold increases the effect threefold, while increasing the antidot generates the reverse effect, i.e., a strong decrease in the caloric phenomenon under study. Due to the great diversity in technological applications with antidots in electronics, the possibility of controlling their thermal response simply by varying the intensity of the internal current inside the solenoid (i.e., the intensity of AB-flux) can be a platform of interest for experimental studies.

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Charge-transfer processes in the MoS_2/WS_2/hBN and MoS_2/WS_2 vertical heterostructures coupled to a plasmonic grating.

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2D-Transition metal dichalcogenides heterostructures are becoming prominent models for studying physics at interfaces, particularly emphasizing the dynamics of excitons [1]. Literature reveals that exciton dynamics in these Van der Waals heterostructures may involve interactions among electron-hole pairs, electron-phonon coupling, spin-orbit, and spin-valley effects [1]. When coupling these heterostructures with plasmonic platforms, we could enhance photoluminescence (PL) emission [2], but charge transfer effects can also be observed due to the disparate work functions between semiconductors and metal. Depending on the efficiency of this latter process, it may induce PL quenching in the semiconductor [3]. Consequently, a common approach to mitigate such effects is employing a few layers of hBN as a protective layer between the heterostructure and the metal. This study investigates charge transfer processes in a hybrid system comprising a vertical heterostructure composed of a monolayer of WS2 and MoS2 on an Au grating. Two systems were examined: one with protective hBN few layers and another without. Analyses from different sample regions reveal distinct emissions from charge exchange processes between MoS2 and WS2 excitons when protected by hBN or in its absence. Furthermore, these processes are mediated by plasmonic effects, which enhance emissions and interact by exchanging charges with the system. Our investigation sheds light on charge transfer phenomena in hybrid van der Waals heterostructures coupled with plasmonic gratings.

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CO2 adsorption on graphene, α-graphyne and α-graphdiyne multi-layered structures through atomistic simulations

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Use of solid sorbents for CO2 capture represents a promising strategy for mitigating climate change impacts arising from anthropogenic greenhouse gas emissions [1]. In this work, we employ molecular dynamics and Monte Carlo simulations to explore the physisorption of CO2 onto graphene, α-graphyne, and α-graphdiyne sheets. These materials, characterized as 2D structures with sp and sp2 hybridization, share a common carbon-based composition and hexagonal lattice arrangement, with differing hexagon diameters [2]. Our study aims to elucidate the influence of this topological diversity on CO2 adsorption capacities. We calculate adsorption capacities for bilayers of the aforementioned materials separated by an interlayer spacing, and with periodic boundary conditions. We systematically vary the interlayer spacing to assess its effect on CO2 uptake. Our analyses reveal a correlation between the presence of multiple CO2 adsorption layers and the interlayer distance, with optimized uptake observed at specific spacing distances and pressures below atmospheric pressure. Additionally, we observe that the hexagonal geometry of these materials serves as 'trap' sites for CO2 adsorption, suggesting an optimal hexagon diameter for enhanced uptake at lower pressures. Notably, graphene exhibits minimal CO2 retention under small interlayer distances whereas graphyne and graphdiyne demonstrate pronounced gas storage within their hexagonal rings. Specifically, graphyne achieves uptakes of up to 9 mol/kg at pressures below 1 atm and at 300 K [3]. These findings contribute to a better understanding of the intricate adsorption behavior exhibited by carbon-based materials, thereby offering valuable insights into their potential for CO2 capture and storage in environmental contexts.

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Construction of a Triple Knudsen-Cell Type Evaporator

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Knudsen-cell type evaporators are commonly used for thin film deposition and constructing complex nanostructures at the surface through a bottom-up approach [1][2]. In some instances, the structure must be prepared using different precursors in varied evaporation conditions. Consequently, employing either multiple evaporators or interchange precursors within a single evaporator is necessary. However, the majority of ultra-high vacuum (UHV) systems have a limited number of insertion ports for this type of instrumentation. Changing the evaporator precursor is laborious and time-consuming. In this regard, we present a triple evaporator Knudsen-cell system's design, construction, and performance analysis. The main objective of this development was to create an evaporator capable of independently and simultaneously evaporating up to three precursors of low evaporation temperature. Halogen lamps perform the heating process of the cells, while cell insulation is achieved through water cooling. Once assembled, the evaporator was placed in a surface analysis system. The conducted tests demonstrate that the designed cooling system efficiently isolates between each Knudsen cell. Furthermore, the well-succeed co-deposition of molecules 1,3,5-tris[4-(pyridin-4-yl)-[1,1'-biphenyl])]benzene (TPyPPB) and Dichloro(1,10-phenanthroline)platinum(II) (DClPh-Pt) on Ag(111) surface exhibit promising results that were only possible by the use of the constructed evaporator.

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CVD growth of Niobium-doped WS2

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Monolayers of transition metal dichalcogenides (TMDCs), specifically in the 2H phase, have emerged as promising semiconductors for opto-valleytronic and opto-spintronic applications due to their strong spin-valley coupling [1]. In recent years, defect engineering has become an attractive avenue for enhancing the properties of these materials. Various approaches have been developed for in situ incorporation of substitutional dopants during growth, such as chemical vapor deposition (CVD) with solid precursors [2]. The doping concentration of substitutional atoms (e.g., Fe, niobium (Nb)) in TMDCs can be effectively tuned by adjusting the amount of dopant precursors, leading to concentration-dependent optical, electrical, and magnetic properties. The ability to control the density and spatial distribution of substitutional dopants in semiconductors is crucial for achieving desired physicochemical properties.

In this study, we employed CVD to grow monolayers of niobium-doped tungsten disulfide (WS2). The growth was characterized in detail using techniques such as photoluminescence (PL) spectroscopy and Raman spectroscopy. Our investigation focuses on understanding the impact of niobium doping on the optical and structural properties of WS2, providing valuable insights for the development of advanced materials in the field of 2D semiconductors and their applications in opto-valleytronics and opto-spintronics.

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Defects in Transition Metal Dichalcogenides: mechanical and electronic properties

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Recently, there has been a significant shift from theoretical predictions to extensive experimental development of new devices using 2D materials. Considerable efforts are being made to develop integrated circuits with these materials. Defects in crystalline materials can both be a drawback or the origin of new phenomena and properties. For example, they can govern molecular self-assembly [1] and ruling new topological states of matter [2]. Transition metal dichalcogenides (TMDs) are currently one of the most explored classes of 2D materials due to the high level of experimental control and the various degrees of freedom in their atomic species [3]. In this work, we have investigated the relationship between defect concentration in TMD systems and their mechanical and electronic properties. We have examined the presence of single types of defects as well as the competitive effects of different defects. Our research can serve as a guide for experimental development of new devices.

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Detection of antibiotics in milk samples using MXene coated-fibers-based impedimetric electronic tongue

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An electronic tongue (e-tongue) is an analytical instrument that uses the global selectivity concept to detect analytes in liquid samples. To design impedimetric e-tongues, usually distinct functionalized interdigitated electrodes are employed as sensing units to provide distinct electrical characteristics, which is imperative to ensure the discrimination of different analytes.[1] However, when the sensing unit has to be replaced, the e-tongue system needs to be recalibrated, since the electrical responses of the new electrode will be different from the replaced one. For the widespread and practical use of impedimetric e-tongues, sensing units that are produced in a fast, easy, and low-cost way are necessitated.[2] Nanostructured materials have been successfully employed as sensing units for e-tongues,[1] however, MXenes (2D carbides and nitrides of transition metals) remain largely underexplored in this type of application. Here, we produced MXene ($Ti_3C_{2-\alpha}N_\alpha$, with α being 0, 0.25, or 0.5) dip-coated nylon filaments in a continuous, scalable fashion to be used as sensing units of an impedimetric e-tongue. The fibers showed different electrical responses and were employed, as a proof of principle, to detect and discriminate distinct types of antibiotics (cloxacillin, tetracycline, and streptomycin) under varied concentrations. Analyses with contaminated goat and cow milk were also performed, showing the potential of the MXene-based e-tongue in detecting antibiotics in milk samples.

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DOPING CHARACTERIZATION OF ULTRATHIN GRAPHENE HETEROSTRUCTURES BY RAMAN SPECTROSCOPY

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Graphene holds great potential for applications due to its high electrical and thermal conductivities [1-3]. Advances in techniques for obtaining ultra-clean graphene enable the development of ultrathin devices in optoelectronics and photonics [1]. Among these applications, it is possible to exploit the high-energy conversion of p-type doped graphene into van der Waals heterostructures (vdWHs) using two-dimensional materials (2DMs) to create novel solar cells [2]. Additionally, Raman spectroscopy stands out as a widely employed tool for characterizing 2DMs and their vdWHs due to its speed and non-destructive nature. Therefore, using Raman spectroscopy is compelling to identify how 2DMs dope graphene and determine which materials are suitable for fabricating high-quality graphene-based vdWHs [3]. In this project, we developed a Python program to analyze Raman map measurements for various vdWHs, correlating them with doping and/or strain in assembled graphene. Furthermore, the program allows us to pinpoint the most homogeneous regions within the heterostructure, promoting higher quality in the graphene-based devices. In the future, we intend to compare Raman spectroscopy measurements with electrical data to enhance our analysis of developed vdWHs and deepen our understanding of these ultrathin nanostructures. Therefore, our work aims to streamline the process of designing vdWH-based devices using a Python program.

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Efficient Catalytic Oxidation of Sulfide to Sulfone Using Layered Ag(I)-Substituted K4Nb6O17

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K4Nb6O17 is a layered n-type semiconductor, showing promising potential for both photocatalytic and catalytic reactions. Its unique structure, characterized by two distinct interlayer regions and the existence of octahedra with different degrees of distortion, confers unique properties to the material, notably in terms of hydration behavior. Moreover, this material offers ample opportunities for enhancing intracrystalline activity through various modifications, such as doping, intercalation, exfoliation, ionic exchange, etc (Souza et al., 2020). Substituting interlayer K+ ions with transition metal ions like Ag+ through ionic exchange can lead to improved properties due to modifications in the conduction band, the existence of d-d transitions and the distortion of octahedra, thus promoting enhanced charge separation and the generation of reactive oxygen species (ROS)[1].

In the present study, Ag(I)-substituted K4Nb6O17 was synthed by treating K4Nb6O17, obtained primarily through the polymeric precursor method, with a solution of AgNO3 for three days with stirring at room temperature. Its catalytic property was investigated through the selective oxidation reaction of sulfides to sulfones and sulfoxides and the mechanism of generation of ROS was studied by utilizing scavenger and probe reactions. The formation of 98% of sulfones was observed.

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Electronic band structure and magnetic properties of doped silicene

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The growing interest in low-dimensional materials has led to the emergence of important ramifications in scientific knowledge such as the emergence of nanoscience and nanotechnology. Nanometer-scale materials exhibit behaviors distinct from those of structural macroscopic. Due to associated quantum effects, these materials can possess new properties such as high electronic mobility and thermal conductivity, in addition to greater mechanical resistance. On the other hand, silicon is a material whose technological application is well established, and obtaining this material in nanostructured form expands its possibility of integration into current technology. Doping with open shell elements can be used to adjust the silicene band gap and at the same time introduce new functions, for example turning the material into a ferromagnet or into a antiferromagnet. This properties could led to spintronic applications. However, several aspects of silicene doped with transition metals still remain unanswered, such as solubility limits of dopant, site preference for adsorption and doping and formation of magnetic domains. In this work we carried out the investigation of diffusion doping of Chromium atoms on silicene. Bilayer silicene was also investigated. We found that some metals introduce new magnetic properties into silicene, in addition to form metal alloys with it. Doped silicene seems to be promising for the application of these materials in electronic and magnetic devices.This work is already available [1].

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Evaluating Carbon Nitride as a metal-free sunblock active component

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The active components in sunscreens must absorb, reflect, or scatter UV rays (λ = 100 to 400 nm) [1]. Carbon nitride, a class of polymeric semiconductors of chemical representation C_3N_4, also absorbs light below 400 nm as TiO_2 and ZnO, typical inorganic materials used as active components in sunscreens. Therefore, it is a positively metal-free alternative for sunblock formulation. Through the thermal condensation of melamine in sodium chloride one crystalline form of carbon nitrides can be obtained, i.e. poly(heptazine) imide (PHI). This synthesis yields Na-PHI, which Na^+ cations can be easily exchanged for H^+ by adding HCl, resulting in protonated poly(heptazine imide) (H-PHI). In this work we aim to determine the SPF of a Na-PHI and H-PHI simple sunscreen formulation by in vitro diffuse reflectance UV-Vis spectroscopy method, comparing to TiO_2, ZnO, and commercial sunscreens to evaluate the potential of carbon nitride as active ingredient. For the SPF determination, we measured the total transmittance using a UV-Vis spectrophotometer with an integrating sphere for diffuse reflectance, and we calculated the SPF according to the reference method [2,3]. Comparing the results of Na-PHI and H-PHI 2M to the usuals active compounds, we concluded that the carbon nitride has similar activity, pointing out as a potential new active material for sunscreens. Nevertheless, we must further explore methods for determining SPF and other important parameters, as well different formulations for testing.

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Exploring the role of the Fe on the physical properties of Fe-doped TiO_2 nanosheets obtained from ilmenite

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In this research, Fe-doped TiO_2 nanosheets were synthesized from ilmenite ($FeTiO_3$), aiming to produce a low-cost photocatalytic material for application in environmental remediation. Raw ilmenite was milled using high-energy ball milling, followed by microwave-assisted alkaline hydrothermal synthesis, employing NaOH as an alkaline agent. Scanning electron microscopy analyses of the as-synthesized material confirmed the formation of nanosheets, while transmission electron microscopy showed that they are extremely thin, consisting of a few atomic layers. X-ray diffraction (XRD) was utilized for the identification of the crystalline phase, indicating the formation of anatase, with preferential growth on the (101) plane, the plane of lowest energy [1]. Photocatalytic efficiency was evaluated by the degradation of methylene blue, demonstrating high efficiency in comparison to the reference photocatalyst P25. Diffuse reflectance and luminescence analyses show a band gap energy and photon emission of 3.1 eV. Mössbauer spectroscopy analyses suggested that Fe is present in three different phases. The major concentration is located in a paramagnetic phase, probably substituting some Ti sites in the anatase lattice. The other phases were identified as Fe oxides, primarily hematite, also detected in XRD. The later displays superparamagnetic behavior and could only be identified through Mössbauer measurements at low temperature (4 K). These phase formations are currently under investigation by Raman and X-ray photoelectron spectroscopies to confirm the Mössbauer results aiming to understand the electronic structure and the role of Fe in the material's property.

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Exploring the use of earth-abundant layered materials in 2D-based studies: from natural mines to van der Waals applications

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Phyllosilicate minerals are an emerging class of naturally occurring layered insulators with large bandgap energy that have gained considerable attention from the scientific community. This layered materials (LMs) class has been explored recently at the ultrathin two-dimensional (2D) level due to their specific mechanical and optoelectronic properties, which are crucial for engineering novel devices. Phyllosilicates have lamellar structures and can be embedded into van der Waals heterostructures due to the possibility of exfoliation down to monolayers (MLs) and easy handling. Here, we will present a high throughput characterization of some naturally occurring LMs by employing several experimental techniques and first-principles calculations. We will demonstrate that these LMs can be applied in different nanotechnological areas [1-3]. Consequently, phyllosilicate minerals can be considered promising low-cost nanomaterials for electronics, photonics, and optoelectronics future 2D-based device applications. We will also present features of these nanomaterials relevant to their use in potential 2D-based applications, discussing the major challenges in working with them.

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Fabrication of pillars on the basal plane of MoS2 using focused ion beam for improved hydrogen evolution reaction

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With the advancement of nanotechnology, the properties of transition metal dichalcogenides (TMDs), such as their chemical nature and atomic structure, have been explored in the energy field [1]. Among the TMDs, molybdenum disulfide (MoS2), stands out as a promising material due to its low cost and high abundance. Its structure features a very stable basal plane and catalytic active sites located at the edge terminations [2]. Thus, the objective of this work is to use MoS2 as a substitute for the noble metals used in the hydrogen evolution reaction (HER) and activate its basal plane through the insertion of edge-like defects. By introducing edge defects in the MoS2 basal plane, we intended to increase the number of active sites for HER. MoS2 crystals approximately 100 nm thick were transferred to a gold substrate and selected after laser scanning confocal microscopy (LSCM) analysis. Edge defects were then introduced on the MoS2 basal plane with controlled position and using Ga+ beam. Pillars of different s were fabricated and the electrocatalytic activity for HER was compared. Characterization by Energy dispersive X-ray and Raman spectroscopies demonstrated the complete thinning of MoS2. Surface topography and kelvin probe mapping by AFM confirmed the thickness measured by LSCM and showed an increase in surface potential in the edge regions. The later suggests chemical alterations on the edges. In addition, HER polarization curves demonstrated better performance for the arrays formed by 5x5 um MoS2 pillars. The overpotential decreased 300 mV when compared to the pristine basal plane.

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Flexile electrochemical sensor based on $NiFe_2O_4$ and laser induced graphene for H_2O_2 detection

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Laser induced graphene (LIG) are electrodes of low cost, with small dimensions, flexible and present high conductivity and stability.[1] Therefore, LIG electrodes have been used in applications such as sensors, battery, capacitors and energy storage.[2] Currently, with objective to increase the sensibility and selectivity of LIG, new strategies have been developed with the inclusion of nanomaterials and metal-organic frameworks (MOFs) to modified the electrode surface. Most strategies are based on drop-casting or electrodeposition, which are not so reproducible because of the higher number of stages for developing the modified LIG electrode. Therefore, the development of enhanced alternatives is demanded. In this context, we present LIG electrodes modified with nickel ferrites ($NiFe_2O_4$) by a novel modification procedure for H_2O_2 determination. $NiFe_2O_4$ microparticles are incorporated within the polyimide film by a single-step laser irradiation procedure. The conditions like velocity and laser potential were studied to obtain the best sensing conditions for H_2O_2. The electrode was characterized by scanning electronic microscopy (SEM) and Raman spectroscopy. SEM images and Raman spectra confirmed the presence of $NiFe_2O_4$ within the graphene matrix. Preliminary study using cyclic voltammetry shows the improved sensing features of LIG-Ni compared with an unmodified LIG for H_2O_2 in PBS buffer pH 7.4. The LIG-Ni sensor was assembled into a 3D-printed batch-injection cell for the amperometric detection of H2O2 with a linear range from 1 to 100 µmol L^{-1} (R2 = 0.996) and sample throughput close to 200 injections h^{-1}.

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Graphene oxide reduction process: monitoring and modeling of reaction kinetics

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Graphene is of extreme importance due to its unique physical properties such as mechanical strength, thermal and electrical conductivity and transparency, among others, making this material ubiquitous in science, technology and engineering. Unfortunately, obtaining this material is complex and, because of that, considerable efforts are devoted in finding mor efficient methods for large-scale and low-cost production of graphene. A viable alternative is the chemical reduction of graphene oxide. Depending on the specific application, a material with properties similar to those of the graphene can be obtained to some extent by removing oxygen, hydrogen and lattice defects. For instance, by the reduction process the electrical conductivity of the graphene oxide, which is an insulator, can be increased resulting in conductive reduced graphene oxide. This changing in the electrical conductivity can be also used for monitoring the kinetics of the reduction process. Despite the importance of the chemical reduction of graphene oxide, there is a lack of studies of the reaction kinetics of this process, whose description would allow its optimization both in time and in cost. This work aims to show a novel scheme for real time and on-line electrical monitoring of the graphene oxide chemical reduction process. The method is teste in different reduction conditions. The electrical conductivity of the reduction solution is measured continuously during the process. A mathematical model is also proposed to determine the reduced graphene oxide concentration from conductivity according to the following expression: $m=\exp((\kappa-c)/a)-b$, where a, b and c are fitting parameters. This model was validated with other expressions found in literature for the conductivity of electrolyte solutions [1].

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Hydrogenation and Elastic Strain Effects on the Electronic Structure of TPDH-graphene

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Since its discovery and synthesis, graphene has been considered a promising material in a wide range of applications, owing to its unique mechanical, thermal, electronic, and optical properties[1]. However, in its pure form, graphene has its limitations, such as for certain applications in electronics due to the absence of a band gap. To overcome this issue, various solutions have been proposed, such as the synthesis of new materials based on graphene, chemical functionalization, and elastic deformation. Chemical functionalization of graphene, through hydrogenation and/or fluorination[2], and elastic deformation have been widely studied, yielding significant results with the emergence of an adjustable band gap in the structure, thereby promoting greater potential for applications of this material.

In this work, based on first-principles calculations using density functional theory (DFT) and reactive molecular dynamics simulations (MD), the structural and electronic effects of hydrogenation and deformation in TPDH-graphene (Tetra-Penta-Deca-Hexa), a metallic character material based on graphene, were studied. The DFT results show a change in the electronic structure, opening a 0.5eV band gap. MD simulations reveal a curious pattern of hydrogenation, where hydrogen lines are formed along the material, consistent with the prediction of the DFT calculations. The simulations also show that the favorable hydrogenation sites are dependent on temperature and applied tension.

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Incorporation of Graphene into SAC Solder Paste - A Prospective Study

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As electronic devices have become more complex and smaller, manufacturing processes for electronic assemblies have improved in recent years. As a result of the elimination of lead in electronic assembly, new solder alloys have been developed in response to this new reality. Intermetallics, the thin layer that forms between the solder joint and the printed circuit board (PCB) in ternary SAC305 or SAC405 solder compositions, can lead to serious reliability problems if the process parameters are not controlled. In order to reduce intermetallic formation, the incorporation of various types of particles into the solder paste has also been researched, including graphene. Although the addition of graphene does not increase the reflow temperature of the solder, several authors have reported that it may not be incorporated into the solder joint and may form agglomerates. A prospective study of the addition of graphene to SAC 405 solder paste was conducted in this paper. Using an orbital mixer, the solder paste was mixed with the graphene at 2000 rpm for 3 min. Optical microscopy analysis revealed the presence of graphene agglomerates in the solder joint and on the surface, and no significant change in intermetallic thickness when graphene was added. These results are consistent with the literature when graphene is added to solder paste already mixed with flux. Research shows that graphene is incorporated into the solder alloy when it is added to the powder prior to mixing with flux or when it is added to the liquid solder alloy. A study is underway to incorporate graphene into liquid solder.

Influence of processing conditions on dispersion and dynamic-mechanical properties of elastomeric compounds containing carbon nanotubes

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There is a current trend in transport sector to improve energy efficiency and vehicle performance. In this context, an option is to use tires with lower rolling resistance, related to energy loss due to hysteresis. The use of silica as reinforcing filler, replacing traditional fillers as carbon black, allows this property to be improved, but prevents the dissipation of electrostatic charges generated due to the tires friction with the ground and friction of mechanical parts. An alternative is the incorporation of carbon nanoparticles as conductive filler. This work aims to develop an elastomeric compound containing silica and multi-walled carbon nanotubes (MWCNT) for application in tire tread, using an elastomeric mixture of natural rubber (NR) and polybutadiene rubber (BR) as matrix. The influence of MWCNT addition and processing conditions on the compounds properties were evaluated through the dispersion state of particles in the vulcanized compound (SEM) and dynamic-mechanical properties (DMA). The nanoparticles incorporation through pre-dispersion (PD) proved to be advantageous by promoting better dispersion of MWCNT and silica, resulting in the enhancement of dynamic-mechanical properties when compared to the direct incorporation of MWCNT in powder form.

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INVESTIGATION OF THE NONLINEAR OPTICAL FREQUENCY CONVERSION IN ULTRATHIN FRANCKEITE HETEROSTRUCTURES

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Layered franckeite is a natural superlattice composed of two alternating layers of different compositions, SnS2- and PbS-like. This creates incommensurability between the two species along the planes of the layers, resulting in spontaneous symmetry-break periodic ripples in the a-axis orientation. Nevertheless, natural franckeite heterostructure has shown potential for optoelectronic applications mostly because it is a semiconductor with 0.7 eV bandgap, air-stable, and can be easily exfoliated down to ultrathin thicknesses. Here, we demonstrate that few-layer franckeite shows a highly anisotropic nonlinear optical response due to its lattice structure, which allow for the identification of the ripple axis. Moreover, we find that the highly anisotropic third-harmonic emission strongly varies with material thickness. These features are further corroborated by a theoretical nonlinear susceptibility model and the nonlinear transfer matrix method [1]. Overall, our findings help to understand this material and propose a characterization method that could be used in other layered materials and heterostructures to assign their characteristic axes.

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Laser-induced graphene in electrochemical sensors for heavy metal detection.

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Laser-induced graphene (LIG) is a material with regions of graphene intertwined with carbon, thus forming a three-dimensional structure, possessing interesting properties such as high electrical conductivity, high surface area, among others [1]. Since its discovery (2014), it has been proving to be a promising material for various potential applications in several technological fields [3]. The methodology used for printing these electrodes was to engrave the LIG on a PI tape over a Teflon sheet [2]. Characterizing them using a multimeter to measure the electrical resistance of the electrodes and electrochemical techniques such as cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS), using a solution of Ferri/Ferro cyanide at 10 mmol·L^{-1} in 0.1 mol·L^{-1} KCl as the supporting electrolyte. Additionally, scanning electron microscopy (SEM) and Raman spectroscopy (RS) techniques were used. The electrodes exhibited an electrical resistance of 144 ± 6 Ω and were electrochemically characterized by CV techniques, which showed a peak separation of approximately 80 mV, indicating the good reversibility of the redox reaction at the electrode interface. In EIS, it was possible to observe the presence of different processes occurring at the interface, such as charge transfer and diffusional processes. And in RS, it was possible to observe the characteristic D and G bands of this material. In SEM, a fairly uniform surface was observed, which corroborates with the electrical resistance data that were measured. Moreover, this electrode detected heavy metals, such as lead, at low concentrations, on the order of µg·L^{-1}. Thus, LIG proves to be a promising material for applications in electrochemical sensors.

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Low-cost and scalable production of few-layer MoS2 via liquid phase exfoliation

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The increasing demand for new advanced materials for technological applications has intensified significantly worldwide. Layered 2D materials, such as graphene and molybdenum disulfide (MoS2), have emerged as versatile materials endowed with distinctive physico-chemical properties for a variety of applications [1]. However, achieving high-quality few-layer dispersions to produce thin films is still a challenge, particularly, when focusing on characteristics such as simple processing, non-toxicity, low cost, and scalability. In this context, liquid phase exfoliation (LPE) can be a promising strategy to produce highly concentrated 2D material-based inks. LPE methods rely on the interaction between the layered bulk material and the solvent to promote exfoliation by effectively overcoming the Van der Walls interactions between 2D flakes and avoiding their reaggregation. This route employs different approaches, such as ultrasound-induced LPE (UILPE), high-shear mixing exfoliation (HSM), microfluidization, electrochemical exfoliation (EE), and others. Here, aiming to investigate the production of exfoliated 2D material dispersions in green solvents we exploit different processing parameters to produce few-flake MoS2 inks[3]. The goal is to obtain high concentration few-flake MoS2 dispersions for the production of thin films towards their integration into electronic devices. Ultimately, this research aims to establish a platform for the exfoliation of 2D materials for printed and flexible electronics.

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Measurement of physical properties of nanoscale bismuth triiodide-graphene heterostructures

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Nanometric heterostructures of BiI3-graphene were obtained by physical vapor deposition in a specialized equipment designed to operate under pressure conditions of 10-7–10-8mBar, which allowed for strict control of variables such as source and substrate temperature, deposition time, and source-substrate distance. BiI3 was grown onto graphene covered SiO2/Si substrates, previously UV/ozone-treated. The growth conditions of the heterostructures include a process involving nucleation, thermal annealing, and post-growth, utilizing a source temperature of 265°C and annealing at 150°C, always working under high-purity Argon atmosphere. The resulting heterostructures were characterized using Scanning Electron Microscopy-Field Emission Gun (SEM-FEG), X-Ray Reflectometry (XRR) and Gracing Incidence X-Ray Diffraction (GIXRD), Raman Spectroscopy and X-Ray Photoelectron Spectroscopy (XPS).

SEM-FEG imaging revealed the uniformity of the obtained heterostructures, while XRR provided thickness measurements ranging from 7,59 to 34,6 nm. GIXRD analysis indicated that BiI3 layers on graphene exhibited a rhombohedral phase R-3, oriented with the c-axis perpendicular to the substrate. Raman spectra exhibited a peak around 115 cm-1, consistent with the out-of-plane Ag Raman mode of bulk BiI3, which does not show a relationship between the thickness and frequency, at least in the range of thicknesses considered [1]. XPS confirmed the chemical composition of the heterostructures, with peaks corresponding to I3d5/2, Bi4f5/2, and Bi4f7/2, attributed to distinctive signals originating from I- and Bi3+ species, respectively. There are not evidence of reaction between BiI3 and Graphene, which are then related with Van der Waals bonds.

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Nanofluids based on aminated-GO and polyacrylamide for oil recovery

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Enhanced oil recovery (EOR) is a tertiary strategy that promotes flooding of fluids into oil wells to increase the sweep of unextracted oil in primary and secondary processes [1]. The polymer partially hydrolyzed polyacrylamide (HPAM) is one of the most used in EOR to increase the viscosity of water, however, HPAM is degraded in reservoir conditions due to pH, high temperature, and salinity, thus losing its rheological properties during the process [1,2]. Polymeric nanocomposites based on graphene oxide (GO) have been an alternative to produce nanofluids as a way of modulating the rheological properties of HPAM, such as viscosity [2]. From these perspectives, the functionalization of GO with amines was carried out in this work using three different methodologies such as microwave reaction (MW), magnetic mixture (MM) at 70°C, and MM at room temperature, focused on comparing the surface modification and level of functionalization of graphene oxide (GO). Aminated-GO was characterized by Fourier transform infrared spectroscopy (FTIR) and thermal analysis (TG/DTG). The FTIR results of the three samples indicated that aminated-GO presented absorption bands that do not appear for GO, such as $1646 cm^{-1}$ and $1034 cm^{-1}$ related to amide-type bonds, and -C-N of amines, respectively [2]. By TG/DTG, a greater loss of mass was observed for aminated-GO compared to GO, in addition to observing that the carbon structure of the material was more preserved due to having been degraded at higher temperatures compared to GO. Given these results, it is inferred that functionalization effectively occurred in all three methods, thus obtaining a promising nanomaterial in EOR.

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Nickel Single Atoms supported on Crystalline Carbon Nitride: a new route for photocatalyzed sustainable H-Transfer

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Hydrogenation of unsaturated organic molecules is an important step on about 25% of all industrial process,[1] and a growing challenge to be overcome revolves around the high energy demand required to perform these reactions on a large scale. This issue has been directing the attention of various researchers towards the largest, yet still underutilized, existing energy source: the sun. In order to achieve a viable and effective process for converting solar energy into chemical energy, it is necessary to use a catalyst active in the visible light spectrum, such as crystalline carbon nitrides in the form of poly(heptazine imides), simple and efficient semiconductors capable of coordinating single atoms of catalytic metals,[2] thus expanding their potential applications. The application of this material discussed in this study is hydrogen transfer, an alternative and refined route of hydrogenation, where the need for molecular H2, mainly derived from fossil sources, is eliminated. The main success of this study was the optimization of the conditions under which this process is carried out, using water as a source of protons to perform the reduction of nitrobenzene to aniline, catalyzed by crystalline carbon nitride coordinated with single atoms of nickel, in addition to glycerol as a sacrificial reagent, ideal due to its low cost and toxicity. This method performed excellently under this conditions, obtaining the total conversion of nitrobenzene, with 100% selectivity to aniline, after 9h of irradiation.

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Obtaining metallic monocrystalline substrates for wafer-size epitaxial growth of 2D materials

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Ultrathin two-dimensional (2D) layered materials offer great potential for electronic and optoelectronic applications. One key challenge with 2D semiconductors is the ability to grow 2D materials with high quality and scalable for wafer- device applications. One of the most promising techniques is through epitaxy due to more favorable growth on metallic single crystals in a highly reproducible way. However, transferring these materials between substrates to enable layer-by-layer integration can still be an obstacle for bulk metallic single crystals. Recently, the successful epitaxial growth of single-crystal graphene and h-BN monolayers on a Cu (111) single-domain thin film on the sapphire wafers and its subsequent transfer to insulating substrates was reported [1, 2, 3]. This method proved compatible with advanced microelectronic fabrication on wafers with monolayers of single-oriented 2D materials. The formation of this Cu (111)/sapphire substrate occurs through the deposition of the metal by sputtering on the sapphire and then performing thermal annealing to achieve single-crystal Cu (111) films. Since Cu (111) tends to form twin-grain boundaries, through kinetic growth processes, the annealing process occurs in the presence of a hydrogen atmosphere close to the melting temperature of Cu. Nonetheless, here we report the successful epitaxial growth of single-crystal Cu (111) thin film on sapphire (0001). The high quality of the single-crystal, with wide terraces and low defect density, was verified using x-ray photoelectron spectroscopy (XPS), low-energy electron diffraction (LEED), and scanning tunneling microscopy (STM).

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Optical and magneto-optical properties of monolayer $WSe_2/\beta\text{-}Ga_2O_3$

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Nano-strain and defects engineering play an important role in controlling optical properties of van der Waals heterostructures, particularly for generating atomic defect-based single-photon emitters, which are the platform for the development of on-chip integrated single-photon sources for quantum technology [1,3]. Monoclinic gallium oxide ($\beta\text{-}Ga_2O_3$) is an ultra-wide bandgap semiconductor which attracted increasing interest for possible applications in power electronics and UV optoelectronics [2-3]. Despite of not being a van der Waals material and having highly strong ionic bonding, the $\beta\text{-}Ga_2O_3$ crystal can be mechanically exfoliated along the (100) favorable surfaces to make ultra-thin layers for device fabrication and nanotechnology [3]. In this work, we investigated optical and magneto-optical properties of a monolayer (ML) $WSe_2/\beta\text{-}Ga_2O_3$ flakes on SiO_2 substrates under perpendicular magnetic field. Interestingly, we observed several sharp emission peaks at low temperatures. These emission peaks have shown valley g-factors values close to -4 which is an unusual result for localized excitons in ML WSe_2. Moreover, some other PL peaks have shown higher g-factor values of ≈ -7 and ≈ -12 and were associated with the hybridization of strain localized dark excitons and point defects. Finally, our studies provide fundamental insights on the impact of exfoliated Ga2O3 substrates and point defects on the optical and magneto-optical properties of monolayer WSe_2. Our results are particularly relevant for the development of devices in optoelectronics and possible applications in quantum information technology [3].

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Photocatalytic oxidation of cyclohexane into KA oil and adipic acid using poly(heptazine imide)

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Industrially, the generation of adipic acid, precursor of nylon, involves the oxidation of cyclohexanol and cyclohexanone (known as KA oil) followed by the co-oxidation of these two compounds. This process occurs using nitric acid as an oxidizing agent and releases N2O, a greenhouse gas under harsh conditions, additionally, the selectivity and conversion for this reaction is low. In this context, the development of sustainable routes to produce adipic acid under mild conditions have been explored. Preliminary results utilizing O2 as a green oxidant and catalyzed by crystalline carbon nitride in the form of PHI, poly(heptazine imide) modified with metallic single atoms (Mn, Co, Fe), an heterogeneous, cheap, stable, atoxic catalyst composed mainly by carbon and nitrogen; demonstrated a selectivity of 10% for cyclohexanol and 15% for cyclohexanone derived from cyclohexanol using visible light (410 nm) and acetonitrile as solvent under mild temperature and atmospheric pressure. Moreover, some results show the production of small amounts of adipic acid, under similar conditions, suggesting a promising direct one-pot oxidation from cyclohexane into adipic acid.

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POLYMER NANOCOMPOSITES FOR APPLICATION AS THERMAL AND ANTIMICROBIAL SMART-COATING IN CIVIL CONSTRUCTION

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Innovative alternatives in civil engineering using polymeric materials with nanometric reinforcements are the subject of recent studies due to the need to improve the performance of buildings in the civil construction [1]. Graphene oxide (GO) and silver nanoparticles (AgNPs) are good candidates for this goal. GO is a graphene-based nanomaterial with interesting chemical, mechanical and thermal properties. Silver nanoparticles can control the growth of many pathogens. In this research, hybrid materials of GO and AgNPs were used as reinforcements in acrylic polymer matrices for application as smart-ink in civil construction. The first part involved synthesizing precursor materials and an experimental optimization of nanocomposites. The chosen method was based on latex technology, mixing the GO and AgNPs dispersions with the latex [2]. The nanomaterials were characterized by atomic force microscopy (AFM) in topography, nanomechanics mode, scanning electron microscopy (SEM), and infrared and Raman spectroscopies. The results have demonstrated a good interaction between the nanocomposite components. SEM indicates a good homogeneity of the materials and GO adherence to the polymer. AFM images show that the insertion of GO and the AgNPs increases the adhesiveness and elastic modulus of the polymer. In the next steps, we will evaluate antimicrobial activity and, through experiments and computational calculations, estimate the thermal properties of the materials. Rheological analyses and other technological characterizations will also be carried out per technical standards. This work is expected to develop nanocomposites with antimicrobial characteristics and thermal properties that can be used for civil construction.

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Probing the influence of strain, chemical composition and dimensionality on the vibrational and electronic properties of layered minerals

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The vibrational and electronic structure of materials carry fingerprints of their structure, besides revealing several physical properties, as their mechanical strength and optical absorption. Thus, the interatomic force constants and electronic interactions are dependent of mechanical strain, chemical composition and the dimensionality of the materials. Here, we present our findings on the influence of strain in the lattice vibrations in monolayer gallium selenide [1], of dimensionality on the Raman and infrared spectra in gallium selenide and talc [2] and on the electronic band gap in phlogopite [3], of chemical composition in the zone-centre phonons in jacutingaite and tilkerodeite and electronic structure in phlogopite [3].

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Production and characterization of MXenes / ethylene propylene copolymer nanocomposites

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MXenes possess very interesting properties such as high conductive, outstanding mechanical properties, compositional and structural diversity and variable surface chemistry. These features allows forecasting. These properties inspire the utilization of MXenes in many-different applications. Among others, these 2D compounds are attractive materials as fillers in polymer matrix nanocomposites[1-3]. In this study, the production and properties of MXenes/ethylene propylene copolymer nanocomposites were investigated. These composites were produced by blade coating method. First, the Ti2C and Ti3C2 MXenes were synthed through the exfoliation and delamination of the commercial Ti2AlC and Ti3AlC2 MAX phases. Solutions of MXenes dispersed into the ethylene propylene copolymer were prepared with different MXenes/ polymer rations. The deposition method of these solutions was studied varying the gap between the substrate and blade, bade velocity and substrate temperature. The obtained films were analyzed by electrical measurements, nanoindentation tests and microscopy techniques. The interplay between the deposition parameters, films quality and microstructures, and materials properties are discussed in this presentation.

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Production and characterization of MXenes/polypropylene nanocomposites

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Two-dimensional MXenes possess exceptional properties, such as high electrical and thermal conductivities, high Young modulus and mechanical strength, low coefficient of friction, and hydrophilic surface functionalities, which have been widely explored for applications in energy storage, sensors, packing, electromagnetic shielding, catalysis and so on [1]. This study focuses on the production of MXene/polypropylene nanocomposites by blade coating method. First, the Ti3C2Tx MXenes was synthed from the commercial Ti3AlC2 MAX phase by chemical exfoliation and delamination. Solutions of MXene and polypropylene were prepared with different MXene/polypropylene rations. The deposition method of these solutions was studied varying the gap between the substrate and blade, bade velocity and substrate temperature. The obtained films were analyzed by electrical measurements, nanoindentation tests and microscopy techniques. The interplay between the deposition parameters, films quality and microstructures, and materials properties are discussed in this presentation.

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Raman Microscopy Characterization of Jacutingaite (Pt_2HgSe_3)

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The Jacutingaite (Pt_2HgSe_3) is a mineral recently discovered in Itabira, Minas Gerais, and it exhibits a robust topological phase, with a recently characterized lamellar crystalline phase. Due to its properties, there has been an increasing focus on studying Jacutingaite to identify its characteristics. Therefore, the objective of this work is to characterize Jacutingaite through scanning electron microscopy, elemental analysis, and Raman spectroscopy, studying its properties, potentials, and applications in real situations with induced defects. The methodology involves experimentation and theoretical foundation. The first part presented here involves the optical and spectroscopic characterization of the material, using white light microscopy and Raman spectroscopy. Simultaneously, literature information about the material's structure is presented, along with calculations and developments in Raman spectroscopy applied to Jacutingaite with induced defects in its structure. The presented measurements show a unique identification of these defects, with characteristic material band modifications in the range between 150 and 220 cm^{-1} when defects are induced. The research proposed in this work is ongoing, and it is expected that the results will bring relevant insights into understanding Jacutingaite defects, which is crucial for future industrial applications.

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RAMAN SPECTRA OF TWISTED BILAYER GRAPHENE CLOSE TO THE MAGIC ANGLE

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In this work, we study the Raman spectra of twisted bilayer graphene samples as a function of their twist-angles (θ), ranging from 0.03º to 3.40º, where local θ are determined by analysis of their associated moiré superlattices, as imaged by scanning microwave impedance microscopy. Three standard excitation laser lines are used (457, 532, and 633 nm wavelengths), and the main Raman active graphene bands (G and 2D) are considered. Our results reveal that electron–phonon interaction influences the G band's linewidth close to the magic angle regardless of laser excitation wavelength. Also, the 2D band lineshape in the θ < 1º regime is dictated by crystal lattice and depends on both the Bernal (AB and BA) stacking bilayer graphene and strain soliton regions (SP) [2]. We propose a geometrical model to explain the 2D lineshape variations, and from it, we estimate the SP width when moving towards the magic angle.

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Structural and microscopic analysis of a new mineral: Roterbärite

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Belonging to the lapieite group, the new mineral Roterbärita ($PdCuBiSe_3$) was discovered in the Roter Bär mine, located in the Harz Mountains, Germany [1-2]. The first studies show that Roterbärita occurs in an orthorhombic crystal structure, with a quasi-2D layered structure with interlayer interactions mediated by metavalent bonds, and its lattice parameters a, b, and c have values of 5.00, 7.99, and 13.59 Å, respectively [1]. In addition, a synthetic version of the mineral, produced at the Experimental Mineralogy Laboratory of the Czech Geological Survey in Prague, has been found to be equivalent to the natural material [2], thus promoting the possibility of reproduction and complete characterization. Ongoing research focuses on the study of the properties and characterizing Roterbärita, using its synthetic analogue, through advanced experimental techniques, such as Scanning Electron Microscopy (SEM) with energy-dispersive spectroscopy (EDS) and Raman spectroscopy. A primary analisis, using the images and spectrum obtained through Raman spectroscopy, with a laser of ~785 nm and an objective of 50X magnification, shows that the material has a metallic luster, a spectrum with various peaks located between 150 and 200 cm^{-1}, providing a fingerprint for future identification. These studies pave the way for understanding Roterbärita's properties and potential applications.

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Study of the mechanical properties of WSe2 Nano-Origamis with Reactive Molecular Dynamics.

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The research addresses the study of the mechanical properties of WSe2 Nano-Origamis through reactive molecular dynamics. Using computational simulations with the LAMMPS software [1] and the reax force field, we investigate the mechanical behavior of molecular kirigamis of WSe2. Kirigami is a process of creating patterns and shapes by cutting, stretching, or twisting materials. In molecular systems, kirigamis can be generated by manipulating the atomic structure of a material to create new molecular arrangements. Our study focuses on investigating the mechanical behavior of molecular kirigamis of WSe2 and their impact on the material's fracture patterns and elastic properties. To minimize modeling stresses, we equilibrate the system with the NPT ensemble for 100 ps and then apply uniaxial tension with the NVT ensemble at 300 K. We simulate the temporal evolution of atoms and molecules in the system using the Newton equations of motion and the Velocity-Verlet algorithm. Similar studies have been conducted on kirigamis of graphene and MoS2 [2], and this work builds on these previous findings to investigate WSe2. Our findings contribute to the fundamental understanding of WSe2, open up new avenues for material science research, and emphasizing the importance of utilizing advanced computational methods to investigate the properties of materials and their potential technological applications.

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Supercell effects on the structural and electronical properties of 2D films

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Materials in their two-dimensional form exhibit distinct properties compared to their bulk counterparts. These differences encompass aspects such as material deformation, response to temperature, work function, band gap, as well as the arrangement of HOMO-LUMO energy levels, among others. This peculiarity has sparked considerable research interest in the last couple of decades. Within this context, arises the question of what is the best way to computationally represent these materials to obtain more precise conclusions that can then be contrasted with experiments.

In the computational representation of such materials, it is crucial to determine the minimum system required to accurately capture the material's properties in its ground state. Furthermore, it is essential to consider how external factors, such as temperature, influence both its structural and electronic properties. In this study, MgO was selected as an example, a material consisting of a layer of Mg and O atoms supported on a Pd (001) structure. Various calculations were performed, varying the lattice parameter and optimizing different structures by modifying the cell to be simulated. Additionally, Ab Initio Molecular Dynamics simulations were conducted in an NVT ensemble, with temperatures ranging from 150 to 900 K. The calculations were carried out at the Density Functional Theory level using the Quantum Espresso and CP2K softwares. From these analyses, various electronic and structural properties were calculated, including Band Gap, Work Function, and monolayer oscillations, among others.. It was concluded that the cell used in the calculations is of utmost importance, especially when considering molecular dynamics simulations. Increasing the supercell allows more relaxation degrees of freedom, bringing new physics to the problem.

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Synthesis and characterization of graphene oxide decorated with niobium pentoxide (GO@Nb2O5)

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Graphene oxide (GO) is a 2D carbon nanostructure composed of functionalized graphene sheets. Functional groups are distributed onto the GO surface (e.g. hydroxyls, carbonyls, carboxyl ethers) attached to both sides and edges of the layers. GO presents unique optical, electronic, and chemical properties, enabling its application in several areas . In the field of photocatalysis, GO has stood out as a material used to improve the photocatalytic activity of a variety of semiconductors. As a result of its high surface area and elevated physicochemical properties, GO can increase the rate of photodegradation reactions based on semiconductor catalysts (metal oxides) [2]. On this basis, niobium(V) oxide (Nb2O5) is a semiconductor with great potential for water treatment due to its long-term stability during photocatalytic processes. However, it presents weak photocatalytic activity under visible irradiationt due to its large band gap energy. This problem can often be solved by combining Nb2O5 with highly conductive materials [3]. The present study aims to produce Nb2O5 decorated GO (GO@Nb2O5) by sol-gel for future application in the photocatalysis of drugs and dyes. The produced sample was characterized by X-ray Diffraction (XRD), Raman Spectroscopy and Scanning Electron Microscopy (SEM). The preliminary results obtained indicate the formation of the Go@Nb2O5 nanocatalyst.

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Synthesis and characterization of graphene oxides by pyrolysis of citric acid in nitrogen atmosphere

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Carbon complexes known as carbon quantum dots (CQDs) or graphene oxides (GOs) have several exceptional optical and electronic properties due to their quantum confinement and edge effects, especially the visible fluorescence of these particles that has been subject of numerous studies in the last decades. These kinds of carbon complexes can be produced by the bottom–up method, controlling the pyrolysis of citric acid (CA) which allows obtaining CQDs by incomplete carbonization of CA or GOs by complete carbonization of CA [1]. These materials are fluorescent and have several applications. Studies have shown that controlling the synthesis process of carbon complexes from CA pyrolysis at different temperatures and atmospheres can optimize and/or potentiate the light emitting properties [1]. Several GQD and GO samples were synthed from CA pyrolysis at temperatures ranging from 250°C to 400°C in open atmosphere and 450°C to 950°C in controlled N_2 atmosphere. Fluorescence and Raman spectroscopy measurements were used to confirm the presence of GQD and GO in samples prepared in open atmosphere and in nitrogen atmosphere. GQD samples prepared in open atmosphere exhibited broadened VIS emission spectra dependent on the excitation wavelength demonstrating that the CA pyrolysis was incomplete and that GQDs were formed. GO samples prepared in controlled atmosphere of N_2 showed blue emission spectra independent of the excitation wavelength, demonstrating a complete pyrolysis with the presence of GO. Raman analysis of the samples prepared in N_2 atmosphere revealed that different synthesis temperatures caused changes in the intensity of the D, G and 2D bands, related to the number of layers, and defects in the GO samples.

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Synthesis and characterization of jacutingaite (Pt_2HgSe_3): exploring solid-state reactions.

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Quantum materials such as: graphene, quantum dots, superconductors, quantum spin liquids, etc. are gaining relevance each year, specially with the development of advanced characterization techniques, that allow us to determine a wide range of material properties, that can only be explained through quantum theories. These types of materials exhibit distinctive properties, with applications varring from biomedicine to devices and computers. Among these materials, the so-called Topological Insulators exemplify this new technological trend very well. Due to relativistic effects and topological orders, this class of materials exhibits conducting states on their surface, despite being insulating in the bulk. Besides this unique property, topological insulators are excellent materials for studying electronic properties of matter, spin-orbit coupling, and phenomena such as the Hall effect and quantum spin Hall for 2D materials. The mineral Jacutingaite, discovered in Minas Gerais in 2008, is considered the first representative natural material of the Kane-Mele model of topological insulators. For this reason, several research groups have focused their attention on the synthesis and analysis of this mineral, which has proven to be a challenge for many. In this work, we present a synthesis method for Jacutingaite (Pt2HgSe3), via high-temperature solid state reaction, in an evacuated quartz ampoule, reacting in two steps for over a month. We varied pressurization during pellet formation to study its effect on the reaction. Promising results were obtained, confirming mineral synthesis and dimensions via X-ray diffraction, Rietveld refinement, SEM, and Raman spectroscopy. These techniques also showed its potential for future exfoliation due to the dimensions of the synthed crystals, and the layered nature of the material. Electrical measurements under alternating temperature and magnetic field were conducted on both PtSe2 and Pt2HgSe3 to compare their properties.

Temperature dependence of the bandgap energies in MoS₂: a photoluminescence study

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In this study, we investigated the transition metal dichalcogenide molybdenum disulfide (MoS_2) thin film. A precursor MoS_2/etanol solution was is drop casted on a silicon dioxide (SiO_2) substrate to create a thin film, later characterized by atomic force microscopy (AFM) , Raman spectroscopy, photoluminescence (PL), and UV-Vis spectroscopy. In particular, the PL of the film was carried out at temperatures ranging from 20 to 400 K. The temperature dependence of the energy band gaps extracted from the PL spectra was fitted by Pässler and Oelgar´s model for exciton peak positions in semiconductors . The temperature dependence of the model parameters, like the effective phonon energy, is also discussed.

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TMD-CARBON- BASED HETEROSTRUCTURES GROWN BY CHEMICAL VAPOR DEPOSITION

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Low-dimensional carbon-based materials have been the subject of several studies in the last two decades due to their interesting physical properties [1]. In particular, graphene has been widely used in various fields, and it can be synthetized by many methods, such as chemical vapor deposition (CVD), which is an efficient method to obtain large-scale and high-quality graphene. A lot of studies have been made regarding CVD growth using metal foils as catalysts. However, for device applications, we have to transfer the as-grown graphene onto another suitable substrate from the metal catalyst surface which needs a series of processes that sometimes may compromise sample quality. Recently, some work has been done towards the direct growth of graphene by CVD on desired target substrates [2,3]. The posterior growth of other materials on top of graphene, such as transition metal dichalcogenides (TMDs), can provide heterostructures that could be interesting in nanoelectronics. In this work, we propose to obtain TMDs or HS grown directly on a sp2 carbon film, all structures grown by CVD method on top of a Si/SiO2 substrate, avoiding any transfer process. We perform spectroscopic measurements to compare these samples with transfer-based carbon-TMD HS in order to infer the differences in layer interaction for both structures.

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Two-dimensional layered MA2Z4 van der Waals heterostructures for high-performance solar cells from first-principles calculations

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MA2Z4 two-dimensional (2D) monolayered materials (M = transition metals Mo, W; A = Si, Ge; Z = P, As, N) have gained a lot of attention in the past few years. After the first successful growth of MoSi2N4 and WSi2N4 in 2020 [1] by chemical vapour deposition, several monolayered materials from the same MA2Z4 family have been proposed and studied theoretically using density functional theory. They present several properties of interest, such as high mechanical strength [1], high piezoelectric coefficients [2], good thermal transport [2], high optoelectronic response [1,3], and magnetism [2]. In this work we propose and study, using density functional theory, 2D layered van der Waals (vdW) heterostructures formed by MA2Z4 layers as candidates for the manufacturing of solar cells. By changing the atomic composition of the MA2Z4 layers, it is expected that the band gaps vary significantly; therefore, we propose tandem solar cells formed by heterojunctions formed by these different materials. To study their stability, we performed lattice parameter optimizations, ionic position optimizations, layer distance optimizations, molecular dynamics calculations, and calculated their vibrational modes. After confirming the stability of the proposed materials, we calculated their density of states, electronic band structure, bandgap, and optoelectronic properties, such as solar energy absorption, and carrier transport properties. This class of 2D layered vdW heterostructures shows great potential to be employed as solar cells, being competitive with other high-performance materials, such as perovskites.

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Two-dimensional materials obtained by defects engineering for hydrogen storage and evolution reactions

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Carbon-based materials have been extensively researched for their unique electronic, thermal, and mechanical properties. Graphene, in particular, has been a focus of study due to its large surface area and potential applications in hydrogen storage and the Hydrogen Evolution Reaction (HER) [1,2]. Various factors such as dopants, vacancies, and defects can influence both hydrogen storage and HER. Stone-wales defects in the hexagonal graphene lattice are well-known for their ability to alter the electronic structure and local reactivity [3]. In this study we investigated the effect of incorporation of random and patterned stone-wales defects on hydrogen storage and HER capabilities. Stone-wales defects were included in a concentration of 5%, 10%, 15%, and 20% in a monolayer graphene. To carry out this work we conducted reactive molecular dynamics simulations using LAMMPS and electronic structure calculations based on DFTB+ to establish a correlation between defect patterns and hydrogen storage. Our results show that defect concentration reduces the structural stability of monolayer graphene, with an energy difference of 0.12 eV with respect to graphene. This study has potential for enhancing hydrogen storage capabilities through the manipulation of defect patterns in graphene, offering promising guidelines for future research.

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UNVEILING OPTICAL PROPERTIES OF LOW-DIMENSIONAL Sb_2O_3

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Antimony is among the most abundant metals in the Earth's crust and It exists in various forms, including the binary oxides Sb2O3, Sb2O5, and Sb2O4. Antimony trioxide, in particular, has garnered attention due to its electronic properties. As a semiconductor with a band gap of 3.3 eV, Sb2O3 finds applications as a flame retardant, and semiconductor dopant [2]. At ambient pressure, Sb2O3 exhibits two crystalline phases: senarmontite (α-Sb2O3) and valentinite (β-Sb2O3). Both phases emit photoluminescence peaks in the 390 to 500 nm range, with β-Sb2O3 showing an extended emission up to 700 nm. Despite its prevalent use in optical glasses, studies on the vibrational properties of β-Sb2O3 remain limited. This study investigates the optical and structural properties of ultrathin β-Sb2O3 nanowires obtained via mechanical exfoliation. Raman spectroscopy and Synchrotron Infrared Nanospectroscopy (SINS) reveal characteristics modes of valentinite, shedding light on its vibrational properties. SINS measurements unveil surface phonon-polaritons (SPhP) in the far-infrared spectral range, establishing β-Sb2O3 nanowires as a potential platform for optical transport studies in nanophotonic applications. Additionally, cathodoluminescence data demonstrate broad emission from 390 to 770 nm, indicating the potential of β-Sb2O3 nanowires to cover a significant portion of the solar spectrum. These findings highlight the excellent room-temperature luminescence properties of these nanowires, suggesting promising applications in advanced optoelectronic nanodevices.

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Water-Driven Selective H-transfer Photocatalysts by Ni-PHI Single-Atoms Catalysts

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Poly(heptazine imides) (PHI) are catalysts based on highly crystalline carbon nitrides, easy to obtain, with robust properties, and the ability to stabilize transition metal atoms, as a nickel. Here, PHI support was synthed in a thermal condensation of melamine assisted by NaCl, followed by an exchange method for the stabilization of Ni single atoms in the PHI structure (Ni-PHI) [1]. The properties of PHI, including its crystallinity, were confirmed by X-ray diffraction, UV-vis and infrared spectroscopy, and transmission electron microscopy. The presence of Ni single atoms was verified through EXAFS and XANES analyses. The catalysts were used to produce styrene from phenylacetylene, using water as the proton source. The results indicated that Ni-PHI converted 98% of phenylacetylene into styrene, with maximum selectivity, while the PHI support only converted 0.2%. Finally, photocatalytic tests using deuterated water confirmed that the protons originate from water.

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FM05-Materials and Devices for Innovation in the Agribusiness

Beeswax lipid nanoformulation with potential for agricultural application.

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Misusing natural resources, including pesticides and fertilizers in agriculture, has led to significant environmental and public health issues. This includes the emergence of resistant pests, ecological contamination, soil degradation, and water pollution. Such practices have escalated concerns regarding both environmental sustainability and public well-being. To address the challenges outlined above, researchers have delved into the extensive study of essential oils. However, their limited solubility, high volatility, and rapid environmental degradation has hindered their widespread application. Nanoencapsulation presents a promising avenue for enhancing their stability and efficacy. This project aimed to create scalable and multifunctional nanoformulations from natural raw materials, such as beeswax and the bioactive compound of clove essential oil (CEO), for agricultural pest management. The study examined the physicochemical properties, stability, encapsulation efficiency, and in vitro biological activity using white mold (Sclerotinia Sclerotiorum) as a model organism. The nanoparticles loaded with clove essential oil (CEO) exhibited a mean diameter of 209 ± 7 nm, a polydispersity index above 0.2, a negative zeta potential (-38 mV ± 0,7 mV), and a high encapsulation efficiency of ≥ 94%. In biological assays, complete inhibition of S. Sclerotiorum was observed after treatment with 1,5 mg of encapsulated CEO. This project holds significant promise for agricultural pest control, facilitating a cycle of bioeconomy and sustainability for farmers.

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Combination of the multifeatured extracts of passion fruit by-product in TPP-chitosomes encapsulation

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This study addresses the sustainable use of passion fruit by-products by investigating ultrasound-assisted extraction of phytochemicals from its peels and seeds separately. The extractions of active compounds were carried out using tip sonication with the amplitude set at 70% and a fixed concentration of 7% dried by-product (DB). Water, ethanol 40%, and ethanol were used as solvents, using different durations of 5, 10, 15, and 20 minutes. The extracts were chosen based on the total phenolic compounds (TPC) and the FRAP (ferric reducing antioxidant power) assay. The increase in extraction time did not significantly improve the results, whilst the solvents influenced the extraction of the active compounds. This is associated with their solubility properties. The 5-minute extraction in 40% ethanol was chosen for the peels' extraction (TPC: 4.67 mg/g DB and FRAP: 87 $FeSO_4$ mM/g DB), as well as the 5-minute extraction in ethanol for the seeds (TPC: 6.13 mg/g DB and FRAP 57 $FeSO_4$ mM/g DB). Both extracts were combined to produce active liposomes coated with chitosan by ionic gelation using sodium tripolyphosphate as a crosslinker (TPP-chitosomes). The combination of aqueous and ethanolic mediums enriches the extracts with lipophilic and hydrophilic compounds, which are co-encapsulated in the particles. During the extraction, a pectin-enriched fraction is obtained from the peel by-products. Alongside, the other extraction residues will be directed to the production of cellulose nanofibers. Beyond using agricultural by-products, this study contributes to the effectiveness of nanoencapsulation for a greater quantity and quality of phytochemicals, thereby promoting sustainable materials development and resource utilization.

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Impedimetric e-tongue for soil analysis

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An impedimetric electronic tongue is a multisensor device using impedance measurements that mimics the human taste sense. It has been applied in food, beverages, pharmaceuticals, environmental analysis, and biosensing, and here we show its use in soil analysis due to the increasing global demand for sensors helping to monitor parameters impacting food production without expanding cropped area. We tested 3D-printed electrodes as a cost-effective alternative for rapid prototyping of the device, which successfully discriminates a soil supplemented with (N, P, K, S, Mg, and Ca), and sandy and clayey soils enriched with different (N, P, K) concentrations. A simple rinsing with distilled water brings the device back to its initial conditions, without cross-contamination signs in independent sets of measurements, and machine learning methods are explored to check the best frequencies discriminating samples. We also compared an e-tongue setup composed of ion-selective membranes as sensing units, with another having sensing units made by non-specific layer-by-layer films. Multiprojection techniques point out that the ion-selective membrane setup presents a higher sensitivity to K content; nevertheless, it degrades in six months of use, while the LbL array, although less selective, operates for over a year without shifts or deviations in the analyses. Our results encourage further investigations on microfluidic, impedimetric e-tongues as valuable tools in precision agriculture developments. Future advances include the fabrication of molecular sieves formed by metallic nitrides, with controlled film thickness, and porosity for a possible selective detection of macronutrients. We look for simplified approaches avoiding pre-treatments for sampling, and looking for machine learning methods supporting faster decision-making in agricultural practices.

Nanoformulations pectin/casein based containing essential oils for use to pests control in agriculture

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Plant Parasitic Nematodes significantly threaten crop production, including economically vital commodities like soybean, corn, and rice, resulting in annual losses of around US$157 billion[1]. Traditional control methods rely heavily on chemical pesticides, but their efficacy is diminishing, and many are being banned due to their adverse environmental impact on non-target organisms [2]. Therefore, there is an urgent need to explore sustainable alternatives to support Integrated Nematode Management. Essential oils are studied for agricultural pest control, but their widespread application could be improved by low solubility, high volatility, and rapid environmental degradation. Nanoencapsulation offers a promising solution to enhance stability and effectiveness. The aim of this study was the preparation and characterization of pectin/casein nanoparticles containing a mixture of Thymus vulgaris, Origanum manjerona and, Cymbopogon flexuosus, Origanum vulgare essential oils. The nanoparticles produced showed from 415 to 650 nm, with a polydispersity index of 0.3 to 0.5, a zeta potential of -29 to -20 mV and high encapsulation efficiency ≥ 80%. Moreover, pre-emergence assays on soybean seeds have demonstrated that encapsulated and non-encapsulated essential oils exhibit non-phytotoxicity at the tested concentration, achieving a germination rate of ≥90%. Our findings suggest that these formulations could serve as promising candidates for nematode control in sustainable agriculture.

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Nanofunctionalization for combating agrochemicals: a perfect match!

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How safe are we from agrochemicals? They are extensively used worldwide but can be highly toxic. Their improper abusive use together with the problematic of threatening stockpiles (unused or prohibited) are of great concern, which require efficient neutralization and monitoring methods. Catalysts-by-design through nanofunctionalization is a promising approach for neutralizing toxic organophosphates (e.g. agrochemicals and chemical warfare). But the quest of site selective functionalization of carbon nanomaterials depends on casting what is good. Although higher coverage is usually pursued, the strategy should also be application-driven. Our group [1-4] has been engaged in correlating catalytic activity with the functionalization route of graphene oxide and carbon nanotubes by varying: (i) site targeted: carboxylic acid (borders) or epoxide (basal plane); (ii) precursors´ degree of oxidation; (iii) group anchored: thiol, imidazole, hydroxamate, amines; (iv) coverage: degree of functionalization and mono/bifunctionalization. The materials were characterized by TGA, FTIR, XPS, CHNS and NMR; and evaluated as nanocatalysts (recyclable) in the neutralization of toxic agrochemicals. The materials with the highest degree of functionalization were not the best catalysts, which was attributed to cooperative effects evidencing the potential of naonstructured backbones. By anchoring thiol groups and nanoparticles, the catalysts promoted the total neutralization in two consecutive one-pot reactions: organophosphate degradation followed by nitrophenol reduction. The nanocatalysts also showed a dual function: could be used as sensors (surface enhanced Raman spectroscopy, electrochemical) for detecting these toxic agents. In summary, nanofunctionalization can greatly boost applications when addressing agrochemicals´ problematics.

Processing of Biomass from Agricultural Waste for Production of Graphene Nanoplatelets for Soil Fertilization

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Agriculture plays a vital role in the Brazilian economy, reflecting impressive numbers of agricultural production in the country. The growing demand for agricultural products has led to significant expansion of agribusiness, which in turn results in significant agricultural waste production [1]. Furthermore, this growth leads to environmental degradation, including unsustainable practices of plant extraction. Agricultural expansion into reserve and preservation areas results in soil fertility loss, reduction of organic matter and emission of greenhouse gases such as CO2, contributing to global warming [2]. Given this scenario, the search for alternatives in waste management and soil nutrients recovering has become imperative. Therefore, this work consists on the utilization of an innovative methodology [3] to produce graphene nanoplatelets from agricultural residues aiming its use as a soil conditioning, simultaneously improving fertility and cation exchange capacity promoting agricultural sustainability. Two types of biomass will be studied, which are banana peel and sugarcane bagasse. These biomass will undergo a sequence of treatments such as UV irradiation, hydrothermal carbonization, vacuum degassing, pyrolysis, and exfoliation by sonication. It is expected that the produced graphene nanoplatelets will exhibit favorable physical, chemical, and biological properties for the soil, such as increased water retention capacity, improved soil structure, and increased nutrient availability. This innovative approach seeks not only to mitigate the environmental challenges associated with agricultural waste but also to promote agricultural sustainability and contribute to the development of sustainable and efficient agricultural systems.

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Soil conditioner based on multimaterial nanocomposite: Thermoplastic starch/Nanoclay/Nanolignin

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The increasing demand for food and the need to enhance soil efficiency have driven the search for innovative soil conditioners. This project proposes the development of a soil conditioner based on a multimaterial nanocomposite composed of Thermoplastic Starch (TPS), Nanoclay (NC), and Nanolignin (NL). TPS, NC, and NL play distinct yet complementary roles in the proposed soil conditioner. TPS provides stability to the conditioner and aids in water retention, which is crucial for plant growth. NC improves soil porosity, facilitates air and water circulation, and participates in cation exchange, promoting plant nutrient availability. NL acts as a binding agent, maintaining the structure of the conditioner, and can also serve as a nutrient source for the soil. Additionally, NL possesses antioxidant, antimicrobial, and UV-blocking properties, offering additional plant protection. The production process involves combining the materials, processing, and analyzing the characteristics of the resulting composite. Together, these materials aim to enhance the physicochemical properties of the soil, promoting a more fertile and sustainable environment for plant cultivation. While this project is ongoing, such an approach contributes to more efficient and sustainable agricultural practices essential for addressing global food challenges.

Keywords: Soil conditioner; Nanoclay; Nanolignin; Thermoplastic Starch (TPS); Sustainable agriculture.

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3D Printing and Nanotechnology: A Promising Alliance for Pest Control in Agriculture

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This study aims to explore 3D printing using sodium alginate (SA) as a base for a controlled release system of methyl salicylate (S_Met), encapsulated into zein nanoparticles (NP-Zein) for pest control in agriculture. Prototypes based on sodium alginate (SA) incorporating loaded NP-Zein were created using 3D printing to enhance the stability and efficiency of the controlled release system. The interaction between the prototypes and NP-Zein was characterized using scanning electron microscopy, atomic force microscopy, and fluorescein isothiocyanate labeling. The results highlight a high encapsulation efficiency of S_Met and good adherence of the NPs to the surface of the prototypes, suggesting a promising synergy between the materials used. The release of both encapsulated and non-encapsulated S_Met was evaluated for comparative analysis. Both systems exhibited sustained release over time, the prototypes containing non-encapsulated S_Met showing a faster release (around 255 ± 143 ng/day) compared to the prototypes with S_Met encapsulated in NP- Zein (around 94 ± 38 ng/day), indicating modulation in release by the NPs. Mathematical models revealed anomalous behavior in S_Met release, attributed to diffusion, polymer wall relaxation, or erosion. Furthermore, the efficacy of NP-Zein in improving the stability and sustained release of S_Met in agricultural pest control applications was emphad. In conclusion, this study demonstrates the potential of combining 3D printing and nanotechnology for designing controlled release systems applied in agriculture. The results opened new perspectives for developing sustainable strategies in agricultural pest management.

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Addition thermoplastic starch in matrix of the PHBV for production biodegradable blend

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This work aimed to produce poly(hydroxybutyrate-co-hydroxyvalerate) (PHBV)/thermoplastic starch (TPS) blends and evaluate its morphology, chemical, and physical properties for application in agricultural mulch film. The pure films (PHBV and TPS) and PHBV/TPS blends (80P20T, 70P30T, and 60P40T) were prepared by melt mixing.[1,2]The SEM micrographs revealed that the blends were immiscible. As the TPS concentration increased, the dispersed phase structure (droplet form) was converted to a co-continuous type structure, indicating the lack of adhesion between the two phases. Moreover, during the first 2 h of immersion in water, there was observed an increase in water absorption percentual of all blends compared to the PHBV film. However, after two weeks, all blends showed an opposite behavior. The partial solubilization of TPS present in the blends might has resulted in a high percentual of soluble material in comparison to pure PHBV (0% for PHBV and 20% for 60P40T). This solubilization in water was confirmed by optical microscopy and FTIR analysis, where after two weeks the blend showed holes on its surface and a decrease in the carbonyl index corresponding to the crystalline region of PHBV was observed. In the tensile strength test, it was observed that Young's modulus decreased with the increased amount of TPS, while elongation at break showed a slight increase. Therefore, the set of results obtained so far indicates that the properties of the materials might be adjusted according to the blend composition, where blends with higher TPS content are more flexible and susceptible to greater swelling in water.

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Adsorption of amoxicillin by chitosan beads

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Amoxicillin, a widely used antibiotic, is often found in water bodies due to incomplete metabolism and improper disposal. This poses risks such as antibiotic resistance and toxicity to aquatic life. Traditional water treatment methods struggle to remove it effectively. This study delves into the application of chitosan beads for amoxicillin adsorption, revealing pH 4 as the optimal condition. The kinetics study indicates that internal diffusion governs adsorption for chitosan, while thermodynamic parameters suggest adsorption is spontaneous and endothermic. This suggests that these beads could be a promising solution for removing amoxicillin from water.

Adsorption of imazaquin by a melamine-based covalent triazine framework

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Imazaquin is a moderately persistent herbicide sold in Brazil and used mainly in soybean plantations. Its direct application to the soil leads to possible leaching into aquatic environment, contaminating the local ecosystem.[1] The present work aimed to apply a nanoporous material for adsorption of imazaquin from aqueous solutions. A melamine-based covalent triazine framework (**SWN-1**), a nanoporous organic network, was synthed from the reaction of melamine with terephthaldehyde in DMSO under reflux with surface area of 160 m^2/g.[2] The adsorption experiments were carried out adding **SWN-1** to aqueous imazaquin solutions, with a concentration of 6 ppm, in the concentration of 1 mg/mL in different pH and in the dark. The evolution of imazaquin concentration over time was measured by UV/VIS spectrophotometry. The adsorption equilibrium was achieved after 21 min, removing 93% of the herbicide from the solution. It was found that the adsorption capacity (qe) of the herbicide was inversely proportional to the increase in pH: 5.31, 4.48, 2.56, and 1.62 mg/g in pH 1.5, 3.0, 7.0, and 12, respectively. The analysis of the concentration in the solution as a function of time indicated that at this pH = 1.5 the adsorption showed pseudo-second order kinetics with rate constant of 3.2×10^{-2} mg/g min. The fit to the Weber-Morris model indicated that intra-particle diffusion is not limiting for the adsorption rate. Studies are being carried out to verify the sites of interaction between the porous material and the pesticide. These preliminary results already show that the melamine-based nanoporous network has potential applicability for removing imazaquin from aquatic environment.

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Analysis of main components of artisanal cachaças produced in Brazil using optical spectroscopy

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In this work, we characterize artisanal cachaça through optical spectroscopy. The samples consist of cachaças registered in MAPA (Ministry of Agriculture and Livestock), Brazil. Namely, some cachaças are blended with Umburana, honey, oak, and balsam, and others possess different classifications like gold, silver, nox, traditional, and premium. The analysis techniques include absorption UV-vis, Near IR, Mid IR, and Raman spectroscopy. In the ultraviolet and visible spectrum, some electronic transitions were obtained ($\sigma \rightarrow \sigma^*$, $n \rightarrow \sigma^*$, $n \rightarrow \pi^*$, $\pi \rightarrow \pi^*$). In the mid-infrared part of the spectrum, various bands are observed in the 400 – 4000 cm-1 range. Raman spectroscopy is used to check the amount of harmful toxic alcohols and to have an insight into the structure of the examined samples. The data were submitted to a non-supervisioned method, Principal Component Analysis (PCA) to evaluate samples from the perspective of artisanal point of view. The regions of Brazil taken into account correspond to Alagoas, and Minas Gerais states. This study focuses on the potentiality of optical analytical methods as a tool for drink security.

A study by SAXS of silver nanoparticles produced by biogenic synthesis

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Nanotechnology applied to the agriculture has highlighted in recent decades, making important contributions, for example, the use of nanoparticles produced by biogenic processes to control phytopathogens. This demonstrates the need of better understand the composition, mechanisms of action and toxicity of these nanoparticles. Their capping by biomolecules, derived from the organism used in the synthesis, contributes to their stability and biological activity. In particular, previous studies demonstrated the potential of Ag nanoparticles to combat the white mold [1], a disease that affects important agricultural species. In this study, Ag nanoparticles were produced by the fungus *Trichoderma harzianum* in aqueous solutions containing silver nitrate as a precursor for the silver nanoparticles. Some of the samples were exposed to the phytopathogenic fungus *Sclerotinia sclerotiorum* responsible for the white mold. After preparation, a fraction of the samples was submitted to physico-chemical processes to remove organic cap layer on nanoparticles surface formed during the preparation process. We used the small angle X-ray scattering (SAXS) technique to determine the effects of the phytopathogenic fungus and cap removal process in the average radius, radius dispersion, and number density of the nanoparticles. The SAXS data analyses suggest that the presence of the pathogenic fungus results in a decrease in number and total volume of Ag NPs without significant changes on average radius and radius dispersion. Our results also indicate that the physical-chemical process applied to remove the organic cap surrounding the Ag NPs leads to a decrease in the fraction of the smaller nanoparticles.

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Chayote shell as an adsorbent for Cu^{2+}

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The contamination of water by various metals is something that has impacted humanity for a long time. Copper is a metal widely used in electrical circuits and in some household utensils. It is an extremely important element for our body but the excess can interfere and cause damage to the dopamine and serotonin neurotransmitters. One of the ways to reduce the amount of impurities in water is by using adsorption. The most used material is activated carbon, but several studies looking for new adsorbents have been reported, including some using food waste, such as passion fruit peel, sugarcane bagasse, pomelo peel and papaya seeds. This work aims to verify the feasibility of using conductimetry for quantitative analysis of copper, as well as verify the viability of chayote shell as an adsorbent agent. In the study of the possibility in quantifying Cu^{2+} using conductimetry, four solutions with Cu^{2+} concentrations ranging between 0.0107 and 0.107 $molL^{-1}$ were prepared and analyzed by conductometry. After linear regression, the curve equation Y= 143X +0.43 was obtained, with a determination coefficient R^2= 0.999. Also the maximum amount of chayote shelll that could be added to a certain mass of water was verified and this value was equal 0.053g shell/20.0g water.

A factorial design 2^2 was carried out using temperature and time as factors. In test number 4, with conditions of 60ºC and 60 min, there was a change in color and viscosity of the mixture, which made it impossible to measure its conductivity. For the other experiments, to determine the concentration of Cu^{2+} that existed after carrying out the process, the found concentrations are gretaer than the initial concentrations of Cu^{2+}, not allowing the calculation of the amount of Cu^{2+} extracted by chayote shell. With this work, it can be concluded that in aqueous solutions, conductimetry is an effective technique for quantifying Cu2+ and the maximun quantity of chayote shell that not increases the turbidy.

Conductivity Analysis and Morphological Assessment of CNF and Monoammonium Phosphate Fertilizer Encapsulation

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Enhanced efficiency fertilizers (EEFs) Enhanced are evolutions in the scientific field, developed to meet the demand for agricultural productivity through food production in an intensified and environmentally friendly way. EEFs requires preparing fertilizer microparticles coated with a biopolymer that allows the material to release nutrients in a prolonged manner. This work produced microspheres from solutions of monoammonium phosphate fertilizer (MAP, NH4H2PO4), a salt widely used in the agricultural sector, being a source of nitrogen (N) and phosphorus (P) macronutrients [1]. Cellulose nanofibrils (CNFs, donated by Suzano Papel and Celulose S.A., Brazil) are used as a biopolymer. The spray drying technique was used to coat the MAP with CNFs and has been applied to agricultural proposals during the encapsulation of fertilizers [2]. The solution was prepared by homogenizing 1 wt% CNFs with MAP in a total volume of 200 mL. Finally, the solutions were dried using a Mini Spray-Dryer BUCHI B-290, employing a 2-fluid atomizing nozzle. Two diameter configurations for the spray nozzle were evaluated: (i) spray nozzle with ø 0.5mm, equipped with nozzle tip 0.5 mm, nozzle cap 1.4 mm and needle 0.5 mm and (ii) spray nozzle with ø 1.4 mm equipped with nozzle tip 1.4 mm, needle 1.4 mm, and nozzle cap 2.2 mm. The equipment was set at an inlet temperature of 140ºC, 100% aspiration rate and 20% pump for all samples. The particle of microspheres influenced the morphology and the solubility of the encapsulated salt.

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CONTROLLED-RELEASE VITREOUS FERTILIZERS FOR PRECISION AGRICULTURE

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Soil nutrients are essential in the efficient production of safe crops and foods to meet the needs of a growing population. Commercial fertilizers present problems, such as the need for successive doses due to their high solubility[1]. Therefore, it is necessary to develop alternative, biocompatible materials that contain the elements necessary for plant growth and have controlled release capacity[2]. Vitreous fertilizers (VF) have in their composition essential elements for plant development, such as phosphorus (P2O5) and silicon (SiO2), which act as network formers, as well as modifiers, such as Ca2+ and K+, responsible for the degree of connectivity network, reflecting chemical stability and dissolution processes. In this work, the glass composition P2O5-SiO2-CaO-K2O was investigated, varying the molar proportions of P2O5 and SiO2. The VF was synthed via melt-quenching and characterized by Raman, DSC, XRF, SEM, and EDX. Structural characterizations revealed that variations in phosphorus and silica impact depolymerizing the glass network. The VFs were evaluated about their dissolution in an aqueous medium and citric acid/sodium citrate buffer solution (pH 4.7), accompanied by losses in mass, pH, and morphology after the test. The materials presented different mass loss profiles, with greater losses in the acid solution. In water, those with greater amounts of P2O5 acidified the medium. Morphological analyses demonstrated that the longer the contact time with the solutions, the greater the surface wear of the material. Thus, this work shows materials with distinct properties that have the potential to be applied in controlled release systems.

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Development and characterization of biodegradable films based on thermoplastic starch and coffee grounds

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Biodegradable materials from renewable sources can be alternatives for minimizing the impacts of plastic pollution and the incorrect disposal of solid waste. The aim of this study was to develop biodegradable films made from thermoplastic starch and coffee grounds. Thermoplastic starch films were prepared using 18g of corn starch, 5.4g of glycerol, and 600mL of deionized water. From this solution, composites were developed with coffee grounds (Coffea arabica), previously dried at 50oC for 12 hours. 48 mesh granules were used in formulations with 15% and 30% coffee grounds in relation to corn starch mass. The film-forming solutions were heated to 60oC and kept under constant stirring for 30 minutes. Then, by the solution-casting
method, the films were formed in an oven with forced air circulation at 60oC for 6 hours. To characterize the materials, digital photographs, photomicrographs, morphological (SEM), thermal (TGA), chemical (FTIR) and soil biodegradation analyses were conducted. The results demonstrated that visually the films presented similar aspects, such as a good distribution of coffee granules and the formation of a starch layer covering them. Morphologically, microcracks were observed in the composite containing 30%. The last stage of thermal degradation occurred at around 300oC [1] and the chemical structure between the films and their raw materials showed no difference [2]. Finally, all films degraded within 30 days. Therefore, it was possible to develop biodegradable composites of starch and coffee grounds, and the film with the lowest filling (formulation with 15%) showing
better results.

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Development and Characterization of Layered Double Hydroxide (LDH) Nanocarriers for Pest Control in Agriculture

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In recent years, pests have slashed agricultural yields by 20% to 40%, propelling farmers towards synthetic chemicals. Yet, the haphazard use of these substances endangers human health, contaminates water and soil, and adversely affects non-target organisms. Enter RNA interference (RNAi) technology—an alternative to sustainable pest and disease control in agriculture. RNAi's allure lies in its precise gene-silencing capability, high specificity, and flexible action mechanisms. Nonetheless, the crux of implementing RNAi in agriculture pivots on developing formulations that stabilize RNA molecules, boost their effectiveness and ensure delivery to target pests' cells. Our initiative focuses on creating double-stranded RNA (dsRNA) nano-carriers using Layered Double Hydroxide (LDH) nanoparticles. LDHs stand out for their exceptional anion exchange capacity, robust stability, minimal cytotoxicity, and superior biocompatibility—ideal traits for gene delivery. By diversifying the metallic ions in LDH synthesis, we aim to engineer platforms with varied physicochemical attributes1. Initial experiments have produced LDHs with nanoparticles ranging from 184 to 518 nm, affirming their nanoscale designation. The uniformity of particle distribution is reflected in Polydispersity Index (PDI) values between 0.19 and 0.39, while positive Zeta potentials (33.4 to 49.4) suggest the potential for electrostatic interactions with dsRNA. This project is poised to revolutionize RNAi application in agriculture by optimizing nano-carrier physicochemical properties, ensuring stability beyond 8 months, and laying the groundwork for efficient, low-toxicity delivery systems. The anticipated success heralds a significant leap in sustainable pest management, aligning with our commitment to agricultural innovation and environmental stewardship.

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Development and characterization of lignin nanoparticles containing plant growth regulators aiming agricultural applications

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Agriculture faces a great challenge, increase food production to feed the global population. In addition, agricultural systems must leave unsustainable practices such as using large amounts of pesticides and fertilizers that result in side effects on the environment [1]. Nanocarrier systems for seed treatment can be an alternative to improve germination, plant establishment, protect against abiotic and biotic stress. The objective of this project was developed nanocarrier systems based on lignin-containing carvacrol essential oil (CVC) and plant growth regulators (PGRs), gibberellic acid (GA3), indoleacetic acid (IA), and kinetin (KN). According to the results, lignin nanoparticles containing GA3, IA and Kn (nanoLn-PGrs) presented s of 176 nm, PDI of 0.2 and zeta potential of -53, and encapsulation efficiency around 90% for all PGRs and 99% for CVC. The same parameters were evaluated over time, showing stability over 3 months. Besides that, the systems have a sustained release of the plant growth regulators over time (24 h). The results showed that systems have good stability and promoted a release profile of PGRs and CVC. In conclusion, lignin nanoparticles have great potential applications in agriculture aiming at sustainable management.

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Development of niobium and mesoporous silica nanocomposites stabilized by PVP (polyvinylpyrrolidone) for potential use in agriculture.

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A synthesis of niobium nanoparticles coated with mesoporous silica with the aid of stabilizing agents is an emerging strategy with great potential for the development of materials with applications in agriculture, such as fertilizers and other agrochemicals. Therefore, this study aimed to investigate the controlled synthesis of niobium nanoparticles coated with mesoporous silica, employing PVP (polyvinylpyrrolidone) as a bivalent molecule. PVP exhibits amphiphilic properties, providing colloidal stability during synthesis and positively influencing reaction kinetics, resulting in more uniform particles. Additionally, the affinity of PVP with silica facilitates the formation of a homogeneous coating. The characterization of the synthed material was conducted through Fourier-transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), and scanning electron microscopy combined with energy-dispersive spectroscopy (SEM-EDS). The analyses indicated interactions between the compounds and the predominance of an amorphous phase, suggesting encapsulation of the metallic oxide by mesoporous silica. The images obtained by SEM-EDS highlight the presence of a uniform silica coating on the niobium nanoparticles, in addition to their monodispersity, confirming the efficacy of PVP as a stabilizing agent. These combined techniques offer a comprehensive understanding of the structural and chemical characteristics of the obtained nanocomposite, providing a basis for its potential applications in agriculture.

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Electrical transport in copper oxides with metallic nanostructures and their behavior as gas sensors

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The agricultural industry faces a significant challenge: the accelerated ripening of products due to the natural emission of ethanol. Early detection of this gas is crucial to reduce costs associated with crop losses. This research focuses on studying and enhancing the sensitivity of gas sensors for application in the agricultural sector.

With this aim, the intention is to improve upon the results obtained in previous researches [1,2] that utilized copper oxide (CuO) ultra-thin films, through the incorporation of cobalt oxide nanostructures (Co3O4)[3,4]. To fabricate these nanostructures, cobalt ultra-thin films were deposited with a thickness ranging between 0.5 and 2 nanometers on a 20 nanometers thick CuO film on an insulating substrate.

The research was divided into two phases: the first phase aimed at characterizing cobalt oxide thin films under controlled conditions using techniques such as Raman spectroscopy, UV-Vis spectroscopy, and subjecting the samples to magnetic fields, in order to detect Co3O4. Meanwhile, the second phase analyzed the electrical properties of CuO thin films with Co3O4 nanostructures, by measuring changes in electrical resistance as a function of temperature and under different gas pressures.

The results demonstrate a significant improvement in ethanol detection at increased concentration levels in the environment, in contrast to sensors fabricated solely with CuO. This improvement suggests the possibility of creating a hybrid system that combines both types of sensors, with the purpose of broadening the spectrum of gas detection.

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Electrolyte-Gated Transistor Applied As A Bovine Milk Fat Sensor

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Sensors are devices designed to detect, measure, or respond to different types of stimuli or environmental variables, such as light, temperature, pressure, humidity, or even the presence of certain chemicals. They convert this information into electrical signals, e.g, that can be measured and interpreted helping to take decisions, issuing alerts, or monitoring specific conditions. An interesting area of exploration is the development of sensors applied to the food analysis. In this work, it was developed a sensor to detect the percentage of fat in bovine milk based on an electrolyte-gated transistor (EGT) platform. The EGT structure is: gold source, drain and gate in-plane electrodes, poly(3-hexylthiophene-2,5diyl) (P3HT) channel. The electrolyte layer is composed by a gelatin foil hydrated with bovine milk. Gelatin foil has acts only as an anchoring matrix. Two commercial and pasteurized bovine milk were tested: whole milk, with the manufacturer's indication of 3% fat and; skimmed milk with 0% fat. Under these conditions, the EGTs showed good results in distinguishing between whole and skimmed milk. For the gate voltage range up to -1V, the EGT with whole milk operates as an electrochemical transistor, while the EGT with skimmed milk operates by field effect only. Based on the field-effect transistor extracted parameters [1], the analysis was performed on cyclic transfer curves and the measured threshold voltage shift from the EGT with whole milk is lower than from the EGT with skimmed one. This sensor depicts promising results to be applied as a portable and low-cost device, aiming to benefit small dairy producers to make measurement of the fat percentage in milk, and add due value to the product.

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Enhancing Micronutrient Solubilization through Acidifying Microorganisms: Exploring Their Potential in Fertilizer Granule Coating.

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Fertilization is essential to provide suitable conditions for plant development and crop productivity, but the environmental cost of fertilizers is a drawback for achieving sustainable agriculture. A potential alternative is the use of unprocessed (raw) nutrient sources such as mineral oxides (ZnO, MnO, CuO) as fertilizers. However, these low-reactivity sources are not readily available to plants. In light of this, this project aimed to develop a bioactive coating material containing microorganisms that enabled the release of different nutrients from unprocessed nutrient sources. To achieve this, the coating material composed of maize starch, mineral oxides (ZnO, MnO, CuO), and a microbial source (Aspergillus niger or Aciditiobacillus thiooxidans) was applied to monoammonium phosphate (MAP) granules, serving as a model fertilizer. Our results revealed that the bioactive coating did not affect phosphorus (P) release, as it did not create a physical barrier. However, the acidifying capacity of both microorganisms significantly enhanced oxide solubilization. The presence of Aspergillus niger or Aciditiobacillus thiooxidans promoted local acidification, and the bioactive coating material with Aspergillus niger achieved solubilization of Cu, Zn, and Mn up to 10.9%, 14.6%, and 34.3%, respectively, within 42 days of soil incubation. This phenomenon suggests that the organic acids produced by Aspergillus niger chelate cations, reducing soil immobilization and thereby increasing their solubilization. This innovative system can effectively supply nutrients to plants using inexpensive and low-reactivity nutrient sources, with the advantage that it can be applied simultaneously to currently used fertilizer granules in a single delivery, facilitating adoption by producers.

Enhancing Rhizobium performance in common bean plants through Fe_3O_4 nanoparticles

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This study investigates the effects of Fe_3O_4 nanoparticles (NPs) on nodulation, nitrogen fixation, and growth of common bean plants. Plants were exposed to Fe_3O_4 NPs, Rhizobium inoculation, and Fe_3O_4 NPs + Rhizobium inoculation. Results showed that treated plants exhibited improved symbiotic performance, with increased nitrogenase activity, nodule leghaemoglobin, and iron content. Additionally, the number of active nodules per plant and nodule dry weight significantly increased. Symbiotic nitrogen fixation was enhanced, leading to higher shoot and root total nitrogen content. Treatment combining Fe_3O_4 NPs and Rhizobium inoculation yielded the best results. Fe_3O_4 NPs were taken up by plants, accumulating in organs including nodules. Moreover, treated plants displayed increased root and shoot lengths, leaf area, and dry weights. Magnetization curves indicated the accumulation of Fe_3O_4 NPs in nodules, enhancing symbiotic performance. The study suggests a novel strategy for improving common bean growth through Fe_3O_4 NPs and Rhizobium inoculation, offering potential benefits for sustainable agriculture, and reducing nitrogen fertilizer use. These findings contribute to a non-genetic approach in legume research, emphasizing long-term improvements in common bean growth and symbiosis [1-2].

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Evaluation of lignin nanoparticles containing plant growth regulators on Zea mays

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The increase in global population demands intensified food production, becoming a key challenge for agriculture [1]. In this context, nanocarrier systems for seed treatment have the potential to improve crops production as well as plants resistant against biotic and biotic stress. The objective of this project was to evaluate the effects of seed treatment using lignin nanoparticles containing the plant growth regulators (PGRs), gibberellic acid (GA3), indoleacetic acid (IA) and kinetin (KN) in corn seeds (Zea mays). For evaluation, seeds were treated with lignin nanoparticles containing PGRs, PGRs solution and water (as control). The seeds were treated according to recommendation of commercial formulation (0.75 µg of PGRs for 1 gram of seeds). The Zea mays plants were evaluated in relation to morphology, the results showed that lignin nanoparticles at 0.37 and 0.18 µg of PGRs per gram of seeds, increased root length and dry mass compared to the control. This effect can represent seed priming effects on Zea mays. These results showed the potential of lignin nanoparticles as nanocarrier systems for PGRs, aiming to enhance seedling development for agriculture application. Modification in the seed priming methodology (as concentration and time of exposition) or alternative treatments as “on farming” or foliar application must be evaluated to check the potential of these nanoformulations.

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Evaluation of the addition of epoxidized soybean oil and citronella oil on the properties of cellulose acetate films

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Cellulose acetate is a polymer obtained from cellulose, undergoing the acetylation process, and is widely used to create polymeric films due to its biocompatibility, non-toxicity, transparency and low cost [1]. For the production of polymeric films, plasticizing agents are commonly added in their manufacturing process, in order to facilitate their processability and also increase their ductility [2]. In this work, different proportions of epoxidized soybean oil (ESO) and citronella oil (CO) were incorporated into the cellulose acetate films to evaluate their potential as plasticizing agents. Characterization studies were subsequently conducted to investigate the interaction between these oils and the polymeric matrix, as well as to examine the resulting film properties. Fourier Transform Infrared Spectroscopy (FTIR) analyses were conducted and similar FTIR spectra were obtained for all the films due to the relatively small amount of the oils compared to the cellulose acetate. Differential Scanning Calorimetry (DSC) analyses confirmed the reduction of glass transition temperature (Tg) with the incorporation of both ESO and CO, in all proportions tested. Notably, lower Tg values were observed with an increase in the proportion of CO relative to ESO, indicating a more pronounced plasticizing effect of citronella oil [3]. The mechanical properties of the films were determined through a tensile test, revealing a substantial improvement in tensile strength, elongation at break, and toughness parameters with the addition of oils across all concentrations. The incorporation of plasticizers into polymeric films typically enhances flexibility, elongation percentage, and toughness. The obtained results, evidenced the efficacy of citronella and epoxidized soybean oils as potent plasticizing agents for cellulose acetate, promising advancements in the development of flexible polymeric films with sustainable applications.

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Evaluation of the repellency efficacy of cellulose acetate mulching films containing citronella oil

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The use of mulching films in agriculture has been a widely used practice, as it has several benefits for crops, such as humidity control, barrier to sunlight and soil erosion control [1]. In addition to these advantages, it is possible to incorporate agents such as essential oils into mulching films, which may give these films properties such as insect repellency [2,3]. This approach eliminates the need for synthetic insecticides that can lead to soil, plant, and groundwater contamination. Based on this, the current study aims to evaluate the potential insect repellency achieved by incorporating varying proportions of citronella essential oil (CO) and epoxidized soybean oil (ESO) into the polymeric matrix of cellulose acetate for mulching film production. Repellent studies on Bemisia tabaci were conducted through mortality and also oviposition of the prepared films, to evaluate its potential as an insecticidal agent.The results were promising, demonstrating a direct correlation between CO concentration and population elimination, with 100% mortality within just 24 hours at the highest concentration of CO. Oviposition tests also yielded excellent results, preventing flies from laying eggs on the substrate at higher CO concentrations and film incorporation levels, consequently indicating substantial repellency.

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Exploring the mobility of poly-ε-caprolactone magnetic nanocapsules in soil columns

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Nanotechnology demonstrates a wide range of applications in various fields, including agriculture. Farmers face a significant challenge in producing enough food of adequate quality to meet the needs of the growing world population while also needing to preserve soil health. This challenge is exacerbated by degradation and contamination resulting from the increased use of agricultural inputs. The use of agrochemicals is, however, limited by their low efficiency due to loss (through volatilization and leaching) contaminating the environment. In this way, the development of nanocarriers for encapsulating active ingredients appears as a potential system for application in agriculture, providing a controlled release of agricultural inputs into the environment[1]. In this study, positively and negatively charged hybrid poly-ε-caprolactone nanocapsules (NCs) containing hydrophobic magnetic nanoparticles were synthed by the emulsion/solvent evaporation method as a potential pesticide delivery system. Leaching studies of both nanocarriers in soil columns were carried out to investigate the mobility of the nanocarriers using magnetic approaches and atomic absorption spectroscopy. Both NCs exhibited average particle distribution of 592 nm, PDI < 0.25 and excellent magnetic collectability. Moreover, negatively charged hybrid NCs exhibited greater mobility in the soil compared to positively charged NCs. Therefore, this study represents an advancement in understanding the mobility of various agrochemical nanocarriers in the environment, thus contributing to more sustainable agricultural practices.

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Extruded active films enriched with chitosan nanoparticles loaded with essential oil for food

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Improper disposal of packaging, especially those made from fossil-origin materials, poses a significant environmental concern due to the resistance of these materials to degradation. In this context, biodegradable packaging emerges as a promising alternative, as it decomposes more rapidly [1]. In this study, we explore an innovative approach in the production of biopolymeric blends, incorporating chitosan nanoparticles encapsulated with clove essential oil into the polymeric matrix for potential applications in food. To achieve this, the study was divided into two stages. In the first stage, the preparation of chitosan nanoparticles with essential oil was carried out using the oil-in-water emulsion and ionic gelation method. These nanoparticles were characterized using different techniques such as Fourier-transform infrared spectroscopy (FTIR), thermogravimetry (TGA), scanning electron microscopy (SEM), and zeta potential. Additionally, analyses of antioxidant and antimicrobial activities were conducted. In the second stage, active blend films were developed using an extruder, comprising biodegradable materials (solid phase) and a liquid phase containing whey protein isolate (16% w/w), corn starch (36% w/w), chitosan (8% w/w), glycerol (24% w/w), and water with nanoparticles encapsulated with essential oil (16% w/w). Their properties were also assessed by FTIR, TGA, SEM, water permeability analyses, mechanical tests, color, and transparency. Finally, the antioxidant activity and the ability to inhibit pathogenic microorganisms in the films were also evaluated. Our results highlight the formation of chitosan nanocapsules encapsulated with essential oil, as well as the creation of immersive blends, suggesting their favorable application as active and biodegradable packaging.

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Fabrication of zinc oxide supraparticles as a potential sustainable material for nutrient release

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Nanotechnology is a rapidly expanding scientific field with numerous promising applications in the agricultural sector. Nowadays, several tools are being designed to improve the efficacy and reduce the impacts of agrochemicals. For instance, supraparticles (SPs), synthed from clusters of smaller colloidal particles, can offer sustainable nutrient release and reduced leaching capacity compared to nanofertilizers [1]. This is due to their unique properties, including coupling, synergism, and co-location. In this study, novel supraparticles (SPs) were developed for potential application as a slow-release system for zinc. Initially, Zn NPs were synthed using the co-precipitation method [2], employing a factorial design, and subsequently characterized via Scanning Electron Microscopy (SEM), Fourier Transform Infrared Spectroscopy (FTIR), and Dynamic Light Scattering (DLS). Supraparticles (SPs) were synthed by the evaporation-induced self-assembly method on a hydrophobic surface and characterized by SEM, FTIR, optical microscopy, etc. The SPs exhibited a spherical morphology and displayed FTIR peaks corresponding to the stretching vibrations of the Zn-O bond, indicative of successful self-assembly. Furthermore, the in vitro release kinetics of SPs and Zn NPs were evaluated, revealing a slow and gradual nutrient release profile for the SPs compared to that of standard nanofertilizers. These results are innovative and offer a new perspective on the field of controlled release of fertilizers.

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Feasible and Low-Cost Autonomous Irrigation System Powered by Solar Energy

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Due to population growth and global warming, with greater irregularity in rainfall, the relevance of irrigation in agriculture has increased given the need to expand food production. In this sense, new technologies are needed that increase the efficiency of water use at the lowest cost. Our project aims to develop an automation system, powered by solar energy, with an automatic control function (on and off) of water flow in an irrigation system for small rural properties. Initially, we purchased equipment and assembled the automation system with a low-cost Arduino microcontroller, model uno, powered by an off-grid inorganic solar system [1] where we connected sensors responsible for measuring soil and air humidity, which will be used in the autonomous drive of the irrigation pump. Subsequently, we will test the effectiveness of the prototypes developed in our laboratory by collecting data in a previously approved area. As a result, it is expected that a viable and low-cost automation system with Arduino, powered by solar energy, will be developed in an irrigation system for small rural properties in the south of Tocantins.

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Improved properties in polysaccharides films for eco-friendly packaging apllication

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The study focuses on the behavior of the reinforcement properties of nanocrystals with fractions around the percolation threshold, and the interaction with the matrices to prepare a multifunctional film for food packaging. Therefore, the work was based on obtaining, characterizing, and adding bacterial cellulose nanocrystals (NCCB) to water-soluble biopolymers for the production of packaging films by casting. The matrices were: gelatin (cationic), hydroxypropylmethylcellulose (neutral) and pectin (anionic). Mechanical properties, water vapor permeability and humidity were analyzed. NCCB were obtained by acid hydrolysis from industrial waste. Thus, 5, 10, and 15% NCCB in gelatin was diffused; 4, 9 and 14% NCCB in pectin; and 3.5, 8.5, and 13.5% NCCB in HPMC. Table 1 shows the thicknesses of the control films and those with NCCB incorporation, as well as the mechanical properties of the films. The water vapor permeability, in general, decreased with the addition of nanocrystals. In gelatin films, without the addition of nanocrystals, with 5%, 10% and 15% the permeability was, respectively, 0.2386, 0.2242, 0.2026 and 0.2002 (g.mm)/(KPa.h.m^2), whereas for films based on pectin, without the addition of NCCB, with 4%, 9% and 14%, it was, respectively, 0.3404, 0.3306, 0.2602 and 0.2362 (g.mm)/(KPa.h.m^2) and for the HPMC matrix, without NCCB, with 3.5, 8.5, 13.5%, it was, respectively, 0.3572, 0.2992, 0.2822 and 0.2698 (g .mm)/(KPa.h.m^2). The moisture content of gelatin and pectin films decreased by an average of 20.18% and 8.72%, respectively. Nanocrystals, in general, have contributed to improving the mechanical properties of biopolymeric films and are promising for obtaining packaging films that require high strength.

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Interaction of oil-based polyurethane and nanoclay as a coating in urea granules reduces greenhouse gas emissions

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Despite the indispensable use of agricultural fertilizers to achieve current levels of productivity, chemical nutrients have their effectiveness limited by problems such as NH3 volatilization and soil immobilization. One strategy to minimize these problems is to protect the fertilizer with nutrient-release barrier materials. It is desirable that the formed polymer should have a homogeneous adhesive line on the granule surface and be able to control the diffusion of soluble nutrients through its structure, allowing the barrier to assume an active role and not just that of a physical obstacle, which release would occur by polymer fracture. The permeation through a polymer can be significantly reduced by the presence of internal diffusional barriers such as finely dispersed nanoclays. Thus, we proposed a nanocomposite system based on castor oil-derived polyurethane (PU) for controlling the release of fertilizers by an ion-exchange mechanism. PU coatings modified with less than 5% montmorillonite, a cation-exchange material, successfully retarded the N release from urea granules, with less than 50% of the nutrient released within 18 days of immersion, as confirmed by soil incubation experiments. The release times were proportional to the contents of the cation-exchange materials, which exhibited specific correlations with the nutrient released, confirming the diffusion barrier promoted by the PU coating structures. Moreover, the results showed that the combination between controlled release and nanoclay reduced the N2O and NH3 emissions in Palisade grass (Brachiaria brizantha). Our results demonstrated that the use of PU nanocomposites can significantly reduce the coating thickness with improved N-release control, opening a new field for the investigation of controlled-release fertilizers.

Low-cost device for thermal conductivity characterization of organic compounds

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The characterization of the thermal conductivity of organic compounds, pure and mixtures, is useful for industry in general and more specifically for the food industry. The present work aimed to design, produce and apply a device capable of determining the thermal conductivity coefficient of fluid or high viscosity organic and inorganic compounds, through the slope of the controlled heating ramp of a sample, before its temperature saturation. The device was designed and printed in Acrylonitrile Butadiene Styrene (ABS) polymer, incorporating the sample heating and temperature detection systems and their respective electrical circuits communicating via Arduino UNO board. The sample inserted inside the device is heated via a nickel-chromium (Ni-Cr) filament that is homogeneously arranged and immersed within the material to be characterized. The temperature of heating can be controlled by limiting the basal temperature of the filament. The detection system is made up of a type J thermocouple circuit inserted in the center of the prototype and its respective circuit for obtaining the temperature values collected in the sample. Calibration of the prototype was carried out with samples of distilled water (0.598 W/m·K at 20 °C) and castor oil (0.180 W/mK at 26.0ºC) in triplicate and the results obtained are in agreement with the data present in literature. The use of the present prototype to obtain thermal conductivity allows the integration of the physical-chemical characterization of materials in order to determine the quality and even originality of food products and organic and inorganic compounds. The primary focus of our team is to analyze artisanal organic products from the mountainous region of Espírito Santo, for example puína (derived from milk). The prototype is in the patent filing phase and its average production cost is around $36 US dollars, a value well below other similar devices found commercially.

Nanocellulose-based nanocomposites as versatile pesticide delivery vehicles: hydrophilic and morphological characterizations

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Nanocellulose-based nanocomposites exhibit excellent physical properties due to 3D nanofiber networks and high absorptive capacity, serving as reservoirs for carrying water and nutrients to agricultural fields [1,2]. The aim of the study was to synthesize and characterize the hydrophilic and morphological properties of the nanocomposite hydrogels based on polyacrylamide, carboxymethylcellulose and different concentrations of bacterial cellulose nanofibers (BCNF). All nanocellulose-based nanocomposite hydrogels, obtained from free radical polymerization, presented good reproducibility. From swelling degree results, it was possible to observe a decrease in water absorption of these nanocomposites caused by increasing in BCNF content. This indicates that the BCNF is acting as a mechanical reinforcing agent. Additionally, strong influence in the hydrophilic properties is observed as the salt valence increased in the swelling solution. The matrix without BCNF showed a slightly higher pKa value, confirming an interaction between nanocellulose-matrix. Scanning electron microscopy technique revealed that the structure of the hydrogel without BCNF are well defined, without roughness and highly connected, having homogeneous distribution, featuring a porous matrix compatible with that expected from a hydrogel. On the other hand, hydrogels with 2.0% BCNF has a small roughness and this is accentuated in the hydrogels with 7.0% BCNF. The results indicated that these matrices are potential materials for the application in agriculture fields.

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Optimizing magnetic nanoparticles for supraparticle design for agricultural applications

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The development of engineered nanoparticles for agriculture has significantly expanded in the last decade. However, designing smart delivery systems for controlled release with traceability capacity remains a challenge [1]. In this study, we synthed magnetic supraparticles (SPs)—complex structures formed by colloidal particles of micrometric —for a slow-release system of micronutrient in soil, enabling easy tracking on the soil. Initially, Fe_3O_4 nanoparticles coated with sodium citrate (Fe_3O_4@citrate NPs) were synthed using the co-precipitation method [2], based on a factorial design, and characterized using Dynamic Light Scattering (DLS). Subsequently, magnetic SPs were fabricated by surface templated evaporation-driven technique and characterized using several analytical techniques. Fe_3O_4@citrate NPs exhibited an average of 260 nm, polydispersity index (PDI) of 0.230, and a zeta potential of -24 mV. The SPs presented spherical morphology, with good affinity between nanoparticles and strong magnetic properties. In vitro release kinetic analysis revealed a controlled release of iron into the soil, as well as easy traceability using a magnetic field. Therefore, this study provides new insights into understanding the micronutrient release and fate of SPs and NPs in the environment.

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PlyB221-Modified Silver Nanoparticles: A Novel Strategy for Antibacterial Applications in Agriculture

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The rise of super-resistant bacteria in livestock farming is a global issue exacerbated by antibiotic overuse. Developing new therapeutic strategies for these pathogens is crucial for food safety and public health. Silver nanoparticles show promise in combating antimicrobial resistance, especially when combined with endolysins, enhancing their antibacterial activity. In this study, we developed new nanobioconjugates combining AgNPs and PlyB221, a bacteriophage endolysin, and investigated protein corona formation, as well as its activity against Bacillus cereus. Results revealed protein binding to AgNP surfaces, indicated by decreased surface plasmon resonance (SPR) peak absorption and a shift in wavelength. Dynamic Light Scattering measurements showed increased AgNP and altered zeta potential. Isothermal titration calorimetry (ITC) analysis revealed a negative value for free energy, indicating spontaneous PlyB221 adsorption onto the AgNPs interface, corroborating surface potential neutralization observations. The binding reaction was driven by an unfavorably distorted entropy change and a favorably inclined enthalpy modification. These parameters collectively highlight that protein introduction onto nanoparticles triggered an exothermic binding reaction. These findings were further validated through Fourier Transform Infrared Spectroscopy (FTIR) and Transmission Electron Microscopy (TEM) analyses. Lytic activity results indicated that the combination of AgNPs with PlyB221 (at 8.125×10^{-6} M) successfully reduced B. cereus turbidity by 80%. These results were further supported by resazurin assay, where inhibition percentage against B. cereus reached 60% at a concentration of 4.06×10^{-6} M, and confirmed by TEM, revealing the lysed morphology of B. cereus cell wall. Our findings have significant implications for developing biocontrol agents aimed at selectively discerning and eliminating super-resistant bacteria in agriculture.

Preparation and characterization of lignin nanoparticles as potential herbicide release system

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Some human choices have altered the climate and unnaturally fluctuated the Earth's temperature, leading to tragedies such as floods and droughts that have devastated crops [1]. These events have compelled scientists to enhance creativity in developing sustainable agricultural technologies. Recently, organic nanocarriers emerged as low toxicity and practical tools for controlled release of agrochemical [2]. However, the majority are made of synthetic polymers, and some are non-biodegradable or have high polymerization costs. In this sense, the present study aimed to prepare and characterize a novel polymeric nanocarrier consisting of lignin, the third-largest constituent of biomass plant from agro-industrial waste, for the controlled release of agrochemicals. Lignin nanoparticles (LNPs) was synthed using the nanoprecipitation method and their physicochemical characterization was performed by Dynamic Light Scattering (DLS). LNPs exhibited distribution of ca. 190 nm, polydispersity Index (PDI) of 0.334, and Zeta Potential of -33 mV. In addition, Scanning Electron Microscopy (SEM) showed spherical morphology and good colloidal dispersion of LNPs. Moreover, atrazine was utilized as a model herbicide for encapsulation within LNPs, revealing a gradual 60% release over time during the in vitro release kinetics. Therefore, LNPs and atrazine loaded LNPs were successfully obtained, demonstrating a promising nanocarrier for weed control in sustainable agriculture.

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Production of Zinc Oxide Nanoparticles via Green Synthesis Using Aqueous Extract of Astrocaryum aculeatum Pulp

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Zinc nanoparticles (ZnNPs) have been gaining prominence the packaging industry due to their anti-UV and antibacterial properties, which help to extend the shelf life of food products. However, the production process, is expensive and environmentally harmful, as it generates toxic by-products.Therefore, New synthesis methods are being explored with an interest in mitigating this process. With an interest in mitigating, Green synthesis is gaining space in the production of this material. I Tucumã (Astrocaryum aculeatum) is a typical fruit of the Amazon. Recent studies have shown that this species has a wide variety and quantity of biomolecules, such as phenolic compounds, flavonoids, among others, which can serve as antioxidants for zinc metal ions. The objective of this work is to synthe ZnNPs through the aqueous tucumã extract, varying parameters such as pH and reaction temperature. The mixture of zinc nitrate solution (Zn(NO3)2) 0.1 mol/L and plant extract was prepared in a ratio of 1:5 (20 mL of extract to 80 mL of Zn(NO3)2). The synthesis was monitored by UV-visible spectrophotometry (UV-Vis) with the monitoring of the plasmonic band near the region of 326 to 394 nm. The condition that obtained the best production of ZnNPs in a shorter time interval was at a temperature of 40 ºC, with the reaction medium at pH 7. The UV-Vis results, together with XRD and FTIR, confirmed the presence of zinc oxide (ZnO). After the mentioned analyses, the sample was calcined for 4 hours at 400 ºC to remove the organic matter from the plant extract. UV-Vis analyses showed the disappearance of the band near 200 nm related to biomolecules, indicating that the ZnNPs were pure. Subsequently, DLS and Zeta Potential analysis were performed, which indicated a moderate polydispersity, consistent with that found in the literature. The next step of this work is to subject this material to biological systems, such as bacteria and fungi.

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Removal of methylene blue from water using magnetic nanoclay

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Water bodies contaminated with industrial dyes, such as methylene blue (MB), can bring a series of disasters environmental, including the processes of photosynthesis due to the decrease of the dissolved oxygen in the water. Adsorption process is a promisor technology for removing dyes from wastewater [1]. Magnetic nanoclays are an actual and efficient adsorbent materials used for removing cationic dye from different aquatic environments [2] because great surface area and possibility of recovery and reuse after application. The objective of the study was to evaluate the removal efficiency of MB from aqueous solution using magnetic nanoclay@Fe_3O_4 as an adsorbent matrix. The amount of MB adsorbed was quantified by UV–Vis spectrophotometry by applying a calibration curve ($R^2 = 0.9992$). Contact time (or adsorption time), adsorbent and dye amounts were investigated to evaluate their efficiency. After only 10 minutes, the dye was completely adsorbed by magnetic nanoclay, reaching 100 % of removal. The maximum efficiency of dye adsorption was obtained for 9.0 ppm of MB and 100 mg of adsorbent, obtaining adsorption of 4.5 mg of MB / g of nanoclay. The results confirmed that these materials are potential adsorbents for the application in technologies of the water remediation.

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Scaling synthesis of carbon-based photoluminescent particles

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Carbon quantum dots show important properties such as zero-dimensional, quasi-spherical morphology, and fluorescence.[1] This carbon-based photoluminescent particles (CPP) present various applications such as in agriculture,[2] due the functionalization, dispersibility in water, biocompatibility, and simple synthesis including biomass as precursor, which offer to scale-up and sustainability. Due to the current biodiesel production, glycerol become as advantageous precursor to CPP synthesis. Actually, the International Energy Agency[3] estimate in 5 billion liters of biodiesel per year from 2024, which 2/3 will be demanded by emergent economies. We developed CPP synthesis from glycerol with citric acid (GCA) or urea (GU), into scale of 100 g and 500 g. For this, it was used a system consisting of heating mantle, round-bottom flask, and thermometer. The temperature and time synthesis were 200 oC and 2 hours. Citric acid or urea were added as 1, 4, 8, and 16% mol with respect to glycerol content. CPP showed narrow particle distribution from emission spectra, and CPP from GCA or GU provided higher quantum yields than CPP from pure glycerol, at least higher 3 times. Furthermore, CPP-GCA presented acid pH and there are no emission shift as function the excitation wavelength. However, CPP-GU (alkaline pH) and CPP pure glycerol (pH 5) presented emission shift as function the excitation wavelength. Thus, we reached out the scaling CPP synthesis from a simple method, which can provided higher sustainability to a strategic important industry as the biodiesel, and mainly CPP presents a huge perspective as photosensitizer in plants.

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Soil electrical resistivity analysis for plant growth monitoring: Low-cost Proof of Concept

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Monitoring plant growth can be done by determining the change in the electrical resistivity of the soil due to plant rooting. Therefore, monitoring the direct and indirect performance of plants can be obtained through direct determination of the electrical resistivity of the soil. The present work consisted of the production and manufacture of low-cost equipment for analysis, definition and characterization of the electrical resistivity of soils. The device as a proof of concept, is composed of two copper metal plates fed by a voltage generator, and two test leads, coupled to a voltmeter, the entire apparatus (plates, test leads and spacing of these items) was designed and printed in ABS polymer. The arrangement is inserted in a portion of soil close to the plant, which allows the definition of resistivity through the resistivity equation associated with a cylindrical conductive body. Minipa's commercial voltage generator imposes an alternating voltage to filter the capacitive properties of the soil. The total production cost of approximately $80 US dollars for the proposed device is lower when compared to commercial devices that realizes the same characterizations. In proof of concept, we changed the applied voltage profile (sine, square, and sawtooth waves), the nominal voltage values (10-100V) (intensity peaks), the duty cycle time of the waves, and the wave frequency sweep (20-200Hz) and duty cycle. The characterization of a soil sample containing clay and humus was carried out in triplicate. for a thickness of approximately 0.1 m thick we found ~4000ohm/m, which is close to literature results. We hope to plant beans and analyze the influence of these legumes on the calculation of electrical resistivity, characterizing the values as a function of time, pointing out the final feasibility of the proposal as an auxiliary tool that can be turned into a sensor that can be made remote/autonomous.

Strenx® steels – Application in headers frame for grain harvesting.

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The proposed study aims to re the welded assembly of a grain harvesting header called frame, aiming to reduce weight by increasing or maintaining mechanical resistance through the replacement of conventional HSLA NBR6656-LNE380 [1] steels with steels from the Strenx® 700 family [2]. This change not only aims to improve the mechanical properties of materials, but also to reduce the environmental impacts associated with pollutant emissions and soil compaction [3]. The scarcity of specific studies on the application of Strenx® steel on agricultural headers motivated the search for information related to the different ways of using this material and its limitations in this context. To achieve this, a header frame was redesigned using Solidworks® software and maintaining the essential assembly dimensions of the existing set. During the development of the project, a finite element analysis was carried out to optimize the design and guarantee the structural integrity of the set. An evaluation of the behavior of the materials and manufacturing processes was carried out, with the aim of filling the gap in the understanding and application of these materials in the agricultural industry. Prototypes of this frame were subjected to real field work conditions for validation. The main expected results include approximately 10% weight reduction in the new frame, an optimized stress distribution and satisfactory performance of the materials in real operating conditions.

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Synthesis and Characterization of La2NiPtO6 Double Perovskite for Glycerol Oxidation Applications

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Perovskite oxides (POs) exhibit promise for electrocatalysis in alkaline conditions due to their cost-effectiveness and customizable properties. However, the exploration of double perovskites (DPs) with the A2BB'O6 structure, remains limited in this context. Despite attention to their structural and magnetic properties, their potential as Glycerol Oxidation Reaction (GOR) catalysts has been overlooked. DPs offer chemical stability, conductivity and ability to create crucial hydroxyl groups on their surface, like single POs. [1]. The ability to adjust their composition, including forming mixed valence states, allows for the development of novel support materials. Additionally, DPs maintain a higher level of oxygen defects compared to single POs, potentially enhancing catalytic activity for GOR [2]. Our study focuses on the incorporation of Pt into the B-site of LaNiO3, as a catalyst for GOR. Herein, we synthed La2NiPtO6 by hydrothermal method, considering influential factors of pH (7, 10, 11, or 12) and calcination temperature (650°C or 800°C) to control crystal , homogeneity, and composition. Characterization involved employing cyclic voltammetry, Scanning Electron Microscope and X-ray Diffraction techniques. Based on our findings, high pH and temperature conditions favor the formation of La2NiPtO6 perovskite with catalytic activity comparable to LaNiO3 single perovskite [2]. Ongoing research explores exsolution techniques to enhance catalytic activity by exposing Pt NPs from La2NiPtO6 perovskite [3]. Exsolution of NPs from this DPs creates a promising electrocatalyst for selective glycerol oxidation, potentially leading to better polyol oxidation catalysts.

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Synthesis of hydroxyapatite nanoparticles and their performance as fertilizer in semi-arid soils

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The use of fertilizers is a crucial factor in agriculture, maintaining adequate plant nutrition and consequently increasing the quality and productivity of crops. The use of chemical fertilizers is common, but this strategy is generally associated with high costs and potential toxic effects [1,2]. An alternative for releasing micro and macronutrients in agricultural applications is hydroxyapatite, one of the crystalline structures of calcium phosphate, biodegradable and biocompatible, and widely used in biomedical and environmental applications. Hydroxyapatite nanoparticles have been investigated for application as nanofertilizers, acting as a source of controlled release of phosphorus, essential in agriculture, in addition to calcium, important in cell formation. Furthermore, hydroxyapatite allows its doping with different chemical elements that can be beneficial in agriculture, such as Zn, B and Mg [3]. In this context, the present work aimed to develop synthetic hydroxyapatite nanoparticles containing different micronutrients, using the chemical precipitation method, and their properties, structure, chemical composition and potential for controlled release of phosphorus in semi-arid soils were evaluated. Results show a synergistic effect of the controlled release of phosphorus and macronutrients, with the potential to increase productivity in semi-arid soils in Minas Gerais, being an innovative alternative for agricultural fertilizer.

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Tailoring the composition of electrospun metal oxide nanofibers with oxidase-like activity for the colorimetric evaluation of total antioxidant capacity

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Metal oxide nanozymes, i.e., metal oxide nanomaterials with intrinsic enzyme-like activities, are emerging as promising materials for colorimetric detection, facilitating the rapid, effortless, efficient, and precise detection of analytes in different matrixes. Efforts have been made to improve nanozyme catalytic properties, including strategies focused on composition regulation. Herein, we investigated the influence of the composition on the catalytic performance of binary metal oxide nanofibers (NFs). We developed ZnO/MnO_2 NFs via an electrospinning followed by a calcination and evaluated their capacity to oxidize the 3,3′,5,5′-tetramethylbenzidine (TMB). By adjusting the amount of the metal salt precursors ratio, NFs with different Zn:Mn mass ratios were obtained (1:0 (I), 3:1 (II), 1: 1 (III), 1:3 (IV) and 0:1 (V)). The morphology and composition of the NFs were analyzed by SEM and XRD, and the kinetic studies were carried by catalyzing the TMB oxidation. All the reactions were performed in acetate buffer (pH 4.0), and the absorbance value was measured at 652 nm by UV–vis. The kinetic parameters (K_m and ν_{max}) were predicted from the Michaelis-Menten model. Materials I, II and III had their nanofibrous morphology confirmed by SEM, while IV presented a mixed phase of fibers and plates, evidencing the favored formation of the fibrous structure in the presence of ZnO. NFs III presented a lower K_m value and higher ν_{max}, indicating greater affinity and high reactivity to TMB oxidation. Taking advantage of the superior oxidase-like activity of NFs III nanozyme, a sensitive method for Total Antioxidant Capacity (TAC) assay in food samples was proposed based on the reduction abilities of antioxidants in reducing the oxidized TMB, resulting the blue color fade.

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FM06-Advances in Welding Science and Technology for Metallic Materials

A Review of Laser Beam Welding

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Laser beam welding is a consolidated process in the industrial environment and involves joining two or more components through localized fusion produced by the light intensity coming from a laser source [1]. The process is fully automatable, fast, and reproducible on an industrial scale; however, its full use requires greater technical knowledge than conventional welding processes. This contribution aims to contribute to the discussion on the current problems and future perspectives of laser welding of metallic materials based on the experience accumulated in 20 years of research and development at the Institute for Advanced Studies [2]. In particular, issues regarding the weldability of dissimilar alloys, the issue of defect mitigation, the means of preventing the high reflectivity of some non-ferrous alloys to infrared radiation, and the most relevant optical and electronic instrumentation are discussed. Future challenges include the trend towards laser welding in the area of renewable energy, the use of artificial intelligence in the production process, and quality control of welded joints.

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Ultrasonic spot welding of dissimilar light alloys

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Lightweighting is not only a major concern in the automotive and aerospace industries to improve fuel efficiency and reduce emissions, but also important for improving the sustainability, material saving and performance, and reducing manufacturing cost. It also leads to increased payloads and longer driving ranges of battery electric vehicles, yielding a ~14% improvement in electric range for a 10% reduction in weight [1]. The global automotive lightweight materials market was valued at USD 72.16 billion in 2022, which is expected to reach USD 137.8 billion by 2032 at an annual growth rate of 6.7% [2]. Vehicle lightweighting can be achieved via stronger materials (e.g., advanced high-strength steels (AHSS)) or lighter materials (e.g., magnesium and aluminum alloys) along with the essential manufacturing methods. While AHSS has a weight reduction potential of 10-19%, aluminum and magnesium alloys have a higher weight reduction potential of 50-65% and 64-72%, respectively [3]. Thus, an innovative "multi-material" concept has been adopted to maximize the lightweighting potential, where the characteristics of different materials are optimized for the desired application for lightweighting, cost effectiveness and value addition. The structural applications of multi-materials inevitably involve welding and joining, especially dissimilar welding. This poses significant challenges due to different thermophysical and mechanical properties and the related requirements on the safety, reliability and durability of welded joints. Dissimilar welding between magnesium and other alloys represents a great challenge, since intermetallic compounds may occur to potentially cause premature failure. Some emerging solid-state joining techniques, such as ultrasonic spot welding, friction stir (spot) welding, have been developed to join the lightweight alloys. In this talk, several examples on the welding of dissimilar magnesium-to-aluminum, magnesium-to-steel and aluminum-to-steel using ultrasonic spot welding will be presented. The weld interface underwent dynamic recrystallization during similar welding, while an intermetallic layer or eutectic layer was formed during dissimilar welding, depending on the material combinations and welding parameters. To eliminate or lessen the occurrence of intermetallic compounds, an interlayer (tin or zinc) was used during dissimilar welding. It was observed that the tensile lap shear strength and fatigue life of the dissimilar welded joints were effectively enhanced. The evolution in the microstructure and texture as well as fatigue fracture mechanisms of the welded joints will also be presented.

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Welding of dissimilar materials: from harfacing to functional graded materials

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Hardfacing typically involves the the metallugical bond of dissimilar materials. This procedure allows the processing of parts with high performance at the surface exposed to wear or corrosive demands while the bulk of the parts exhibits adequate structural properties. Before hardfacing it is important that engineering consider the impacts of processing parameters on the dilution of deposited material with the alloy of the substrate and solidification structure both influencing te performance of hardfacing coatings. A review on the impact of processing conditions on the dilution and solidification structure and their impact on the performance of hardfacing coating of complex metallurgical alloy is discussed. Boundaries for the welding of dissimilar materials are moved forward when multilayers can be deposited by directed energy deposition processes (DED) wit a gradient of properties. This can be achived imposing a gradient either with in the composition or microstructure of each deposited layer. Gradient materials offer a step further towards enhanced performance smoothing the transition between the substrate and the high performance material of the coating. Further enhancements include expanding these procedures to the processing of functional graded materials allowing to manufacture costumize parts to attend specific demands. The challenges associated with processing property gradients using welding of dissimilar materials are bring forward including a discussion on the opportunities presented by costumization of mechanical parts.

Effect of solubilization and aging treatments on the microstructure evolution and mechanical behavior of Inconel 718 alloy processed by a laser-based Directed Energy Deposition

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The laser-based Directed Energy Deposition is an additive manufacturing (AM) method that offers a high accuracy and deposition rate [1]. Due to the development of materials for gas turbine engines, focused on materials with high mechanical properties and corrosion resistance, Inconel alloys were designed, such as the Inconel 718 (IN718) [2]. The precipitation hardening heat treatments recommended for IN718 focused on appropriate temperatures and times to promote the precipitation of the fine γ' and γ” coherent phases to enhance the mechanical properties. Previous works coincide in applying a solubilization treatment before the double aging, carried out in two stages (DA: 8h at 720°C followed by another 8h at 620°C). The solubilization heat treatment at temperatures above 1000°C, followed by double aging (DA), aims to produce fine precipitation of the γ' and γ” phases that increase the mechanical resistance of IN718 [3]. However, heat treatments suggested by books for conventional processed IN718 does not apply for AM parts. As a result of the thermal cycle that each part undergoes, the phase transformation kinetics are affected in subsequent heat treatments, which in turn affects the thickening of γ', γ” precipitates and the formation of deleterious phases such as δ and Laves that can happen at different times. Consequently, in this work, we explore the effects of the as-built condition, homogenization (H – 1100 °C for 1,5 h), solubilization (S – 1000 °C for 1h) and double aging (DA) heat treatments and combinations of these (S, H, DA, S+DA, H+DA and H+S+DA). The microstructural evolution and mechanical properties were assessed, and the best overall microstructural and mechanical properties were achieved with the H+S+DA.

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Effect of solubilization treatments on the microstructure evolution and mechanical behavior of Inconel 625 alloy processed by a laser-based Directed Energy Deposition

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The high strength, creep, rupture resistance, fatigue, thermal fatigue, and good weldability of the Inconel 625 (IN625) alloy make it very attractive for aerospace applications of large components, mainly by using additive manufacturing (AM), specifically the laser-based Directed Energy Deposition, that offers high accuracy and deposition rate [1]. The mechanical properties of as-built components depict heterogeneities due to thermal history and micro segregations. Therefore, heat treatments and machining operations are needed after AM. Two types of heat treatments are recommended for additively manufactured IN625 components: stress relief (SR) and solubilization (S). The SR is recommended for large components to reduce residual stresses, and solubilization intends to reduce or fully dissolve potentially formed deleterious phases, such as the δ-phase. The presence of δ-phase can compromise the ductility and corrosion of IN625 welded joints [2]. Solubilization above 1000 ºC in a DED-processed IN625 decreases the presence of δ-phase, and above 1100 °C will fully dissolve this phase in a wrought IN625 alloy. Previous studies explored the effect of SR heat treatment, finding that SR led to the hardest condition while the solubilization softened the matrix. Bon et al. [3], using DED-LB, found similar results using SR (800 °C for 1h) and SR + solubilization (1100 °C for 1 h). Consequently, in this work, we explore the effects of the temperature and time of homogenization (H – 1200 °C for 1h), solution 1 (S1 – 1100 °C for 1h) and solution 2 (S1 – 1100 °C for 3h). The microstructure and mechanical strength were studied, and the best mechanical behavior was found after using the S1 heat treatment.

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Microstructure and mechanical properties of the 316L stainless steel parts fabricated by WAAM.

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Wire Arc Additive Manufacturing (WAAM) presents a swift method for producing large metal components while maintaining cost-effectiveness and material efficiency [1,2]. This research delves into the microstructure and mechanical property anisotropy of 316L stainless steel parts crafted via WAAM, employing diverse deposition strategies. By optimizing parameters, the study achieves successful component fabrication, highlighting the pivotal role of deposition parameters in determining surface quality. Examination of XRD peaks unveils post-weld crystallographic texture development, corroborated by EBSD analyses indicating notable texture presence. SEM analyses distinguish varied ferrite phase morphologies across different component regions. Mechanical assessments suggest a tendency towards anisotropic behavior in WAAM materials, with samples featuring a 45° overlap angle displaying marginally superior mechanical properties. Consistent microhardness along the build direction underscores the reliability of the deposition strategy.

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Non-Destructive Evaluation of SAF 2507 Thermal Aging and Phase Transformations via Nanoindentation and Pulsed Eddy Currents

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Super duplex stainless steels (SDSS's) are highly recommended for corrosive environments [1]. However, detrimental phases tend to precipitate in the austenite-ferrite interfaces at certain temperatures [2]. In this study, the elastic moduli and hardness of ten specimens of SAF 2507 aged at 900ºC for different amounts of time were determined using nanoindentation, an instrumented indentation technique widely used for measuring the mechanical properties of materials with state-of-the art precision [3]. An investigation of isothermal phase changes, employing optical microscopy (OM) and X-ray diffraction, in addition to the instrumented indentation data, enabled elucidation of how SAF 2507 microstructure influences these properties. As the ferrite content decreases and the sigma phase content increases, the elastic modulus increases until a treatment time of 45 minutes and remains stable for higher aging times. Moreover, the potential of the Pulsed Eddy Current (PEC) NDT technique in assessing SDSS mechanical properties is also explored. Analysis of the SAF 2507 specimens reveals a relationship between ferrite content and PEC signal amplitude, corroborated by hardness measurements and OM. These findings support the applicability of NDT's for assessing microstructural changes and determining mechanical properties of SDSS's, which is vital for ensuring equipment integrity in the industry.

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The application of electrical pulses as an innovative technique of self-healing in aluminum alloys

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Extrinsic self-healing in metallic materials has great potential for application in industrial components, but is little studied in the literature. The action of external stresses acts to generate defects, such as microcracks and hardening, being clear indicators of the reduction in the useful life of a structural component. The application of the electric pulse technique (EPT) in self-healing in metals has the great advantage of little temperature rise, which better preserves their original microstructure. The present work proposes an innovation in the application of (EPT) in pre-deformed materials to verify its effectiveness in repairing microstructural defects and, consequently, in extending its useful life. Two aluminum alloys with different behaviors were chosen, the high-strength aeronautical alloy Al-Zn 7075 and the high-ductility naval alloy Al-Mg 5083. Both were subjected to tensile pre-deformation and subjected to EPT application with current densities of up to 66.7 A/mm2 for up to 21 seconds. EPT promoted an increase in the ductility of both alloys, where analyzes via scanning electron microscopy (SEM) showed the promotion of softening mechanisms and, mainly, the effective partial closure of microcracks! The results corroborate the diffusional mechanisms of action of electrical pulses discussed in the literature [1-3], with the applied procedure being effective in promoting the microstructural and mechanical regeneration of the analyzed samples.

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Towards Enhanced Understanding of Defect Formation in WAAM Processed Steel: Integrating Sensor Fusion and microCT analysis

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WAAM processes have been increasingly studied both due to their strategic applicability in the additive manufacturing of large metal parts [1] and in relation to their mechanical behavior and the presence of defects such as porosity [2]. This study investigates the utilization of sensor fusion techniques, coupled with evaluating defect formation in steel samples processed through Wire Arc Additive Manufacturing (WAAM). A series of experiments were conducted using AWS ER410NiMo wire on ASTM A36 substrates, with parameters adjusted to induce defect formation. Multiple sensors, including voltage dividers, ammeters, microphones, and cameras, were employed to capture real-time process data. Defect analysis was performed using microCT. The results demonstrate the effectiveness of accurately identifying porosity and pore diameter (in the range of 50 µm) and crack length using microCT. Findings highlight the potential of integrating sensor fusion with microCT characterization to improve quality control and process optimization in WAAM applications.

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Bimetallic flanges for ultra-high vacuum applications in synchrotron light source manufactured by friction stir welding

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Aluminum-based vacuum chamber applied in synchrotron light sources machines are joined by bimetallic flanges of aluminum 6xxx series alloy and stainless-steel SAE 304 [1]. The aluminum side is joined by Shielded Metal Arc Welding (SMAW) to the vacuum chamber. The stainless-steel side is used to deform the copper ring and guarantee the sealing for ultra-high vacuum of the interface between the flanges. The process used to produce the bimetallic blank can not achieve high temperatures because it reduces the hardness of the aluminum alloy to the point that the torque used to fix the flanges cause a deformation that decrease the efficiency of the ring copper sealing. In this work it was proposed the use of the Friction Stir Welding to joining both materials. Friction Stir Welding is a welding process that uses A non-consumable rotating tool inserted into the touching edges of plates to be joined and go across along the line of junction [2]. It was made a dissimilar overlapping welding of AA6061 and SAE 304LN plates using a 9.5 mm WC-Co tool who's the path is like internal flange shape. The flanges were produced from the welded plates by electrical discharge machining and milled in a CNC machine. For evaluation of the performance of the flanges, these components were submitted to leak test with helium gas after heating cycles at 180 °C - simulating the baking used to clean the vacuum chambers. The mechanical characterization was performed by microhardness measurements, near the interface of the plates and by tensile test of sub specimens. The flange was approved in the tests, and it has been used at Brazilian synchrotron light source (SIRIUS) in vacuum pressure of 10^{-11} mBar.

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Characterization of Arc Welding Coating of Metal Matrix Nanocomposite based on CNTs/Ti6Al4V/CaF_2

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Welding coatings based on metal matrix nanocomposite (MMN) nanoreinforced by Carbon Nanotubes (CNTs) [1] are promising due to its balancing hardness and ductility and, thus, reducing equipment maintenance costs. In this sense, this research presents the microstructure, vibrational interaction and hardness tests of a nanostructured welding coating. For this, a flux-cored wire based on a low-carbon steel metal sheath filled with CNTs/Ti6Al4V/CaF_2 (mass ratio 1:40:4) was used as a consumable electrode in the coating of an ASTM A131 grade A steel plate via tungsten arc welding at 160 A protected with argon gas (12 L/min). Optical microscopy and field emission scanning electron microscopy (FE-SEM) micrographs revealed the formation of cross-, rod- and petal-shaped titanium carbides (TiC) in Fe alloy matrix. Using FE-SEM with magnification up to 200,000× and Raman spectroscopy, CNTs were detected in a petal-shaped TiC, demonstrating that the welding process did not promote its complete structural disintegration. In this case, this phase transformation contributing to a 60% increase in the degree of amorphous carbon compared to the CNTs as received. Additionally, blueshifts were observed in the Gouter and Ginner subbands of the coating's Raman spectrum show that residual stresses in this region of the weld promoted compressive deformations in the external and internal walls of the CNTs. In the Rockwell A hardness test, the nanostructured coating performed around 7.0% and 22% better than the base metal, in the top and cross-sectional, respectively. In this way, the welding of MMN promoted the incorporation of TiC/CNTs and improved in the mechanical property.

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Effect of aging heat treatment on the microstructure and pitting corrosion resistance in SAF 2205 duplex stainless steel

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The SAF 2205 duplex stainless steels are alloys with two metallurgical phases that consist of austenite and ferrite, which provide good mechanical properties and corrosion resistance. However, the exposure of these stainless steels from 600°C to 1000°C for a certain period induces the precipitation of the deleterious sigma phase, originating from ferrite and austenite decomposition, and consequently can cause embrittlement in the material [1]. This work investigated the effects of the aging heat treatment at 800°C for 60 minutes, 120 minutes, 180 minutes, 300 minutes, and 900 minutes. It was inferred that there was intense sigma phase precipitation from 120 minutes of aging, verified by the X-ray Diffraction (XRD). Tensile tests were conducted to evaluate the mechanical properties of the duplex stainless steels after microstructural modification induced by heat treatment. The obtained results revealed that the material exhibited higher tensile strength as well as microhardness with increasing heat treatment time. This finding indicates that the sigma phase significantly reduces the material's resistance to plastic deformation. To assess the pitting corrosion resistance of these materials, cyclic potentiodynamic polarization tests were performed in a sodium chloride solution of 35 g/L at 60°C. Based on the test results, it is evident that the samples exposed to longer periods of aging are more susceptible to pitting corrosion. This observation suggests that the increased presence of the sigma phase (σ) in the microstructure may have reduced the material's resistance to pitting corrosion.

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Enhancing Tribological Performance of Automotive Dies with Nickel-Based Alloy Coatings Reinforced with Boron Carbide

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Nickel-based alloys are widely used in the automotive industry, particularly in the manufacture of punches for nodular cast iron dies. These alloys are crucial for stamping Class A surfaces, offering enhanced durability and wear resistance, essential for the production of high-quality automotive components. The addition of high-hardness carbides in these alloys can significantly increase wear resistance, thus expanding their applicability [1]. In this study, powder mixtures of Ni-5Al alloy (used as matrix material) and boron carbides (used as ceramic hardening phase) were employed for the production of metal matrix composite (MMC) coatings, aiming at improved tribological performance. Ni-5Al powder was added with 5, 10, and 20% B4C agglomerated with an organic binder, in the form of suspension, and previously deposited on nodular cast iron samples. The composite coatings were fabricated using a continuous Nd:YAG laser operating at 300 W, with a scanning rate of 350 mm/min and a 0.25 mm overlap between passes. The coatings and substrate were characterized by optical microscopy, X-ray diffraction, Vickers microhardness, and microabrasive wear test. The addition of 5% B4C to the Ni-5Al alloy resulted in a high-hardness coating, comparatively superior to the nodular cast iron substrate. The additions of 10 and 20% B4C produced coatings with 10 and 15% higher hardness, respectively, compared to the coatings with 5% B4C. Proportions greater than 5% B4C resulted in coatings with vertical cracks at the coating/substrate interface. The wear resistance analysis was performed only on the coating with 5% B4C addition, due to the absence of cracks, ensuring the integrity of the coating during the wear tests. It was found that the addition of 5% B4C increased the wear resistance of the substrate by 27%.

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Influence of the Oxide Layer on Laser Welding of Dual Phase DP800 Steel

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Laser beam welding (LBW) has been adopted as a replacement for spark welding in continuous strip lines of high-strength steel, owing to the need for a fusion zone (FZ) with fewer oxide inclusions, which can weaken the weld bead. This study focused on the weldability of dual-phase DP800 steel with an oxide layer using LBW. Yb:Fiber lasers from IPG were used, with powers ranging from 700 W to 2000 W and speeds between 10 and 60 mm/s, without process gas. The samples had dimensions of 100 mm × 200 mm x 2.8 mm, and the oxide layer was intact. Microstructural analysis and tensile tests showed that power levels of 1800 and 2000 W and speeds of 40 and 50 mm/s resulted in weld beads with full penetration and an average width of 0.8 mm. The tensile strength was 730±12 MPa and the yield strength was 440±3 MPa. The weld bead, which is mainly composed of martensite, reinforces the material and reduces its ductility without affecting its tensile and yield strengths. The required heat input ranged from 45 to 50 J/mm, without the need for a shielding gas.

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MICROSTRUCTURAL EVALUATION OF WELDED JOINTS BY ELECTRIC CONDUCTIVITY

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For a full characterization of welded joints several techniques, that are usually destructive or performed in a local and precarious way, are needed. The search for the development of new methods, preferably non-destructive, is still a current need. Recent studies have shown that electrical conductivity can be used to identify different welding zones, as it has a good correlation with microstructure and hardness. This work aims to develop a system capable of tracing electrical conductivity profiles, using the four-point method, in order to correlate them with the microstructure and microhardness of welded joints. For this, interstitial free steel plates and copper plates were welded by tungsten inert gas. At the cross section and on the surface of the samples, profiles of electrical conductivity and Vickers microhardness were traced, later correlated with their micrographs. The results indicated that electrical conductivity measurements can be used as an effective method to identify the welding zones, in addition to being promising for in situ application.

Optimization of vacuum Cu-Cu diffusion welding for cryogenic structure purposes

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Widely used in aerospace and nuclear applications, diffusion welding provides a metallurgical bond between parts, joining them across the entire material interface, without the use of filler material, thus maintaining the chemical compositions of both parts, thus maintaining the strength and resistance of the base materials. This type of welding is based on the process of joining two or more parts by applying pressure and temperature to the parts to be welded, promoting the diffusion of the first atomic layers of the materials. The main objective of this study is to characterize the influence of the experimental parameters of time under pressure, temperature and surface roughness in order to develop a greater understanding of copper-copper diffusion bonding and to apply this method to weld metals for cryogenic purposes. The application includes the welding of thermal belts to be used at cryogenic temperatures, due to the high thermal conductivity of copper at low temperatures. Optical microscopy and scanning electron microscopy (SEM) were used to characterize the microstructure of the welded part, to validate the bonding interface of the base materials. Tensile strength tests were carried out for mechanical characterization.

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Residual stress in 316L Si stainless steel produced by wire arc additive manufacturing

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X-ray diffraction analysis of 316L steel parts produced by Wire Arc Additive Manufacturing (WAAM) faces challenges due to the particularities of this manufacturing process. To overcome them, specific approaches are necessary, such as the use of appropriate sample preparation and combining X-ray diffraction with Electron backscatter diffraction (EBSD). In this context, this study aimed to evaluate residual stress by X-ray diffraction and correlate it with the grain and texture resulting from the material solidification process.The results showed the presence of coarse grains, on the order of tens of microns, and a preferential growth of columnar-dendritic grains along the [100] direction. These factors made it difficult to measure residual stress by X-ray diffraction, requiring surface preparation to overcome this difficulty. The magnitude residual stresses were high and trative in both conditions analyzed of current and contact tip-to-work, being even higher in the condition with higher current and shorter working distance.In light of these results, it is suggested to use longer working distances and lower currents as an alternative to minimize the formation of residual stress during the deposition of 316L Si stainless steel by WAAM.

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Study of corrosion behavior in API 5L X7O steels applied in the oil and gas industry.

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API 5L X70 MS and MO (MS support more corrosion than MO with contact of petroleum), steels are used in oil pipelines, where both purposes are to contribute to the microstructural understanding of the causes and mechanisms of corrosion. Starts with the preparation of specimens for microstructural characterization was carried out; The sample is presented as received and the corrosion resistance of the specimens has been calculated: Immersed in deaerated NACE 177-B or with H2S for 96 hours solution and subjected to the steam of this solution at room temperature of 24°C. Analysis of corrosion products by scanning electron microscopy (SEM), EDS and X-ray diffractometry. The received samples were also attacked with 2% Nital solution for 7 seconds, evaluating the grain , with predominantly ferrite and perlite microstructure. MS revealed a ferritic matrix and intergranular ferritic aspects, whereas MO has a banded ferritic microstructure caused by the microsegregation of the alloying elements during the manufacturing process. The corrosion resistance of the specimens was evaluated by mass loss, making it possible to observe that the MO samples exhibited greater resistance to the environment without H2S due to its greater homogeneity and refinement of the microstructure, however, are exhibited banding characteristics, leading to the formation of MnS inclusions compared to MS. The microhardness HV of the steels was determined, in such a way that the HV microhardness of the steels was the mean and the standard deviation of the MO sample in the banding, the corrosion resistance of the specimens was evaluated, the mass losses with the reduction of the MO samples showed a higher resistance to the environment without H2S than the MS. Scanning electron microscopy and EDS in secondary electron mode revealed a homogeneous microstructure related to grain and the presence of sulfur and manganese, probably nucleated by the inclusion of MnS.

STUDY OF PIN PROFILE AND ROTATION SPEED EFFECT ON THE FSW WELDING OF AA1100 AND AA5052 ALUMINUM ALLOYS

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Since Friction stir welding (FSW) does not lead to fusion, it has attracted considerable attention, both for production and repairing in the industry, mostly when low weldability alloys, like aluminum alloys, are involved (ALVES et al., 2010). The FSW tool is basically composed of stem, shoulder and pin. A number of variables determine the success of FSW operations, among them, pin geometry and rotation speed. Pin geometry influences the level of deformation imposed on the volume of material moved during the operation and rotation speed determines heat generation during the operation (PANKUL, 2019). FSW has been used for aluminum alloys, since it does not reach the melting point and leads to lower residual stress (MA, 2008). The purpose of this work is to study the welding of the AA1100 and AA5052 aluminum alloys using three different pin geometries (circular, square, triangular) and two rotation speeds (828 rpm; 1356 rpm). Advancing velocity of the tool was always 28 mm/min. Tensile tests showed that the best results were obtained with triangular pin, leading to comparable resistance level and higher ductility; the square pin led to intermediate values and the circular pin led to the poorest results. Microhardness mapping of the welding beads confirmed the results observed with tensile tests.

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Study of the formability of DP780 and CP1000 automotive sheets welded dissimilarly with a laser beam

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The dissimilar laser welding of advanced high-strength steels (AHSS) is gaining prominence in the automotive industry owing to its potential for lightweighting and structural integrity enhancement. Among the possible combinations, dual-phase (DP) and complex-phase (CP) steels are gaining increasing relevance in the security envelope of car frames [1]. This study investigates the feasibility and characteristics of dissimilar laser welding between DP780 and CP1000 steels with reference to their mechanical behavior. The experimental setup involved a high-power continuous-wave laser system with tailored process parameters to achieve an optimal weld quality. In particular, the in-line rolling of steel sheets provides a close-gap mechanism that improves weld reliability. Microstructural analysis, including optical microscopy and electron backscatter diffraction (EBSD). Mechanical properties, such as tensile strength, hardness distribution, and Erichsen test , were evaluated to assess the structural integrity of the weld. Finite element simulations were employed to model the thermal history and residual stress distribution in the welded joint. In particular, softened material near the heat-affected zone is considered an important issue for successful dissimilar welds. According to the current results, it is possible to produce sound welds between the steel sheets by fine-tuning the experimental results. These findings shed light on the microstructural evolution, mechanical behavior, and process optimization strategies for dissimilar laser welding of DP780 and CP1000 steels, offering valuable insights for enhancing the performance and reliability of automotive structures.

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SS02-Towards a Sustainable Bioeconomy: Innovations in Biomass Conversion for High-Value Bioproducts and Biorefinery Integration

On the versatility of lignin: from sustainable derivates for thermoplastic blends to photo-promoter in organic chemistry

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From an industrial perspective, Lignin, the second most abundant biopolymer, represents a cheap byproduct for pulp and paper production and, currently, it is incinerated to recover energy for the cooking process. Framed in a sustainable development perspective, however, lignin is gaining more and more attention as a versatile feedstock for several applications ranging from the polymeric sector to the synthetic field.

The first example presented here underscores lignin's significant potential to replace petroleum-based derivatives in material science.[1] Its multiple functional groups facilitate chemical modification, while its aromatic structure can enhance thermomechanical properties. Although various lignin modifications are emerging, they often involve unsustainable chemicals, conditions, and purification steps, hindering the scalability of industrial processes. The results discussed in this example focus on optimizing the chemical modification of lignin through reactive extrusion to create innovative biomaterials. These materials, containing up to 40% lignin and produced through simple, scalable, and sustainable processes, have proven to be suitable for film-blowing, recyclable, and compostable.

The second example serves as a proof-of-concept, highlighting how lignin structures and their interaction with visible light open new opportunities for developing green photochemical processes. Specifically, technical lignin was refined using solvents to obtain fractions with controlled molecular weights and fully characterized structural features. These refined fractions were then tested as photo-initiators for the direct functionalization of terminal olefins with radical precursors under visible light irradiation. The results demonstrated that low molecular weight refined lignin effectively promoted significant photo-induced radical reactions, yielding several densely functionalized alkyl halides.

The Impact of Enzymatic Catalysis on Enhancing the Sustainability of Biobased Furan Polymers

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Environmental issues due to plastic pollution have become so prevalent that tremendous efforts to develop sustainable polymer alternatives from renewable resources have become an urgent necessity. Biomass-derived molecules like adipic acid, lactic acid, camphoric acid, and furandicarboxylic acid have emerged as key components in the development of biobased chemical platforms for polymer synthesis. Within a large variety of biobased monomers, furan derivatives and furan chemistry hold special attention in polymer chemistry. The similarity between furan and phenyl rings unveils the opportunity for a biobased alternative for phenyl-based polymers. However, current research involving furan polymers is predominantly at the stage of material development and faces some limitations e.g. due to poor thermal stability. Achieving sustainable and effective synthetic processes of furan polymers remains a formidable challenge. Here we present a strategy for integrating enzymatic catalysis for the synthesis of novel furan polymers. By enzymatic polycondensation, a series of furan (co)polymers are successfully tailored from biobased furan building blocks, rendering a library of polymeric materials with versatile properties. Enzymatic catalysis enables lower reaction temperatures and avoids the use of toxic catalysts, thereby improving sustainability and overcoming the limitations of conventional chemical routes. We demonstrate the fundamental impact of enzymatic catalysis in furan polymer synthesis, highlighting its potential for a scalable, environmentally friendly synthetic approach.

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Tung oil-based building blocks: Exploiting a non-edible vegetable oil for the synthesis of polyfunctional monomers and polymers

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The fast spread of the polymer sector within the last century, along with its inherent dependency on petroleum-derived compounds, has been negatively contributing to serious, and sometimes irreversible, environmental impacts. The use of less harsh processes, as well as transitioning to renewable platforms, are promising strategies for the sustainable preparation of macromolecules. The combination of the two approaches is encouraged, which has been motivating a myriad of research initiatives focusing on the design of novel macromolecular materials based on renewable resources and respecting the principles of green and sustainable chemistry. Tung oil is a non-edible vegetable oil that bears a peculiar chemical composition of approximately 80% of alpha-eleoestearic acid, a polyunsaturated, conjugated fatty acid that has a huge potential to be exploited as a source of monomers and polymers. In this study, tung oil was considered as a bio-based building block for synthesizing novel polyfunctional monomers via the straightforward Diels-Alder 'click' reaction. Specifically, methyl alpha-eleostearate, directly obtained from tung oil via transesterification, was applied as a diene in Diels-Alder reactions with either dimethyl itaconate, n-butyl methacrylate, or 1,1′-(methylenedi-4,1-phenylene)bismaleimide. The monomers were characterized by FTIR/ATR, 1H NMR, and GC-MS, and then submitted to step-growth polymerization reactions with diols of different molecular structures. The choice of different dienophiles allowed the production of bi- and tri-functional monomers, with aliphatic or aromatic structures, leading to novel linear and crosslinked polyesters with different thermal and mechanical properties. In general, opting for a reaction which is aligned with the principles of green chemistry to modify tung oil proved to be an effective approach for generating monomers with diverse architectures. This opens up new avenues for synthesizing bio-based polymers with customizable p

Adaptation of a tung oil-based thermosetting resin for binder jet 3D printing

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In this work, a tung oil-based thermosetting resin was synthed via thermal polymerization and reinforced with thirteen different types of sand. The viability of this process inspired the adaptation of the resin for its use as a binder and sand as a powdered material in binder jetting, an additive manufacturing process. Firstly, it was shown that the resin could have its initial viscosity (~2 cP) increased by preheating it at a certain temperature for a certain time, making it tunable according to each necessity. The curing process of the resin was assessed via dielectric analysis (DEA), combining the utilization of heat and ultraviolet (UV) light, showing that a resin with a viscosity of 10 cP can be fully cured after 250 min at 90 °C, or 300 min at 75 °C, both under a 365 nm light exposure. Rudimentary tests simulating the 3D printing process successfully formed a solid object, which was post cured, giving a hard piece. This collection of results is promising and suggested that the tung oil-based resin can serve as a bio-based binder for 3D printing applications.

Chitosan supported WO3 as catalyst for highly efficient sulfides oxidation

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Molecules such as sulfones and sulfoxides have great aggregated value when it comes to their use in the production of pharmaceuticals and medicines [1]. Therefore, finding ways to acquire said molecules is of great importance. The main way these molecules are produced is through the oxidation of sulfides, but the challenge is to selectively form one of the two products of oxidation, either sulfoxides or sulfones. The main process utilized for this reaction is through heterogeneous catalysis, and the use of semiconductors is very common [2]. Therefore, using WO3 in pair with chitosan can be an interesting combination to be explored in this scenario. To obtain that, coprecipitation method was used to acquire the oxide in its monoclinic state, with help of microwave stove. Four different concentrations of WO3/chitosan were tested at 0, 10, 20 and 40% w/w, named QT, QT1W, QT2W and QT4W. The obtained catalysts were tested in different times, temperatures, solvents, oxidants and catalyst load using thioanisole (methylsulfonylbenzene) as model sulfide molecule to be oxidized. They were then analyzed through X-ray diffraction, Raman spectroscopy and SEM and EDS. Following the finding of optimal conditions, tests for recyclability, scaling and determination of mechanism were conducted. QT2W showed itself as a great catalyst, being capable of selectively obtaining sulfones and sulfoxides with specific conditions and different solvents.

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Development and Characterization of Castor Oil-Based Biopolyurethanes: A Sustainable Alternative to Conventional Polyurethanes

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The aim of this study was to develop and characterize a biopolyurethane (BPU) based on castor oil and evaluate its potential as a sustainable alternative to conventional polyurethanes derived from fossil resources. The materials utilized were castor oil (Mw= 928 g/mol), polyol polyether (Mw= 1000 g/mol), and modified diphenylmethane-4,4' diisocyanate (MDI), supplied by Purcom. The formulations were prepared in accordance with the stoichiometric calculation and subsequently cast onto glass plates to form 1.5 mm thick membranes. The specimens were then subjected to a 14-day curing period at 25°C and 65% RH. The study compared the mechanical, surface, thermal, and morphological properties of BPU and conventional PU. The results indicated that BPU exhibited superior mechanical properties, with a tensile strength of 19.18 MPa, which was higher than that of fossil PU (12.94 MPa). In terms of performance, both membranes demonstrated comparable Shore A hardness values. The BPU had a value of 89, while the fossil PU presented a value of 86, indicating adequate surface resistance. Additionally, both membranes exhibited less than 0.1% mass loss in the abrasion resistance test, demonstrating potential for heavy traffic applications. The BPU exhibits significant hydrophobicity and minimal water absorption, which makes it a promising option for waterproofing applications. These characteristics are supported by a contact angle of 81.05° and a water absorption rate of 0.45%. Furthermore, the thermogravimetric analyses suggest that the BPU may have lower thermal stability compared to traditional PU. However, this does not necessarily affect its applicability. These findings suggest that further research and development of biopolyurethanes is necessary. By reducing the use of petroleum-derived polymers, these materials can promote sustainable and innovative solutions. Acknowledgements: The authors would like to acknowledge Purcom and the Mackenzie Research Fund (Project n° 231021).

Eco-friendly graphene nanoplatelets synthesis with syngas generation from biomass sources

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The technological concept of the patented method developed by the National Institute of Metrology, Quality and Technology (Inmetro) "Method of transform lignin into nanocarbon for application as a graphene precursor obtained by the method" is based on a nanostructured carbon material fabrication process using biomass waste [1]. With this approach, it is possible to make full use of biomass that nowadays, is treated as industrial waste, generating high-value-added by-products in the process, in addition to the possibility of generating thermal energy and biofuels in the process [2]. The aim of this project is to scale the production of lignin nanocarbon from biomass sources, such as rice husk, for a kilolab scale, generating graphene nanoplatelets, as well as syngas. The process will provide a method of producing low-cost graphene nanoplatelets (R$60/Kg) with the possibility of recovering synthesis gases during the vacuum degassing stage for the production of thermal energy and biofuels. One of the biomass to be used in this project will be rice husk so that, at the end of the transformation process, a graphene and silica nanocomposite will be obtained aiming different applications as: additive for concrete, with a 30 % reduction in specific mass and an increase of 25 % in compressive strength, and substrate for fertilizers, with a 10-fold increase in surface area. For both applications, nanocarbon will be achieved from the pre-treatment and pyrolysis of rice husk, following the methodology developed and patented by Inmetro.

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Extraction and Esterification of Fatty and Resin Acids from Tall Oil Soap: a co-product of Pulp and Paper mills

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The process of converting pulp mills into biorefineries has led to the creation of a wide range of bioproducts. This is achieved by upgrading the waste and by-products of the Kraft process. In the specific case of the softwood Kraft pulping process, fatty and resin acids (extractives) react with the white black liquor and are saponified, resulting in the production of Tall Oil Soap (TOS). From TOS, we can extract Crude Tall Oil (CTO). In this study, CTO was extracted using standard methods, resulting in residual lignin and an aqueous fraction as co-products. Subsequently, esterification reactions were conducted using microstructured acid catalysts (Beta Zeolites) with different Si/Al ratios to produce biodiesel. TOS and CTO were analyzed for viscosity, density, and elemental content. They were also characterized using various techniques such as X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDS), thermogravimetry (TG), and differential scanning calorimetry (DSC). The XRD results of dry TOS revealed the presence of crystalline sodium salts, including sodium oleate and linoleate. EDS analysis of dry TOS showed high levels of Ca, Na, O, and C, as well as trace amounts of K, S, Cl, and Si. SEM images displayed non-uniform particles dispersed on the sample holder. TG analysis indicated that TOS starts to lose mass at 100 °C and the loss is gradual up to 546 °C, with the maximum rate at 500 °C. DSC results showed exothermic and endothermic events at 85 °C and 150 °C, respectively. Finally, the use of Beta zeolites was found to be effective in converting CTO into biodiesel and potentially other renewable fuels.

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Fabrication of Micromotors from Natural Sources

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Self-propelled microscale devices exhibit considerable potential in the fields of environmental remediation, drug delivery, and sensor applications [1]. In recent decades, there has been a significant emphasis on the exploration and development of micro- and nanomotors employing biodegradable materials, driven by environmental concerns and sustainability imperatives [2-3]. In this study, we investigated the interaction between alginate (anionic polyelectrolyte) and chitosan (cationic polyelectrolyte) biopolymers to fabricate micromotors capable of propulsion in diluted hydrogen peroxide solutions. To assemble these micromotors, we employed metal wire templates of varying diameters (1, 0.2, and 0.1 mm). Two propulsion strategies were applied: manganese oxide microparticles and catalase enzyme, serving as hydrogen peroxide catalysts. Movement analysis was conducted using an optical microscope revealed that micromotors with smaller diameters exhibited greater speed compared to larger ones, suggesting that energy availability did not compensate for the larger mass. Additionally, catalase enzyme demonstrated comparable catalytic activity to manganese oxide microparticles, enhancing micromotor movement. Furthermore, owing to the biodegradability of alginate and chitosan, these micromotors exhibit gradual degradation in solution. The findings of this study highlight the potential of these micromotors for applications in biological environments.

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Lignin/cellulose polymer networks via Diels-Alder click chemistry: a sustainable approach towards dynamic thermosets

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Thermosets play a key role in modern plastic and coating industries. However, the crosslinking responsible for their valuable properties, including chemical and thermal resistance and tensile strength, also comes at the expense of their environmental footprint, as it renders them unable to undergo reprocessing or recycling. Herein, fully biobased crosslinked polymers were prepared from lignin and cellulose via Diels-Alder (DA) click reaction, while envisioning the properties of dynamic networks. Soda lignin was functionalized with furan and maleimide moieties, and cellulose nanofibers were grafted with furan groups. At first, DA reactions were carried out using different combinations of functionalized lignins and bismaleimide, forming crosslinked networks while simultaneously enabling a reversible control over thermally induced decrosslinking and recrosslinking. In contrast, thermoreversibility was not achieved when both lignin and cellulose were associated via DA-based crosslinks, even though mild reaction temperatures and lower degrees of crosslinking were considered. Ultimately, the study contributed to widening the use of furan-maleimide DA click chemistry for the preparation of sustainable materials providing insights into a green and versatile platform that may be considered in future applications.

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Phase fractionation of the SiO_2-Graphene Nanoplatelets nanocomposite obtained from rice husk pyrolysis

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Rice husk is an agricultural waste with 20% inorganic materials, predominantly silica, and 30% lignin, the second most abundant natural polymer. Crystalline carbon materials can be obtained from biomass by processing them at high temperatures [1]. This approach was used in the present work to convert aromatic carbon of lignin, present in rice husk, into graphene-like nanoplatelets (GNP). The chemical structure of rice husk was modified by pre-treatment steps as: UV irradiation, hydrothermal carbonization in an autoclave, vacuum degassing, pyrolysis, and exfoliation [2]. After completing this process, the SiO2-GNP nanocomposite material biphasic was obtained. This sample was submitted to a fractionation procedure in a water column that used a combination of flotation and sedimentation phenomena of fluid dynamics in order to separate sample's fractions according to particle and density with eventually different silica and GNPs contents in each fraction. The obtained fractions are intended to be applied as additives in cement pastes in order to improve such properties of the final concrete as compressive strength, lightness, acceleration of hydration kinetics and water impermeability. X ray diffraction analysis presented the amorphous phase of silica, in the beta quartz phase and nanostructures of silica, both associated with GNPs and graphitic carbon. The appearance of the graphitic carbon was more pronounced in the denser (bottom) fractions, while mostly nanosilica fraction floated during the fractionation process, remaining at the top of the water column. The possibility to adjust the phase composition of SiO2-GNP mixture from mostly SiO2 to mostly graphitic opens up opportunities to tune the properties of SiO2-GNP nanocomposites according to the required needs.

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Scalable methods to isolate cellulose nanofibers from sugarcane bagasse

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Cellulose nanofibers (CNFs) are sustainable advanced materials with potential applications in diverse fields. Methods to isolate them from plant-based biomass are often time, energy, and water-intensive, mainly due to lignin removal. As so, large-scale commercial utilization of CNFs is still at an early stage. Previous studies showed that TEMPO-catalyzed oxidation with sodium hypochlorite (NaClO) leads to a simultaneous removal of lignin while still chemically defibrillating cellulose [1]. Additionally, using sugarcane bagasse as the initial material enables fibers to reach nanoscale without requiring mechanical treatments [2]. Herein, we adapted the one-pot TEMPO oxidation to sugarcane bagasse using a low-energy mechanical treatment (Ultra-Turrax). High CNF yields (up to 30%) with different carboxylate contents (from 0.37 to 1.1 mmol/g) were obtained by modulating the NaClO content (10-50 mmol of NaClO/g of fibers) and the bagasse granulation. Fourier transform infrared spectroscopy (FTIR), thermogravimetric analysis (TGA), and acetyl-bromide lignin determination showed a decrease in lignin content compared to the initial biomass, with a lignin content of 6 wt.% for 50 mmol NaClO/g. Atomic force microscopy (AFM) images revealed the presence of flexible nanostructures with high aspect ratios (diameters smaller than 5 nm and lengths around 1 µm) when using NaClO contents higher than 20 mmol/g. Aqueous suspensions (0.5 wt.%) of highly charged CNFs (30 and 50 mmol/g) showed highly viscous shear-thinning power-law behavior, as observed for CNFs prepared by conventional methodologies. Overall, this study demonstrated a simplified methodology for biomass delignification and CNF extraction, with potential applicability on an industrial level.

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Study of the influence of andiroba oil (Carapa guianensis) on Poly(3-hydroxybutyrate)

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The environmental impact of synthetic polymers has led to an increased interest in the use of biodegradable materials. One such material is PHB (poly(3-hydroxybutyrate)), which is produced from natural organisms. However, its use is limited due to its low mechanical performance, high fragility, and high crystallinity [1]. The addition of additives to the PHB polymer can result in changes to its properties [2]. This study assessed the impact of andiroba oil (CAPARA GUIANENSIS AUBL.) as a natural additive on the properties of PHB. Andiroba oil is a versatile natural product composed of oleic acid glycerides and is commonly used as an additive in polymeric materials [3]. The study produced four samples, one containing pure PHB and the others with 1%, 2%, and 4% andiroba oil, respectively. The morphology of pure PHB exhibits numerous cracks and voids. The study found that the crystallinity of andiroba oil decreased as the percentage of andiroba oil increased, which is a behavior expected with the addition of a plasticizer. It is important to note that this information is based on objective measurements and not subjective evaluations. Additionally, andiroba oil affected the degradation temperature and reduced roughness and the presence of defects.

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Surface hydrophobization of pulp and cellulose nanofibrilated (CNF) using blocked diisocyanates

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Cellulose fibers and cellulose nanofibrillated (CNF) stand at the forefront of sustainable material innovation, thanks to their unique structural properties that pave the way to produce remarkable all-cellulose products. Despite their promising attributes, challenges such as high hydrophilicity and lower durability in wet conditions highlight the need for simple and cost-effective hydrophobization techniques. In this study, we explore the potential of a novel two-step hydrophobization process of pulp plates and CNF films using blocked diisocyanates. The synthesis of the hydrophobic adducts utilized phenol and linear chain alcohols, with the chain lengths varied from 3 to 18 carbons, to tailor the hydrophobic characteristics of the treated materials. The hydrophobization processes consisted of dipping and heating steps. The resultant hydrophobized plates and films were analyzed employing scanning electron microscopy (SEM), atomic force microscopy (AFM), Fourier-transform infrared spectroscopy (FT-IR), and water contact angle (WCA) measurements. These evaluations revealed that the effectiveness of the hydrophobization was intricately linked to the length of the adduct moiety and the inherent roughness of the cellulose surfaces. Notably, the treated pulp plates exhibited WCAs ranging from 109° to 144°, while the CNF films demonstrated improved water resistance with WCAs between 93° and 114°, highly above the 50° presented by the neat CNF film. This study not only sheds light on the critical role of chemical modification in enhancing the water resistance of cellulose-based materials but also opens new avenues for the development of cellulose products with enhanced durability and sustainability.

Synthesis, characterization, and evaluation of Iron-based Metal-organic frameworks as catalysts for biomass upgrading reactions

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There is an increasing interest in searching for renewable sources that can be used as alternatives to meet the demand for fossil fuels. Different high-added-value chemicals can be obtained through biomass-derived platform molecules such as furfural (FUR). Using a one-pot approach diminishes the use of solvents, enhancing the economic availability of the process.[1] Metal-organic frameworks (MOFs) are promising for catalytic reactions since they present tunable properties such as pore, volume, and acidity. Therefore, its use in catalytic transfer-hydrogenation reactions must be evaluated.[2] Hence, in this work, Fe-MIL-88B and the amino-functionalized Fe-MIL-88B-NH2 MOFs were synthesized by a hydrothermal route following a method described in the literature. The synthesis involved the use of 10 mmol of FeCl3·6H2O, ten mmol of terephthalic acid or 4-aminobenzoic acid, 8 mL of 1 M NaOH, and 50 mL of dimethylformamide (DMF) as reagents. The materials were evaluated as catalysts for furfural transfer hydrogenation reaction using isopropanol as the hydrogen donor. Their crystalline, textural, and morphological features fully characterized the materials. The catalytic studies were performed using 0.34 mmol of furfural, 1500 µL of isopropanol, and 25 mg of catalyst at 130 °C for 24 h using ACE tubes. GC-MS equipment analyzed the resultant reaction liquid, and the preliminary results (non-optimized) indicated an excellent furfural conversion (>55%) and furfuryl alcohol selectivity (>65%).

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Synthesis, characterization, and evaluation of Nb and Sn-based graphitic carbon nitride nanocatalysts in biomass valorization reactions

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Using lignocellulosic biomass as a complementary source for petroleum presents several environmental advantages and allows the obtention of renewable high-value-added products, such as ethyl lactate and solketal, that can be used in a biorefinery context. These products have been evaluated as feedstock for food, polymer, and especially petrochemical industries since they can be applied as fuel additives. Different catalysts have been proposed in the literature to obtain those products using more economical and green methods, and the development of nanocatalysts presents the advantage of higher exposure to active sites and control of the arrangement of surface atoms. [1] Graphitic Carbon Nitride (g-C3N4) has brought attention as a support for catalysts since it presents low toxicity and semiconductor properties. Its electronic structure and molecular arrangement allow the coordination of metals in its cavities, giving rise to a highly dispersed material.[2] This work presents the synthesis and characterization of Sn or Nb catalysts (1, 2, and 5%wt) based on g-C3N4 and their use in several biomass-derived compounds. TGA, XRD, FT-IT, XPS, SEM, TEM, were used to characterize the materials. The catalytic evaluation revealed high conversions of the substrates (dihydroxyacetone, glycerol, and levulinic acid) and high selectivity to value-added compounds that can be applied as green solvents, biofuels, and polymers precursors, such as solketal, ethyl lactate and γ-valerolactone.

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Valorisation of the xylan fraction of rice-husk to produce furfural or xylose syrup.

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Rice husk is an agro-industrial waste generated in rice mills during the peeling process. The husk material constitutes approximately 20% by weight of the rice grains and is characterised by a low density, high ash content and low heating value. This lignocellulosic material, due to its high content of hemicelluloses (particularly xylans), has potential application for the for value added products as xylose syrup or furfural. In previous works, the production of furfural was evaluated in one step using sulfuric acid as a catalyst. In order to improve the process, especially through the characteristics and use of the spent-solid, within the framework of a biorefinery, this work proposes two-stage process. Firstly, an hydrothermal (autohydrolysis) treatment was studied, were temperature (170–200 °C), time (30– 60minutes), and stirring conditions were evaluated to solubilise xylosaccharides from biomass. In the extracted liquid phase, different conditions were used to produced furfural, using sulphuric acid (0-1.5%), temperature (190-230°C) and time (1-30 minutes).Alternatively, in order to obtained a stream rich in xylosaccharides and minimizing the inhibitors, resin treatments were performed using two polymeric adsorption resins (Amberlite XAD-4 and Amberlite XAD 16N) and two weak anionic resins (Dowex 66 and Diaion WA 30). Resins were tried in column, at ambient temperature with a liquor: resin ratio of 3:1.Under the best autohydrolisis conditions, it is possible to extract 72.0% of the pentosans present in the starting material. Furfural production reached 60%, which is higher than values reported elsewhere using sulphuric acid. Regarding xylosaccharides syrup, Dowex 66 resin presented the most satisfactory results, with a complete reoval of insoluble lignin and HMF and high remotion yields (over 65 %) of the other common inhibitors (acetic and formic acid, acid soluble lignin and furfural).

Advancing into circularity for the life cycle of polymer blends obtained from post-consumer multilayer packaging films

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In previous works, three post-consumer multilayer films composed of 1.5-10 wt% of ethylene vinyl alcohol (EVOH) and polyamide (PA), and 77-93 wt% of high-density polyethylene (HDPE) and low-density polyethylene (LDPE) were recycled in order to produce blends with virgin HDPE and high-density polyethylene-graft-maleic anhydride (HDPE-g-MA) as compatibilizer in different formulations. As recycling has become an extremely important route for development of circular economy [1-3], it is desirable that these blends are recyclable as well. Thus, neat HDPE (control) and two compositions that exhibited the greatest performance in tensile and impact strength were selected to be recycled, 74.75HDPE/25FILM/0.25HDPE-g-MA (A) and 49HDPE/50FILM/1HDPE-g-MA (B), respectively. The blends were shredded in the knife mill and processed once more in a thermokinetic homogenizer followed by a hydraulic press (8 ton and 250 °C). After recycling, the blends properties were mostly preserved, presenting a tensile strength of 18,5 MPa (A) and 15,4 MPa (B); tensile modulus of 865 MPa (A) and 667 MPa (B); and impact strength of 5,06 kJ/m2 (A) and 12,26 kJ/m2 (B). Morphological and thermal analyses showed no difference at all between the original blends and the ones submitted to the recycling process. Therefore, the results confirmed the possibility of producing recyclable blends from post-consumer multilayer packaging with great potential for application in the furniture industry, construction and packaging industry, advancing into circularity for the life cycle of these materials.

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Analysis of the Impacts of Mercerization on the Production and Characterization of Wood Particle-Reinforced Composites

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The increasing production of lignocellulosic agro-industrial waste from the timber industry has posed significant environmental challenges. Effectively redirecting these waste materials can not only contribute to reducing improper disposal but also create a value chain around this new activity [1]. One such possibility lies in using this waste for the manufacture of medium-density fiberboard (MDF). However, to provide better satisfactory interface between matrix and reinforcement, surface treatments can be performed. Chemical surface modifications, such as mercerization, these techniques are particularly effective in removing hemicellulose, lignin, and greases from lignocellulosic materials, thereby enhancing adhesion between desired surfaces. So, this study aims to evaluate the physical, mechanical, and thermal properties of composites produced with polyurethane resin derived from castor oil, reinforced with timber waste, specifically Louro Itaúba species (Mezilaurus itauba), arranged in three formulations: natural, treated with 5% and 10% NaOH solution. The composites were produced by thermocompression and underwent flexural tests, achieving an average elastic modulus of 435.5 ± 46.4 MPa. Flame resistance did not meet established safety standards. Thickness swelling after 24h of immersion complied with norms in all treatments, and specific density remained stable without significant variations. Morphological analysis of the residues used, and fracture surface revealed degradation in treatments with higher content.

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ANALYSIS OF THE MICROBIOLOGICAL AND OPTICAL PROPERTIES OF SODIUM ALGINATE BIOPLASTIC WITH CINNAMON

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Plastics are mainly destined for landfills, and take up to centuries to degrade, which generates a huge amount of waste. Brazil is classified as the fourth largest producer of plastic waste in the world and has a low recycling rate of this material, just 1.3%. Waste derived from non-renewable sources can cause environmental pollution and public health problems. In this sense, this work aims to offer a more sustainable alternative through the production of a bioplastic made from the polymer sodium alginate plus additives from cinnamon. With a quick and simple synthesis methodology, which requires few materials, such as sodium alginate, glycerol and additives obtained from the infusion of cinnamon in water, the process involved immersing the cinnamon in water for 24 hours. To produce the biomaterial, sodium alginate (2%), glycerol (0.6%) and cinnamon solution (97.4%) were added with a concentration of 1.001 g.cm-3. The process included incorporating the polymer with glycerol, followed by adding the solution to the mixture and maintaining thermo-agitation at 65°C for 20 minutes. The reaction medium was then deposited in 15 cm x 15 cm Petri dishes and left to dry for 2 days at room temperature. After synthesis, the material was subjected to microbiological and optical analyses. The cinnamon present, known for its antimicrobial properties, presented a positive aspect when considered to evaluate its applicability in biodegradable packaging, as it demonstrated the ability to delay the growth of undesirable microorganisms. However, it can significantly affect color parameters. In conclusion, the research highlighted the viability and potential of biofilms produced from the combination of sodium alginate with cinnamon additives as a promising alternative for biodegradable packaging, suggesting its applicability in the conservation of food products.

An evaluation of the thermal properties and pyrolysis kinetics of the invasive macrophyte *Urochloa arrecta*

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The production of renewable and sustainable energy from biomass has been identified as one of the most promising sources of energy. Biomass consists of lignocellulosic materials collected from a wide variety of natural sources. Macrophytes have emerged as prominent biomasses in recent decades, particularly for their energy conversion potential and the development of carbon-based materials, given their sorption capabilities. Among the macrophytes, one of those explored is *Urochloa arrecta*, originally from Africa, considered a very aggressive and invasive weed in humid areas [1], which threatens to destroy the biodiversity of vegetation in Brazilian biomes and to damage hydroelectric power plants [2]. Therefore, this study examined the thermal degradation of *Urochloa arrecta* in an inert environment at four different heating rates, aiming to evaluate its potential as a low-cost source of bioenergy. In order to conduct the pyrolysis kinetics experiment, a thermogravimetric analyzer (TGA) was used. A TGA analysis of *Urochloa arrecta* indicated a thermal profile characteristic of lignocellulosic materials, with three main mass loss events occurring between 30°C and 800°C due to the structural degradation of hemicellulose, cellulose, and lignin. Through isoconversional methods, thermal data were used to analyze the kinetic parameters of *Urochloa arrecta* and activation energy (Ea) for different conversion ranges was determined. Based on the results, it was possible to observe higher values for conversion rates of 0.3 to 0.6 because an increase in energy was required to break the lignocellulosic chains during decomposition.

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Application of catalysts based on Sn1-XSixO2 binary oxides in biodiesel production

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The use of solid catalysts such as simple or modified oxides applied in heterogeneous catalysis to obtain biodiesel from different oilseeds, has been a frequent focus of a variety of research, since biodiesel production aims to reduce the environmental impacts caused by fossil fuels [1]. The present work aims to obtain binary oxide catalysts Sn1-xSixO2(x=0.05; 0.10; 0.15 and 0.20) obtained by the polymeric precursors method, aiming to evaluate the influence of Si on the structural modifications of SnO2 and its catalytic effectiveness for the production of biodiesel from the transesterification and simultaneous esterification reaction with soybean oil acidified, simulating residual oil. The Sn1-xSixO2 systems obtained were characterized by X-ray diffraction, Fourier transform infrared spectroscopy, particle distribution and textural analysis by nitrogen adsorption. The catalytic test products were characterized by acidity level and gas chromatography. The catalytic tests were carried out in a Par reactor, using the ethyl route under the following conditions: ethanol and oil molar ratio (15:1), 4% catalyst, 180ºC/1h. Through the XRD results it was possible to identify the crystalline planes (220), (002) that are related to the formation of the tin dioxide, as well as the respective Sn1-xSixO2 systems. Through BET analysis it was observed that the Sn0.80Si0.20O2 catalyst has a greater surface area (82.26 m^2/g) compared to the other samples studied, confirming that the presence of Si influenced the expansion of the surface area of these materials, proven by granulometric analysis that highlights the heterogeneous characteristics of particles with a micrometric profile. Although the catalytic effect of all catalysts was on average only 46.6%, with a deviation of ± 1.8%.

Keywords: Polymeric precursors, Binary oxides, Ethyl esters

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Bamboo: exploration and development of a renewable material with environmental regeneration potential

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Discussing sustainability holds paramount importance for both academia and industry, especially in light of the ongoing climate changes. Within this context, the Environmental, Social, and Governance (ESG) acronym underscores the significance of economic, environmental, and social sustainability in the goods and services management. This framework advocates for the conscious utilization of natural resources, exemplified by materials like bamboo [1]. Therefore, the main objective of this study is to advance new applications and foster the production and commercialization chains of bamboo-derived materials, leveraging their commendable mechanical properties, socio-environmental regenerative potential, short cultivation cycle, and wide range of applications [2].

In the experimental phase, different bamboo species were collected and subsequently stored for drying. Then, they underwent heat treatment under air atmosphere across a spectrum of temperatures ranging from 200°C to 800°C for four hours. The resulting heat-treated fibers undergo characterization employing techniques such as optical microscopy, electron microscopy, and thermal analysis methods including thermogravimetry (TG), differential scanning calorimetry (DSC) and dynamic mechanic termal analysis. Following this, a composite material incorporating bamboo fibers within a cementitious matrix will be produced, and its mechanical properties will be investigated. The results will be presented at the forthcoming scientific congress.

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Carbon-based photoluminescent particles as acid catalyst in glycerol acetylation

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The glycerol acetylation provides solketal (2,2-dimethyl-1,3-dioxolane-4-methanol), which has been used as a solvent, a reagent for chemicals, and a fuel additive.[1] For this reaction, an acid catalyst such as H2SO4, HCl, or H3PO4 is necessary.[2] Carbon-based photoluminescent particles (CPP) present a promising catalyst due to their surface acid sites.[3] Additionally, CPP can be obtained from glycerol. This scenario presents a significant opportunity for both CPP synthesis and the subsequent glycerol acetylation reaction. CPP was synthed from glycerol (CPP-G), glycerol with citric acid (CPP-GCA), and urea (CPP-GU) at 200 oC for 2 hours. The photoluminescent emission spectra indicated a narrow particle distribution, independent of the precursor. However, CPP-G provided lower quantum yields than CPP-GCA and CPP-GU. CPP-G and CPP-GCA presented a pH of 5, while CPP-GU showed a pH greater than 9. The glycerol acetylation reaction was performed using the CPP synthesis product. Therefore, we added acetone to CPP-G, CPP-GCA, and CPP-GU at 45 ºC for 2 hours. Conversion to solketal was observed only for CPP-G and CPP-GCA. We have obtained and used CPP as a catalyst for the conversion of glycerol to solketal by a simple method, which can provide more sustainability to a strategic industry such as biodesel, which produces a high volume of crude glycerol.

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Conversion of Eucalyptus grandis biomass into amorphous carbon via photoelectrochemical reaction

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Environmentally friendly refers to an industrial process that is considerate of the environment. One of the significant challenges in chemical engineering and biomaterials engineering is to develop methods for green carbonization to achieve sustainable production of amorphous carbon [1–2]. The clean production of amorphous plant carbon contributes to the decarbonization of the planet. This work aims to develop a green production method to obtain amorphous carbon at temperatures below 180 °C. The photoelectrochemical reaction method via oxidation-reduction of lignocellulosic biomass was adapted from Santos (2017A)[3] and Santos (2017B)[4]. The structure of the eucalyptus extract and products was analyzed by X-ray diffraction. It was found that the photoelectrochemical reaction of eucalyptus extract produces a powdery solid, black in color, with a molten carbon odor and a homogeneous appearance when viewed freely. The product is comparable to charcoal. It is concluded that the photoelectrochemical reaction of Eucalyptus grandis extract produces amorphous vegetable carbon at low temperatures (25 °C).

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Copper Single Atoms on Titanium Dioxide for Selective Oxidation of Benzene to Phenol

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Single-atom catalysis has been gaining attention from the scientific community due to its unique ability to resemble homogeneous complexes on solid supports and to maximize metal utilization.[1] Recently, benzene oxidation using single atoms (SAs) has been studied with carbon-based supports such as carbon nitrides or N-doped carbons.[2] Titanium dioxide (TiO2) is one of most applied catalysts in the world, but few reports are devoted to stabilize single-atoms (SAs) on its 3D structure. Herein, we demonstrate that copper single-atoms stabilized on TiO2 (3D materials) can efficiently promote the catalytic oxidation of benzene to phenol, with high phenol yields (55%). In addition, our data suggest that Cu SAs are more active than supported larger particles such as copper oxides. Moreover, we verified that Cu-TiO2 does not produce CO2 as side-product, while other Cu SAs supported on carbon-based materials (carbon nitrides or N-doped carbons) display low phenol yields, as well as higher CO2 amounts. This study expands the applicability of TiO2 as suitable support SAs for selective oxidation reactions.

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Development of materials for CO2 capture from biomass of aquatic macrophytes

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The few technologies for Carbon Capture, Utilization, and Storage-CCUS used today are technically complex and restricted, mainly due to high material costs and somewhat limited storage capacity, directly affecting the CAPEX and OPEX of CO2-emitting institutions. The use of renewable materials during the development of CCUS technologies is aligned with the Sustainable Development Goals and the desired concepts in Environment, Social & Governance-ESG, contributing to sustainable transition by producing more sustainable materials. Macrophytes are plants that grow in aquatic environments, developing constantly or periodically in aquatic ecosystems, playing a crucial role as a food source for various aquatic and terrestrial species, as well as stabilizing sediments, helping to mitigate the effects of waves and water flow. However, under unfavorable conditions, such as in regions with high organic matter content or pollution in general, macrophytes proliferate rapidly, becoming problems for the aquatic ecosystem and the well-being of riparian populations. Therefore, the development of innovative, low-cost, and sustainable materials capable of CO2 capture is of paramount importance for the environment and the entire global production chain, requiring the selection of suitable raw materials and parameters as well as the optimization of operating conditions for different gas compositions. In this context, the present work aims to present the results of the use of macrophytes for the production of activated biochars, aiming to evaluate their CO2 capture capacity. The biochars were characterized for their composition to evaluate the functional groups present, and their morphology was assessed for determination of surface area, volume, and pore diameter, and evaluated for CO2 adsorption capacity under industrial gas, aiming at their application as materials developed for CO2 capture.

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DYES ADSORPTION BY NANOMODIFIED PLANT-BASED BIOSORBENT

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Among the techniques used to remove dyes from water, biosorption is a promising approach based on the adsorption of chemical substances using biosorbents. A nanocomposite (LR-NP), prepared from hydroponic lettuce roots biomass (LR) and magnetite nanoparticles (NP), was used to remove methylene blue (MB) and Congo red (CR) dyes from water. The maximum MB and CR adsorption was reached at pH 6.0 and 3.0, respectively, and 60 min contact between adsorbate and adsorbent. In the kinetics studies, the pseudo-second order equations exhibited the best fit according to r2, both for CR (LR = 0.997 and LR-NP = 0.996) and MB (LR = 0.995 and LR-NP = 0.962). The experimental sorption capacity (SCexp) found for both dyes were 305.75 10.9 mg/g (LR), 260.50 17.57 mg/g (LR-NP) and 188.89 3.94 mg/g (NP), and 173.66 0.86 mg/g (LR), 167.50 3.62 mg/g (LR-NP) and 20.88 1.43 mg/g (NP) for CR and MB, respectively. Six isotherm models (Langmuir, Freundlich, Sips, Temkin, DR, and Hill) were used to evaluate the best fit for the experimental data. The biosorbents were characterized by Fourier Transform Infrared Spectroscopy (FTIR), X-ray diffractometry (XRD), and scanning electron microscopy (SEM) to investigate their morphology and chemical composition. The pH at the point of zero charge, 5.96 and 6.50 for LR and LR-NP, respectively, allowed to assess the materials' surface charge [1].

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Eco-Friendly Photodegradation of Direct Red 80 Dye Mediated by Biochar Decorated with Cobalt Ferrite

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Cobalt ferrites are highly catalytic, structurally stable, and magnetic. However, their aggregation reduces their catalytic activity[1] The use of supported nanomaterials with biochars is an alternative to avoid this aggregation, increasing the surface area and reactivity[2]. In this work, a biochar (BC) decorated with cobalt ferrite (BC/CoFe2O4) was synthed using the co-precipitation method. The material was characterized by different techniques and applied to remove Direct Red 80 (DR80) dye. BC and BC/CoFe2O4 presented moisture content of 5.8 and 8.4%, ash content of 24.1 and 30.0%, volatile content of 75.5 and 69.5%, respectively. The H/C ratio was approximately 0.5, and the O/C ratio was around 0.2 for both materials. The materials showed thermal stability observed by TGA. BC presented peaks related to quartz, dolomite, and calcite, while BC/CoFe2O4 exhibited characteristic peaks of CoFe2O4. The selected area electron diffraction (SAED) pattern of BC/CoFe2O4 showed crystalline planes of CoFe2O4. Oxygen (74.97%), cobalt (8.86%), and iron (16.17%) elements were detected in BC/CoFe2O4 by energy dispersive analysis (EDS), which was later confirmed by ICP-OES Fe. The materials were applied as a photocatalyst in the degradation of DR80. A removal efficiency of approximately 100% was achieved within 180 minutes under the following conditions: BC/CoFe2O4 dose of 1 g L−1, initial DR80 concentration of 25 mg L−1, pH 3, temperature of 30 ± 5 °C, and exposure to UV light. The species responsible for degradation were identified as photogenerated holes (h+) and O2•−. The material can be reused for up to two cycles without significant loss of efficiency.

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Evaluation of cupuaçu shell as an organic filler in thermoplastics: preliminary studies

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In order to reduce the environmental impacts caused by pollution and inefficient management of solid wastes derived from petroleum-based materials, many researchers have applied the use of vegetal residues in polymers, due to their low cost and high availability, which can also enhance specific properties of the material [1]. Cupuaçu (Theobroma Grandiflorum) shell, commonly discarded by frozen pulp industries, has significant technological potential [2, 3]. Therefore, the aim of this work is to investigate the potential of cupuaçu shell as a filler in thermoplastics. Initially, the shell was dried at 100 °C for 7 days and then ground in a ball mill until passed through a 200-mesh sieve. The chemical composition (ashes, lignin and extracts) was determined. The ashes were characterized using X-Ray Fluorescence (XRF). The residue was characterized through Scanning Electron Microscopy (SEM), Thermogravimetry (TGA) and Differential Scanning Calorimetry (DSC). The low contents of extracts (4.51%) and ashes (1.94%) suggest that the residue can be suitable as reinforcement filler in a polymeric matrix. XRF analysis of ashes found high potassium content in the residue. TGA and DSC present similar events related to water loss and degradation of its major components (lignin, cellulose and hemicellulose). SEM images revealed that the residue has varied particle s and an irregular morphology, which can increase the contact area with polymer.

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Evaluation of the use of post-consumer diatomite for the development of high-density polyethylene (HDPE)/diatomite composites

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Diatomaceous earth or diatomite is an amorphous sediment, silica-based, originating from frustules or shells of unicellular plant organisms, and its color can vary between gray and white. Due to its porous structure and unique properties, diatomite is frequently used in the beer filtration and clarification process in the brewing industries. Reverse logistics aims to plan, operate, and control the return of industrial waste to the production cycle through reverse distribution channels, adding value to the product, primarily focusing on recycling, disposal, and reprocessing. This has motivated the search for viable alternatives for the disposal of industrial waste, especially solid waste, which occupies significant physical space, such as diatomite used by breweries. In this work, post-consumer diatomite was dried by two methods: oven drying and spray-drying. Afterwards, high-density polyethylene (HDPE)/ post-consumer diatomite composites were prepared in a high-speed mixer rotation at 3000 rpm followed by hot pressing. The composites were prepared with the addition of 5 wt% diatomite. The test specimens were evaluated by tensile test, Izod impact strength, and Shore D hardness. In the mechanical tests, it was noted that the addition of diatomite contributed to an increase in tensile strength and hardness. Regarding the impact test, it was observed that both compositions did not fracture, meaning that the addition of the filler did not modify the impact properties. Thus, it is concluded that the addition of post-consumer diatomite contributed to improvements in the mechanical properties and can be an alternative to reduce the amount of diatomite disposal.

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Evaluation of the use of swine liquid waste as organic fertilizer: a cleaner approach using FTIR spectroscopy and chemometrics

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Swine liquid waste (SLW) is an effective option for crop fertilization, as it is rich in organic matter (OM) and essential nutrients for plants. When properly applied, it can replace mineral fertilizers. Though OM can rapidly mineralize due to heightened microbial activity, the organic carbon (OC) within it undergoes a gradual stabilization process on mineral surfaces or microaggregates. Soil OC stabilizes aggregates, improving soil porosity and structure, and thus reducing erosion. Therefore, assessing OC levels in SLW-fertilized soils is essential. The study evaluated FTIR as an eco-friendly method, along with chemometrics, to determine OC in cerrado soils with varied crops, fertilized with SLW at different times. PLS regression served as a multivariate calibration approach, using MATLAB software, assessing models using coefficient of determination R^2, root mean square error of calibration (RMSEC) and cross-validation (RMSEV). The Walkey-Black method [2] was used to obtain reference values, and OC contents ranged from 9 to 54 g kg-^{1}. The calibration and validation R^2 values were 0.892 and 0.751, respectively, indicating good correlation. The RMSEC and RMSEV were 4.48 and 6.82 g kg^{-1}, respectively, considered adequate as they are lower than the lowest carbon concentration in the samples (<9 g kg^{-1}). The characteristics of FTIR together with chemometric models (PLS) proved to be a powerful tool for obtaining information about soil fertilized with SLW quickly and with minimal waste generation. The development of these greener technologies could strongly affect the sustainability of the agricultural and swine sectors.

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HYDROCHAR DERIVED FROM BABASSU (*Attalea speciosa*): SYNTHESIS AND CHARACTERIZATION

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Wastewater produced from industrial practices leads to water contamination. Adsorption is among the most used methods to remove contaminants from wastewater, due to the many limitations of conventional approaches, such as inefficiency and complex purification processes. In this sense, the objective of this work is to develop a hydrochar derived from babassu endocarp that has stable chemical properties, and serves as a cheap and accessible carbon-based material. An accessible raw material like this agricultural waste makes the babassu fruit a potential candidate in removing contaminants from wastewater by synthesizing cost-effective adsorbents like hydrochar from babassu coconut endocarp. Babassu coconut fruits were collected, washed and separated into various parts, the endocarp was sieved to obtain a particle of 63 nm for the hydrochar synthesis. After, the sieved biomass underwent hydrothermal treatment in a temperature range of 120ºC to 240ºC and a fixed time of 180 min. From X-ray diffraction and Fourier Transform Infrared Spectroscopy analyses, the hydrochar was amorphous and presented O-H and C=O functional groups. The amorphous nature was associated with the presence of amylose-lipid complexes and the functional groups were found to increase adsorptive capacity. The reuse of an agriculture waste as a raw material for hydrochar aimed at water remediation promotes sustainability and aligns with the sustainable development goals (SDG 06, 07, 12 and 13) of the UN.

Incorporation of polyaniline into ultrafiltration membranes: a study on fouling mitigation

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Membranes have stood out as filtration technology because they have exceptional characteristics, but the fouling process is still a challenging issue [1]. Knowing that fouling agents have negative charges, inserting a material with conductive characteristics into the membrane can result in electrostatic repulsion field, which ultimately reduces fouling formation [2]. In this investigation, polyaniline (Pani) was obtained by aniline polymerization. The polyethersulfone (PES) membranes were prepared using the phase inversion method and the relationship between Pani concentration and antifouling effects was studied. The samples s were characterized by UV-Vis spectroscopy, scanning electron microscopy (SEM), and fouling mitigation assays. Pani structural characterization by UV-Vis showed a maximum absorption at 760 nm, being this peak correlated with the delocalized polarons formation, confirming that the Pani is in conductive oxidation state. The spectra of the Pani-doped membranes show the shift of these peaks to 600 nm, demonstrating the presence of a polymer in conductive form. SEM images indicated the appearance of pores on the surface of the membrane in addition to having different average diameters. In the transverse SEM images of the membranes, the elongation of these pores is seen in the finger shape, characteristic of assymetric membranes Preliminary fouling mitigation tests indicate that for any incorporated concentration of Pani into the PES membranes, the antifouling capacity was enhanced when compared to the pristine PES membranes. This result suggests that the PES-Pani membranes can be used in membrane processes, such as drinking water and wastewater treatment, where fouling is an issu to be overcome.

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Investigation of the catalytic activity of $Sr_{1-x}K_xTiO_{3-d}$ in the transesterification reaction for ethyl esters production

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This study presents the results of an investigation into the catalytic activity of the compound $Sr_{1-x}K_xTiO_{3-d}$ in the transesterification reaction between soybean oil and ethanol for the formation of ethyl esters, intended for potential use as biodiesel. The $Sr_{1-x}K_xTiO_{3-d}$ compounds, where x varies from 0 to 0.5, were synthed via the Pechini method and thermally treated at 850°C for 2 hours. Catalytic tests were conducted in a Parr reactor, using a stoichiometric ratio of soybean oil to ethanol of 1:18, a reaction temperature of 80°C, for 9 hours with 15% by mass of catalyst relative to the mass of soybean oil. X-ray diffraction (XRD) results showed the formation of the $SrTiO_3$ phase, with a perovskite structure (JCPDS 35-0734), with a decrease in the intensity of diffraction peaks as a function of the partial substitution of Sr^{2+} cations by K^+. The specific surface area, obtained by BET, showed slightly higher values for the materials containing potassium in the structure compared to the pure material. TPD-NH_3 and TPD-CO_2 techniques showed that the materials exhibit active sites with acidic and basic characteristics, as well as an increase in acid and base strength as a function of potassium substitution in the $Sr_{1-x}K_xTiO_{3-d}$ structure. The reaction yield was monitored by GC-FID and H-NMR. The results showed an increase in the reaction yield as a function of the amount of potassium present in the structure, indicating that the acidic and basic properties strongly influence the catalytic activity. The highest reaction yield was obtained with the catalyst $Sr_{0.5}K_{0.5}TiO_{3-d}$, with 95% conversion of soybean oil and ethanol into ethyl esters and glycerol as a byproduct.

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Photocatalytic properties of Biochar@Nb2O5-Nanoneedles composites and their application for degradation of methylene bue

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The production and application of biochar to prepare composites for photocatalytic (PC) systems had recently gained attention and also become a key factor for the treatment of industrial waste. From the optimization of materials with metal oxides it also enhances the degradation of chemical compounds. Because of the strong chemical stability between oxidative composites and functional groups on the biochar surface, it was possible to capture and immobilize various pollutants, promoting their degradation under UV radiation [1,2,3]. In our work, we obtained the biochar composites through the one-step thermochemical synthesis of sugarcane biomass, urea and niobium compounds. From XRD characterization it were identified the peaks attributed to Nb2O5–orthorhombic phase (JCPDS card n° 2710-03) and a broad region observed between ~22–33° indexed as C<002> diffraction peak related to an amorphous carbon structure with randomly oriented aromatic sheets. The SEM reveals morphology as nanoneedles (diameter width of ~30–80 nm) well-distributed on the biochar surface. From Raman Spectroscopy it were clearly identified the characteristics D- and G-bands of carbon materials at ~1340 cm^{-1} and 1600 cm^{-1}, respectively. Through photodiscoloration by UV radiation of MB aqueous solution (5 mg.L-1) it was achieved efficiency degradation over than 80% after 3 hours of experiment.

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MAGNETIC NANOMODIFIED BIOMASS FOR CATIONIC AND ANIONIC DYES BIOSORPTION

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The production of dyed fabric generates high amounts of wastewater containing pollutants as reactive dyes, the most common textile dyes employed in industries. Biosorption emerges as a promising and low-cost alternative for treating wastewater contaminated with dyes using natural adsorbents, such as sugarcane bagasse. This work proposes the production of a nanomodified biosorbent (SB-NP) prepared from sugarcane bagasse (SB) and magnetite (Fe3O4) to remove cationic (methylene blue) and anionic (Congo red) dyes in water. Ferromagnetic nanoparticles and the nanocomposite were synthed using the coprecipitation method, employing FeCl2 and FeCl3 to produce Fe3O4 and SB-NP [1]. The efficiency of removing dyes at different pH and increasing contact times was evaluated using 10 mg of SB or SB-NP and 10 mL of dye solution (25 mg/L). The dyes were determined by UV-Vis spectrometry and all assays were performed in triplicate. The results showed that SB and SB-NP's ideal pH for removing the dyes was between 5.8 and 6.0. Compared to SB-NP, SB exhibited slightly better dye removal capacity, possibly due to its larger surface area and more active functional groups. The adsorption of the dyes reached equilibrium around 30 minutes for both SB and SB-NP. The dyes sorption capacity (SCexp) was 125.06±5.08 and 123.42±4.82 mg/g (CR), and 27.30±0.11 and 24.61±0.16 mg/g (MB), respectively, for SB and SB-NP. Eight theoretical isotherm models were fitted to the experimental data.

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New $Sr_{1-x}K_xZrO_{3-d}$ Type Catalysts for the Synthesis of Ethyl Esters from Soybean Oil

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Zirconates have been studied as heterogeneous catalysts for the synthesis of methyl esters. However, the effects of substituting Sr^{2+} cations with K^+ in the structure of $Sr_{1-x}K_xZrO_{3-d}$ have never been reported, nor has the study of their catalytic activity for the production of ethyl esters. In this sense, this work aims to study and evaluate these effects on the reaction yield of transesterification between soybean oil and ethanol, for the preparation of ethyl esters. $Sr_{1-x}K_xZrO_{3-d}$ ceramic powders, with x varying up to 50 mol%, were synthed by the Pechini method and calcined at a temperature of 850°C for 2 hours. The reactions catalyzed by the zirconates were studied in a Parr reactor, using the following experimental conditions: temperature of 80°C, reaction time of 9 hours, 15% by mass of catalyst relative to the mass of soybean oil, and a molar ratio of 1:18 of soybean oil to ethanol. X-ray diffraction (XRD) results showed the formation of the $SrZrO_3$ phase, with orthorhombic symmetry (JCPDS 10-268). From 30 mol% of K in the structure, peaks related to the tetragonal symmetry phase of $SrZrO_3$ (JCPDS 48-1049) were observed. An increase in the surface area was also observed as a function of the potassium content. TPD-NH_3 and TPD-CO_2 techniques showed that the material exhibits amphoteric characteristics, however, basic strength is superior to acidic strength. Reaction yields, calculated by GC-FID and H-NMR, showed a strong dependence on acid-base properties, wherein potassium substitution contributed to increasing catalytic activity, which may also be related to tetragonal symmetry. The best reaction yield was observed for the $Sr_{0.5}K_{0.5}ZrO_{3-d}$ catalyst, with 93% conversion of the reactants to ethyl esters.

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Optimization and economic evaluation of alginate extraction from the brown seaweed *Dictyota mertensii* using the response surface methodology.

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With the depletion of natural resources, advanced environmental degradation and the evolution of climate change, producing sustainable science has become an obligation in the face of the challenge. Exploring new raw material possibilities improves the unlocking of the bio-based and sustainable economy, providing advances and perspectives in the creation of value from discoveries. Marine macroalgae are emerging as a sustainable raw material with antioxidant, antimicrobial, non-toxic, biodegradable and biocompatible characteristics. This work extracts alginate from *Dictyota mertensii*, a brown seaweed found on the north coast of northeastern Brazil. A Central Composite Design (CCD) associated with Response Surface Methodology (RSM) was used to optimize the extraction process of different biopolymer fractions present in Dictyota mertensii, depending on the factors time, temperature and Na_2CO_3 concentration. The extraction yield and the economic parameters of the extraction are evaluated and the alginate is characterized. Characterization is carried out in terms of its intrinsic viscosity, viscosimetric molar mass and color. The maximum extraction yield was 29.28±0.02%. The economic evaluation considered the consumption of electricity by the equipment, the consumption of reagents, logistics and labor. The lowest price per gram of alginate obtained was R$ 3.82.

Optimizing Fuel Gas Recovery from Plasma-Treated Sewage Sludge: A Study on Operational Parameters

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The effects of operational parameters on fuel gas production from DC-transferred arc plasma processing of sewage sludge were investigated. The parameters explored were the exhaustion speed, the feedstock supply rate, the reactor chamber operation temperature, and the plasma applied power. The sludge was submitted to the preliminary chemical investigation as follows: Proximate analyses reported relatively high net calorific values of 14.99 MJ/kg and 13.97 MJ/kg for upper and lower heating values, respectively, which are desirable features for fuel gas as a recovered product. X-ray fluorescent spectroscopy results reveal the main composition elements in sludge ashes: Si, P, Al, Ca, and Fe. In the sludge Fourier-transform infrared spectroscopy spectrum, the primary organic bonds, in the range of 4000 – 1200 cm^{-1}, are associated with alkanes and amides, while the fingerprint region, from 1200 – 400 cm^{-1}, is populated with P, Si, Ca, Al, and Fe oxides bonds absorptions. Preliminary results of gas analyses from plasma processing show that for fixed sample mass, the fuel gas production is limited to a few minutes, and the syngas ($CO + H_2$) volumetric fraction and combustion heat are highly dependent on exhaust speed. Continuous feedstock supply stabilizes the gas components (CO_2, CO, O_2, CH_4, H_2, and N_2) volumetric fractions and provides feasible control over gas production under various conditions of exhaustion speed and the reactor's chamber operational temperature. For instance, at 20 kW applied power conditions and the reactor's chamber at 200 °C, the optimal parameters found were a constant feedstock supply of 300 g/min and 36 m^3/min exhaustion speed. The volumetric fraction of syngas was 92 %, with HHV and LHV of 12.9 kJ/m^3 and 11.8 kJ/m^3, respectively. The findings contribute to the worldwide research of wastewater treatment solutions and, more specifically, to developing a consistent methodology for fuel gas production from thermal plasma-treated sludge.

Potential of the Aquatic Macrophyte Egeria najas in natura in the Adsorption of Methylene Blue Dye in Aqueous Solution

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Macrophytes are found from marshes to submerged environments. They play a physical role in sediment stability. However, under adverse conditions, they can cause issues such as accumulation on the surface of water bodies, due to their rapid proliferation [1]. Egeria najas can serve as a renewable source of adsorbent material for removing specific molecules, such as methylene blue (MB) present in dyes [2]. Therefore, this study aimed to assess the potential of Egeria najas in natura for adsorbing MB dye in aqueous solution. The macrophyte was prepared and characterized using elemental analysis techniques (CHNS-O), Fourier-transform infrared spectroscopy (FTIR), and scanning electron microscopy (SEM). For the adsorptive potential assessment, 0.1 g of the in natura adsorbent remained in contact with the MB adsorbate at a concentration of 100 mg/L for durations ranging from 1 to 1440 minutes. Readings were taken on a UV-Vis spectrophotometer at a wavelength of 665.0 nm. The carbon and oxygen contents were approximately 14% and 11%, respectively. FTIR revealed bands corresponding to O-H, aliphatic C-H, C=C, C=O, and C-O stretching vibrations of aromatic rings. The morphology showed irregular heterogeneity with various sizes. Egeria najas exhibited approximately 86% adsorption of MB in 1440 minutes. However, approximately 73% removal was observed in 1 minute. Based on the results obtained, it is feasible to use Egeria najas in natura as an adsorbent for MB removal.

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Production of low-density polyethylene (LDPE) and thermoplastic starch (TPS) blends without and with the addition of compatibilizing agent for application in the packaging sector

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In recent years, the consumption of polymeric materials has increased worldwide, especially during the period of social isolation caused by the Covid-19 pandemic, due to the increase in delivery consumption. In this study, partially biodegradable blends of low-density polyethylene (LDPE) and thermoplastic starch (TPS) (LDPE/TPS) were processed through the extrusion process, with TPS produced by the same process using a 70:30 ratio (w/w) of corn starch and glycerol [1,2]. Blends were produced without and with the addition of a compatibilizing agent, using LDPE grafted with maleic anhydride (LLDPE-g-MA). In these blends, the amount of TPS varied from 10 to 70%(w/w), while LLDPE-g-MA remained fixed at 3% (w/w). Mechanical impact resistance testing, wettability, thermogravimetric analysis, and in some compositions, scanning electron microscopy (SEM) were performed. In general, the higher the concentration of TPS in the material composition, the lower its hydrophobicity. Thus, samples with 10 and 70% TPS obtained contact angles of 89.07 and 69.33°, respectively. The increase in LDPE concentration in the blends led to an increase in impact resistance. Samples with 30 and 50% TPS (w/w) showed impact resistance of 77.24 and 35.72 J/m respectively. The addition of the compatibilizing agent proved indispensable for processability in blends with TPS content above 60% (w/w), resulting in the reduction of TPS domains as observed in the microstructure of all analyzed compositions. In the thermogravimetric analysis, the degradation of each blend component was observed at well-defined plateaus in all compositions.

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Recycling of post-consumer multilayer packaging films by blending process as a sustainable and promising route

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Environmental pollution associated to solid waste accumulation have urged recycling, especially of polymer materials, such as multilayer packaging, which has a challenging recycling due to distinct materials of each layer in their composition [1-3]. Thus, multilayer films for packaging were applied as secondary feedstock for production of high-density polyethylene (HDPE) blends. Three post-consumer multilayer films composed of 1.5-10 wt% of ethylene vinyl alcohol (EVOH) and polyamide (PA), and 77-93 wt% of HDPE and low-density polyethylene (LDPE) were shredded in a knife mill and processed with HDPE in the fractions of 0:100, 25:75, 35:65 and 50:50, with 0 wt%, 0.25 wt% and 1 wt% of high-density polyethylene-graft-maleic anhydride (HDPE-g-MA) as compatibilizer, in a thermokinetic homogenizer followed by a hydraulic press (8 ton and 250 °C). Morphology analysis showed that the compatibilizer enhanced the adhesion of the packages in the HDPE matrix. However, low concentrations of EVOH and PA did not change significantly the blends properties, which makes the recycling of even higher concentrations of packaging feasible. The blend 74.75HDPE/25FILM/0.25HDPE-g-MA obtained the highest tensile strength (19.3 MPa) and modulus (921 MPa), showing great potential for application in furniture industry and construction. On other hand, the blend 49HDPE/50FILM/1HDPE-g-MA exhibited the highest impact strength (12.39 kJ/m), representing a good material for packaging industry. Therefore, their good properties proved the recycling of the multilayer films to be sustainably and technically advantageous.

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Recycling of Tags and Labels Residues with BOPP into Composites for Commercial Use

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In this study, an alternative method of recycling the residue of printing industries, consisting of labels and stickers (parings) containing biaxially oriented polypropylene (BOPP) and polyurethane based-glue, with the addition of recycled BOPP was proposed and studied. This material is hard to process due to the large amount of glue on the residue [1]. This alternative process consists of mixing both materials at different rates before being extruded in order to create composites of varying weight percentages of parings to BOPP, with samples created with 10% weight ratio of parings. The samples were analyzed in order to determine their mechanical properties with the use of tensile, three point flexural, Shore D hardness, density, water absorption and impact tests [2]. The results ascertained the influence of the recycled material (parings) on the composite's properties, resulting in significant increase in rupture strength, a slight decrease in yield strength, hardness and elastic modulus, and a significant reduction in maximum deformation before rupture. The proposed process showed that a new method can be employed in the recycling of tags and labels residue, and allows the study of the potential applications for the resulting composites.

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Removal of iron from water using biochars derived from banana peel obtained through a hydrothermal process.

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One of the essential parameters for controlling water quality is the concentration of iron and manganese, which can impart undesirable color and odor to the water. Ministerial Ordinance No. 888 from the Ministry of Health establishes a maximum permitted concentration of iron after treatment of 0.3 mg L-1. The removal of iron from aqueous systems can be achieved through adsorptive processes utilizing biochars derived from residual biomass. The production of materials from waste is aligned with the United Nations' sustainable development goals. Thus, this study aimed to remove iron from water using biochars obtained from banana peels and produced by a hydrothermal process. A factorial design with a central point was used to screen the main variables that could be significant in the process, such as (1) activation agent (H_3PO_4 or NaOH), (2) temperature (100 and 200 °C) and (3) residence time (8 and 14 hours). The central point (CP) was carried out without an activation agent, using only water in the process, at 150 °C, and 11 hours. The biochars were characterized by FT-IR, which showed characteristic bands of aromatic compounds, hydroxyl, and carboxylic groups. The pH at the Zero Charge Point for the different biochars ranged from 4.39 to 6.00. Adsorption assays were conducted using an Fe at 10 mg L-1, without pH adjustment, at 25 °C, for 24 hours. The response used in the design was the removal of total Fe. None of the variables were significant within the studied range, resulting in removals between 27% and 91%. The best performance was obtained for the biochar obtained at the CP. Thus, it is observed that adsorption by this biochar stands out as a promising and environmentally friendly method for removing iron from water. The authors would like to thank CNPq (Processes: 312400/2021-7 and 405828/2022-5), as well as FAPEMIG (APQ-01275-18 and RED-00144-22).

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Removal of manganese from water using biochars derived from orange peel obtained through a hydrothermal process.

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Manganese can compromise water quality at elevated concentrations, leading to undesirable taste, odor, and color. Therefore, Ministerial Ordinance No. 888 from the Ministry of Health establishes a maximum permitted value of manganese after treatment of 0.1 mg L-1. Several treatment methods have been proposed to remove metals from natural waters, with adsorption being prominent among them. Among adsorbents, biochars stand out due to their high specific surface area, which contains pores of various sizes. Biochars from agricultural waste has attracted interest due to their low cost and high efficiency, contributing to environmental sustainability and the circular economy. Among these residues, orange peel stands out as it is widely consumed worldwide, yet it generates a significant volume of organic waste. Thus, this work aims to remove manganese from water using biochars obtained from orange peel and pulp, produced by a hydrothermal process. A factorial design with a central point was employed, where three variables were evaluated: temperature (100 and 200 °C), residence time (8 and 14 hours), and activation agent (H_3PO_4 or NaOH). The physical-chemical, textural, morphological, and structural properties of the biochars were characterized. FT-IR showed characteristic bands attributed to O-H, C-H, and C=O bonds in the biochars. The biochars demonstrated greater thermal stability compared to biomass, as evaluated by Thermogravimetric Analysis (TGA). The effectiveness of the biochars was also evaluated in removing manganese from water over 24 hours, with orbital agitation at 25 °C, achieving removals close to 70% for some of the biochars tested. These results indicate promising efficacy in manganese removal. The authors would like to thank CNPq (Processes: 312400/2021-7 and 405828/2022-5), as well as FAPEMIG (APQ-01275-18 and RED-00144-22).

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Structural morphology and properties of chitosan from shrimp shell and blue crab waste

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The shells of crustaceans are an abundant waste from the fishing industry. They are rich in chitin, the precursor of chitosan. The use of these wastes reduces the environmental impact caused by their accumulation in places where they are generated or stored. Chitosan has properties that make it a biomaterial with versatile applications, such as in the food industry, agriculture, cosmetics, biomedicine, and pharmaceutical industries [1]. This aimed to extract chitosan from shrimp shells and blue crab waste, both derived from marine environment, to compare the structural morphology and physicochemical properties to investigate their suitable areas of application. Chitin was extracted from ground shrimp shells of Litopenaeus vannamei and crab waste of Callinectes danae by demineralization with hydrogen chloride solution (HCl 0.55 mol/L) and deproteinization using sodium hydroxide solution (NaOH 0.3 mol/L). The chitin was deacetylated in sodium hydroxide solution (NaOH 60% w/v) at 120 °C. The yield of chitosan was 18% and 8% for marine shrimp shells and blue crab waste, respectively. The degree of deacetylation (DD) and viscosimetric molar mass (Mv) of chitosan from shrimp shells was 90% and 115 kDa. The DD and Mv of chitosan from blue crab waste was 87% and 180 kDa. Porous and fibrous structures were observed for both chitosan samples. The high DD of chitosan from shrimp shells makes it suitable as a porous foam for sustainable filter elements while the high Mv of chitosan from blue crab waste suggests its use as a membrane for proton exchange membrane fuel cell. Both applications are under development in our research group. This study provides a sustainable solution to convert marine waste into new biodegradable products.

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Studying the application of carbon quantum dots obtained from pumpkin seed to mitigate corrosion.

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The industry constantly suffers from corrosion-related problems. In the oil industry, several media are considered critical due to their aggressiveness, such as acidic solutions or even waters with high salinity, saturated or not with CO2 [1]. Carbon quantum dots (CQDs) have shown promise in mitigating corrosion due to their characteristics such as high solubility and high degree of functionalization and doping, which, in the case of corrosion inhibitors, increases the adsorption capacity and, consequently, passivation of the substrate. In this work, CQDs were produced from pumpkin seeds through hydrothermal synthesis, and mass loss tests evaluated their inhibitory efficiency (IE) in the following media: HCl 15 %, HCl 1 mol L–1, and 170000 ppm Cl– saturated with CO2. DLS, FTIR, and XPS characterized the CQDs produced, and the results proved that the CQDs were successfully obtained, with a distribution smaller than 10 nm and with the presence of elements such as O, N, and S, which indicates that during the synthesis, self-doping was guaranteed. In the mass loss corrosion tests, using 5 ppm of Pumpkin-CQDs, the inhibitor showed IE of 97.2 ± 0.95, 90.4 ± 0.94, and 73.7 ± 0.57 for the media HCl 15%, HCl 1 mol L–1, and 170000 ppm Cl– saturated with CO2, respectively. In addition to the advantage of obtaining CQDs from waste, which is advantageous not only for the environment but also for industry, the CQDs produced showed good efficiency in all the media tested. Using a functional inhibitor in various media is extremely important when working in conditions susceptible to multiple corrosive media or where contamination is possible. Using CQDs obtained from pumpkin seeds by hydrothermal synthesis appears promising. Note that only 5 ppm was used, which is very low content; its saturation concentration has not yet been evaluated so that the efficiency could be even greater.

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STUDY OF SUGARCANE BIOCHAR SYNTHESIS TOWARDS A RECYCLABLE WASTE APPLICATION

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Sugarcane bagasse is a major agro-industrial subproduct in Brazil, being produced in huge amounts annually. Effective management of this waste plays a crucial role in mitigating various forms of pollution through biomass renewal in value-added products such as biochar, biogas, and biofuel. Biochar (BC) has a wide range of applications such as pollutant removal, energy storage, soil amendment for composting, carbon sequestration, catalysts, and in wastewater treatment [1] with the advantage of low-cost precursor material. In this study, the aim was to develop devolatilization of this residue investigating BC formation. A detailed approach was made about the conversion of lignocellulosic carbon-containing sugarcane bagasse, by using slow pyrolysis method, into a material having high conductivity in order to apply in carbon pastes electrodes (CPEs). Carbonization of biomass was carried out in a tubular furnace with inert argon atmosphere at 600, 800 and 1000 °C, 2h retention time and mean residence time (MRT) of 50min. After the synthesis, the obtained carbon-based powder was characterized by Raman spectroscopy and X-ray diffraction (XRD) to evaluate the crystallinity and amorphous phases influenced by carbonization temperature. Furthermore, scanning electron microscopy (SEM) was performed to observe surface morphologies changes and electrical conductivity values were measured. Results shows that biocarbon material is a promising additive for the enhancing of CPEs proprieties using only residues, thus restraining pollutants and contributing to energy generation.

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Synthesis and characterization of green nanoparticles ZnO (*Abelmoschus esculentus* L.) and Fe_3O_4 (*Solanum Tuberosum* L.) and ZnO-Fe_3O_4 nanocomposites with potential photocatalytic applications

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Green and bio-inspired syntheses have been widely explored as alternatives for obtaining nanomaterials and their applications in environmental fields. In the effort to align materials chemistry with green principles, the improvement of synthetic procedures that minimize waste is of utmost importance. Fe_3O_4 exhibits biocompatibility, and in the field of photocatalysis, ZnO stands out, demonstrating exceptional performance in the degradation of organic compounds using UV and solar light. The intelligent use of the magnetic properties of Fe3O4 allows for the recovery and reuse of nanocatalysts after treatment, pushing the competitiveness and sustainability of heterogeneous catalysis a step forward. In this work, the synthesis of green NPs and the formation of magnetic photoactive composites, which can synergistically enhance the performance of single-component catalysts, were evaluated. Fe_3O_4 was effectively obtained using potato peel extract [1], ZnO using okra mucilage [2], and ZnO-Fe_3O_4 nanocomposites. The green credentials of the proposed methodology were assessed using AGREE software on a scale of 0-1 (with 1 indicating the highest green rating), where ZnO and Fe_3O_4 achieved scores of 0.84 and 0.82, respectively. The NPs were characterized using XRD, confirming the phases, with average crystallite s between 15.3 and 30.7 nm. SEM images indicated spherical morphology for all materials. Diffuse reflectance showed band-gap values between 3.22 and 2.08 eV, a crucial factor for applications in photocatalytic reactions. Promising and low-cost, the syntheses were efficient, and the combination of the nanomaterials proved to be relevant, characterizing a system of green, photoactive, and magnetic NPs with great potential for environmental remediation applications.

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Synthesis, characterization, and use of nanomodified yeast activated carbon in the biosorption of hormones in water

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The pharmaceutical industry plays an essential role in modern society, providing medicines and vaccines to cure and treat various diseases in humans and animals. The use of hormones in various drugs, such as contraceptives, has become progressively common, resulting in an increase in the disposal of pharmaceutical waste in the sewage system and watercourses. Hormones fall into the class of Contaminants of Emerging Concern (CEC) and release persistent toxins, drastically affecting the environment and impacting water, soil, sediments, and biota [1]. Aiming to remedy this environmental problem, biosorption, which involves using materials of natural origin or their derivatives, appears as an alternative for removing these contaminants. Thus, the potential of a nanomodified ferromagnetic activated carbon (YAC-NP) biosorbent, produced from yeast residues of the sugar and alcohol industry, was evaluated in the removal of the hormones estrone (E1) and progesterone (PROG) in contaminated aquatic environments. YAC-NP was synthed by the coprecipitation method [2]. The materials were characterized to assess their morphology and chemical composition by FTIR, XRD, Boehm Method, and pHPZC. The efficiency of impregnation of ferromagnetic nanoparticles in the yeast material and the predominant acidic character of the sample were demonstrated [3]. The experimental sorption capacity for E1 and PROG was 10.16 ± 0.02 and 32.30 ± 0.01 mg/g (YAC-NP) and 1.09 ± 0.38 and 1.58 ± 0.46 mg/g (NP), respectively. The Langmuir, Freundlich, Sips, Hill, D-R, Temkin, Toth, and R-P isothermal models were evaluated to describe the adsorption phenomena.

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SYNTHESIS OF HYDROCHARS FROM *Attalea speciosa* FOR ADSORPTION OF METHYLENE BLUE

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Recently, emerging innovations for the remediation of pollutants from various media contaminated, such as soil, water and so on, have been constantly developed [1]. The study of hydrochar can be considered a promising strategy and innovative approach to pollution control and management of emerging pollutants and dyes using nanomaterials based on agricultural waste, such as babassu coconut shell. At Maranhão, babassu (*Attalea speciosa Mart. ex Spreng*) is one of the most important fruits in the region, since the State is one of the main producers in Brazil [2]. The objective of this work highlights the sustainable remediation of the cationic dye Methylene Blue (M.B.) using hydrochar as an adsorbent, evaluating its capacity as a promising and innovative strategy for pollution control and pollutant management emerging technologies using nanomaterials based on agricultural waste, such as coconut shells babassu. Four hydrochar samples were synthed by hydrothermal method, varying in temperature (120 ºC to 240 ºC) and with a fixed time (120 min). Absorbance was analyzed in triplicate on LAMBDA™ XLS UV-Vis Spectrophotometer. There was a percentage adsorption efficiency of 68.01% in teste with hydrochar from the endocarp of Attalea speciosa in adsorption of M.B. varying in temperature and fixed time, therefore the conversion of babassu waste, the most abundant product in the State of Maranhão, in hydrochar can offer a promising solution for waste management with benefits for the local community, as well as contributing to achieving the Sustainable Development Goals (SDG) of the United Nations (UN).

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The application of Brazilian biomes natural fibers in composite materials: a review

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As the application of natural fibers has garnered interest as a more sustainable reinforcement option for composite materials, it is important to understand the implications regarding its usage in comparison with industrial fibers already established. In a recent review, Silva et al. conducted a "comprehensive examination of recent studies'' addressing the composite materials produced with Amazon natural fibers as reinforcements. The Amazon Rainforest, the largest tropical forest in the world with the world's biggest flora, is just one of the six biomes that make up the ecological diversity present in Brazil - the expanse flora of Caatinga, Cerrado, Atlantic Forest, Pampa, and Pantanal are also worth mentioning. This study aims, then, to expand on the research of the mentioned authors by evaluating composite materials described in the literature that are reinforced by natural fibers extracted from plants native to the five biomes mentioned. The authors intend to utilize articles available on Google Scholar and the CAPES Periodicals Portal as data sources from the research and seek for studies that include information regarding mechanical properties and fabrication process of the final material as well as challenges to the application of the fibers discussed. It is important to mention that, in order to properly understand the relevance of each biome to the discussion conducted, information regarding the plants utilized are also crucial for the study to be considered on the review. With this study, the authors intend to contribute to the advancement of discussions regarding more sustainable materials as well as the role that Brazil can play in the scenario of composite materials reinforced by natural fibers as well as more.

Thermal and chemical treatments for the purification of carbon nanotubes recovered from the biodegradation of PHBV/CNT biodegradable nanocomposites.

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In this study, a biodegradation process in a bioreactor was employed to recover carbon nanotubes (CNTs) from nanocomposites of poly(3-hydroxybutyrate-co-3-hydroxyvalerate), PHBV, a natural and biodegradable polyester. The biodegradation process occurred in an aqueous medium at 32°C and pH 7 for 21 days. Microorganisms were extracted from soil, and samples of PHBV/CNT 2% (w/w) were utilized as a carbon resource. Despite the high amount of exposed CNTs in the biodegradation process waste, the PHBV matrix was not fully biodegraded. Following several washing and centrifugation cycles, the CNTs from the biodegradation process waste (CNTs-W) were lyophilized, then heated in a tubular oven EDG (FT20-10P-LCD) at 350°C for 30 minutes in an inert atmosphere for purification via thermal treatment (CNTs-W-TT). For purification via chemical treatment, the CNTs-W were immersed in a 4 mol L-1 NaOH aqueous solution at 70°C for 2 hours (CNTs-W-CT), followed by washing and lyophilization. Samples of CNTs-W, CNTs-W-TT, CNTs-W-CT, and CNTs-controls were characterized using SEM-FEG (Scanning Electron Microscopy - Field Emission Gun), Raman Spectroscopy, and Fourier Transform Infrared Spectroscopy (FTIR). The SEM-FEG images exhibited a high amount of exposed CNTs in the CNTs-W-TT and CNTs-W-CT samples, as desired. However, they were found to be adhered to high amounts of PHBV matrix. This result is consistent with the FTIR spectrum, which showed typical bands of PHBV (e.g., 1450 cm-1) in the CNTs-W-TT and CNTs-W-CT samples. Bands at 1350 cm-1 and 1620 cm-1 in the Raman spectrum indicate that both treatments can promote partial purification of CNTs-W. Therefore, the results suggest that both treatments hold promise for promoting the reuse of CNTs recovered from PHBV/CNT nanocomposites, although further improvements are necessary.

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Ultrasonic-modified ariá starch for application in biofilms

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The utilization of starch presents itself as a viable option for the production of bioplastics. Among the diverse sources for starch extraction, unconventional options like regional tubers such as ariá (Goeppertia allouia), a native plant of the Amazon region, are gaining attention. However, native starch does have certain limitations that can be addressed through "green technologies" such as ultrasound modification. This treatment can significantly impact the structure and physicochemical properties of starch granules, thereby enhancing its applicability [1]. This study aimed to investigate the influence of ultrasound modification on the physicochemical properties of ariá starch-based biofilms. Starch granules were subjected to different treatment durations (30 and 60 minutes). Biofilms were then produced using the casting method, employing both native and modified starch granules. The films were subsequently characterized using Scanning Electron Microscopy (SEM) and Fourier Transform Infrared Spectroscopy (FTIR), with evaluations conducted on their physical and thermal properties. Results revealed that the treatment did not significantly affect the thickness of the films. However, a noticeable decrease in the enthalpy of gelatinization was observed for both modified-starch films. Analysis of the FTIR spectra indicated a reduction in the intensity of the 340 cm-1 band, associated with hydroxyl groups in amylose and amylopectin molecules, following ultrasound treatment. SEM images demonstrated that films produced with 30-minute modified starch exhibited more homogeneous surfaces. In conclusion, the findings suggest that ultrasound-modified aria starch holds promise for the production of biofilms, offering potential improvements in their properties and applicability.

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Use of scheelite mining residues as neutralizing agent for vinasse for application as fertilizer

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Scheelite is one of the main ores used to obtain tungsten, while its residues are scarcely used and become waste. In this work, the scheelite mining residue from Brejuí Mine/RN, was characterized by X-ray fluorescence, field emission scanning electron microscopy, X-ray diffraction and infrared spectroscopy. Results confirmed a meaningful amount of calcium carbonate after processing of the ore by gravimetric separation, followed by calcination and magnetic separation of the iron oxides. This residue was used as neutralizing agent for vinasse, a residue from sugarcane processing, normally used was natural fertilizer to enrich the soil. Vinasse is known for its high acidity, which is harmful to the soil and may lead to environmental problems. After tests with different proportions of both residues and for different periods of time, a meaningful increase in the vinasse pH was observed after 3 h of process, with a final pH of 5.5, ideal for use as fertilizer. This way, one residue may be used as neutralizer for another residue, making this a valuable process, less harmful to soil and without losing the organic nutrients of vinasse.

Keywords: residue, sugarcane, scheelite, vinasse, fertilizer

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Utilization of Andiroba Cake Residue in Eco-Friendly Composites: Characterization and Influence of Processing Parameters

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Environmental concerns have motivated the utilization of agroindustrial residues in the development of eco-friendly materials. One such example is andiroba cake, a by-product generated in the process of extracting oil from andiroba (Carapa guianensis) seeds. Despite being commonly discarded, this residue holds technological value as a filler [1]. Due to its high residual oil content, mercerization can be applied to remove non-cellulosic components from this residue. Therefore, the objective of this study was to produce and characterize oil-based composites reinforced with 5% NaOH-treated andiroba cake. Initially, the morphology of raw and treated residue was evaluated using Scanning Electron Microscopy (SEM), and their extract content was determined. Five types of composites using only treated residue were manufactured through thermoforming, varying processing temperature (110°C, 120°C, and 130°C) and resin weight (15%, 20%, and 25%). These composites were characterized based on Brazilian Standard NBR 14810-2/2018 for density, swelling, and flexural test. A 2^2+1 experimental design was applied to evaluate the influence of these parameters. SEM images revealed that raw residue particles had irregular shapes and a fat-rich surface, with morphological modifications observed after treatment. This was consistent with a decrease in extract content after treatment (31.30% for the raw residue and 7.93% for the treated one). However, the mechanical performance of the composites did not meet the standard requirements. Nevertheless, the panels exhibited low swelling content. Finally, the experimental design suggests that both temperature and resin amount can influence the properties of the composites.

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Vanillyl alcohol and lignosulfonates as precursors of epoxy resins

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One of the current challenges for biorefineries is to diversify products adding value to the production chain boosting their commercial implementation. Lignosulfonates, a soluble lignin byproduct produced in pulp and paper industries, present high potential for replacing bisphenol A in the production of epoxy resins. These resins are formed by polymerization of epoxylated phenols with varied types of amine compounds. The substitution of bisphenol is a current query because this compound has proved deleterious to the human health. In the current work, to accomplish bisphenol substitution, lignosulfonates were acid condensed with vanillyl alcohol to produce polyphenolic products amenable for epoxylation reactions. UV/vis and infrared analysis indicated the repeatability of the reactions as well as the incorporation of the lignosulfonate on the vanillyl alcohol polymer. Proton [1] and 2D 13C/1H [2] NMR analysis confirmed the reaction sites during acid-condensation reactions, permitting anticipate which polymeric structures were produced. The same techniques demonstrated that the phenolic structures were efficiently epoxylated after reaction with excess epichlorohydrin. Curing epoxylated products with triethylenetetramine produced homogenous blocks with thermoset properties. The use of this epoxy resins for adhesion of pinewood test samples showed that the adhesive produced joints stronger than the internal wood resistance. The work demonstrated that vanillyl alcohol and lignosulfonates can replace bisphenol in epoxy resins pointing out for a new product deriving from biorefineries.

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WO_3 applied as a catalyst in simultaneous transesterification/esterification reactions to obtain biodiesel.

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The global production of biodiesel is predominantly carried out by transesterification or methyl esterification with basic catalysts, using high quality vegetable oils, while acid catalysts can promote the simultaneous reaction of transesterification and esterification, from high acidity materials [1,2]. This work aims at synthesizing tungsten trioxide (WO_3) using the modified-Pechini method for use in biodiesel catalysis, by the methylic transesterification of refined palm oil, esterification of oleic acid and simultaneous reactions (SET). The material was characterized by X-ray Diffraction, Infrared Spectroscopy, Raman Spectroscopy, UV-Visible Absorption Spectroscopy and Scanning Electron Microscopy. The products of the catalytic tests were characterized by kinematic viscosity, acidity index (AI), gas chromatography (GC) and nuclear magnetic resonance (1H NMR). The results indicated a monoclinic crystalline structure, after calcination at 800°C for 4 h. The highest percentage of conversion into methyl esters by transesterification was attained after 120 minutes at 200°C, reaching a conversion value of 14.4% according to GC data. A much better efficiency was attained by esterification reaction, 91.1% of conversion, according to AI data. For the SET reactions, 10% oleic acid was added to the refined palm oil, and a conversion of 69.5% was attained, according to GC data, which is significantly higher than expected, indicating a synergy in the simultaneous reaction. Thus, the WO_3 catalyst has great potential for application and versatility in the production of biodiesel using residual raw materials.

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YEAST-BASED MAGNETIC BIONANOCOMPOSITE FOR ADSORPTION OF DRUGS

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Due to the efficiency of biological waste in removing chemical species from aqueous media and its easy access, it became an economically viable process for water decontamination. Drugs such as paracetamol (PAR) and caffeine are widely used and can be found in contaminated waters as emerging contaminants. Thus, considering the importance of preserving water resources free of toxic substances, a biosorption approach using biosorbents prepared from yeast residues generated in sugar and alcohol industries before (YB) and after (YB-NP) magnetite nanomodification is proposed to remove PAR from water. The biosorbents were characterized by Fourier Transform Infrared Absorption Spectroscopy (FTIR), X-ray Diffraction (XRD), and scanning electron microscopy. The potential of YB and YB-NP in the sorption of PAR was evaluated as a function of pHPZC, sorption pH, kinetics, and sorption capacity of the materials. The biosorption equilibrium of PAR was reached in around 30 min. These biosorbents are promising approaches for water decontamination of drugs since they presented fairly high sorption capacity for the investigated drug in aqueous medium

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Zinc molybdate: a new catalyst for biodiesel synthesis by simultaneous esterification/transesterification reaction

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The search for new solid catalysts for biodiesel production using high acidity raw materials is still a challenge, as it requires that simultaneous transesterification esterification reactions take place, with high efficiency. In this work, a new acid catalyst was evaluated, composed of zinc molybdate ($ZnMoO_4$), synthed by the modified Pechini method and characterized in relation to its structure, morphology and acidity. The catalyst was used in the transesterification of soybean oil, in the esterification of oleic acid and in the simultaneous esterification transesterification reaction of soybean oil acidified with oleic acid, to simulate a residual oil. After the catalytic test, the reaction product was characterized by acidity index, gas chromatography and 1H and 13C nuclear magnetic resonance (NMR). According to the results of 1H NMR, the zinc molybdate was highly efficient in the esterification reaction, with 88% of conversion at 160oC for 120 min, while only 5.7% of conversion was obtained in the transesterification at the same conditions. In spite of this, 69.5% of conversion was obtained in the simultaneous reaction, indicating a strong synergic effect. This behavior seems to be due to the formation of new acid sites after esterification reaction, besides an acid-base character, as suggested by the formation of α-pyridone and pyridinium oxide on the material surface.

SS03-Materials for energy conversion and storage

Controlled synthesis of semiconductor nanoparticles

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The controlled synthesis of semiconductor nanoparticles with the same composition, morphology, and uniform distribution is essential for obtaining materials with the desired properties for energy conversion. In this seminar, we will discuss how factors that affect the mechanism of nucleation and growth can be experimentally controlled to result in materials with desired and reproducible properties. We will also briefly touch on how machine learning can be employed to predict relevant parameters and how the use of robotic platforms for high-throughput synthesis can accelerate the discovery of new materials.

Controlling charge transportation by substrate work function for PEC devices

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Hydrogen production via solar photoelectrochemical (PEC) water splitting has been regarded as one of the most promising directions. For solar energy devices, particularly those based on narrow gap semiconductors, the choice of the substrate is crucial for the overall device performance. This talk introduces the synthesis of the chalcogenide semiconductor (Bi2S3) on four different substrates (FTO, ITO, Au, Mo) by simple electrochemical deposition and sulfurization in a single zone tube furnace. The films behave as photoanodes, producing photocurrents of up to 9.3 mA cm−2 at 1.23 V vs. RHE and photovoltages of up to 0.25 V for the FTO/Bi2S3/Na2S configuration. These values are among the best reported for phase pure Bi2S3 photoanodes. The observed photovoltage trend of the Bi2S3 electrodes (FTO > ITO > Mo > Au) inversely correlates with the Schottky barrier height at the Bi2S3-substrate interface. FTO makes an ohmic contact and causes the smallest barrier and hence produces the largest photo-voltage and photocurrent. These results highlight the importance of matching substrate work function to the chalcogenide Fermi level.

Metal nanoclusters for catalysis

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At the core of our research is a unique method for breaking bulk metals down to single metal atoms (SMA) or nanoclusters (MNC) of precise and chemical composition. The aim of our research group is two-fold: (i) to provide a solution for a sustainable use of scarce metals of technological importance (e.g. Pt, Au, Pd), by maximising utilisation of every atom, and (ii) to unlock new properties that emerge in metals only at the atomic scale, leading to substituting critical metals with abundant ones (e.g. Pt with Ni), and providing a platform for next generation of materials for catalysis. In our latest works: i- we have created Pd nanoclusters that combine the features of both heterogeneous and homogeneous catalysts. We determine the atomic structures and electronic environments of a series of metal nanoclusters in ionic liquids at different stages of formation, leading to a discovery of Pd nanoclusters with a core of ca. 1.8 nm surrounded by a diffuse dynamic shell of atoms in [C 4 C 1 Im][NTf 2]. ii- we have atomically dispersed and stabilized Pt atoms on g-C 3 N 4 using a scalable, ligand-free, one-pot magnetron sputtering deposition process. The deposition of Ni on g-C 3 N 4 improved hydrogen production ca. 370 times (5 h reaction) when compared to bare g-C 3 N 4 , thus demonstrating a high activity compared to other reported systems. We ascribe its high photocatalytic activity to the highly dispersed naked Pt species on g-C 3 N 4 , and due to electron-hole pair recombination decrease, thus enhancing the hydrogen evolution.

Microfluidic fuel cells as promising energy converters from alcohols, pollutants, and CO_2

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Microfluidic fuel cells (µFCs) are miniaturized energy converters that utilize laminar flow to separate the anode from the cathode, eliminating the need for a membrane and the associated ohmic loss, allowing for the use of anolyte and catholyte at independent pHs [1]. Furthermore, the flow-through configuration constructed with porous electrodes enhances surface utilization and electrochemical conversion [1]. µFCs also provide flexibility in catalyst selection, accommodating metallic or light-sensitive electrodes, enabling the development of microfluidic photo fuel cells (µPFCs) [2]. The Electrochemistry Research Group (ERG) at UFMS-Brazil has dedicated efforts to developing new µFCs and µPFCs fueled by alcohols and pollutant models, with CO_2 serving as an oxidant. These endeavors primarily aim to mitigate pollutants and enhance the value of co-products while generating power. Among the achievements, we built a µFC fed by glycerol and HClO to produce the benchmark power density of 315 mW cm^{-2} using Pt/C as catalysts. A comparable 3D-printed system delivered 175 mW cm^{-2}. Regarding µPFCs, we recently developed a 3D-printed µPFC featuring a Pt/PtO_x-decorated $BiVO_4$ photoanode and Pt/C cathode. This µPFC produced 0.48 mW cm^{-2} when fueled by rhodamine B and O_2 for over 5 hours, with energy generation accompanied by approximately 74% pollutant consumption. We also introduced a µPFC equipped with a Pt/C anode and a $CuO/CuBi_2O_4$ photocathode, yielding 0.8 mW cm^{-2} when fueled by glycerol and CO_2 oxidant. These endeavors underscore how µFCs and µPFCs serve as alternative sustainable energy converters.

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Multifunctional materials for emerging solar technologies

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This presentation focuses on structure property/relationships in advanced materials, emphasizing multifunctional systems that exhibit multiple functionalities. Such systems are then used as building blocks for the fabrication of various emerging technologies. In particular, nanostructured materials synthed via the bottom–up approach present an opportunity for future generation low cost manufacturing of devices. We focus in particular on recent developments in solar technologies that aim to address the energy challenge, including third generation photovoltaics, solar hydrogen production, luminescent solar concentrators and other optoelectronic devices. [1-18].

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MXenes: potential materials for electrochemical energy production and storage

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MXenes is family of 2D compounds (carbides or nitrides) obtained through chemical exfoliation and delamination of 3D precursor phases denominated MAX phase. MXenes possesses unique properties derived from their complex bonding (a mixture of metallic and covalent bonds) and electronic structures, atomic stacking, synthesis routes and surface chemistry. Despite the growing interest in these materials, several issues still need to be elucidated concerning their fundamental properties and applications, particularly in clean energy conversion and storage devices. In this talk, new finds on the use of MXenes in energy systems will be discussed, mainly concerning their use in electrocatalysis and supercapacitors. Moreover, the effect of synthesis protocols and terminal groups in MXenes' properties will be depicted.

New materials and strategies for photo(electro)chemical conversion of solar energy into green fuels and chemicals

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This talk will present new strategies for the development of materials and devices based on inorganic semiconductors and metal complexes for converting solar energy into fuel. The topic has great current relevance given the need to reduce the emission of greenhouse gases resulting from the use of fossil fuels. Solar energy presents itself as a more abundant and accessible renewable source, but it needs to be stored in the form of fuel for later distribution and use. During the presentation, recent results from the development of nanostructured materials capable of promoting specific specifications in the presence of visible radiation will be presented. Such responses involve the reduction of CO2, the photocleavage of water and the photoreforming of biomass derivatives to produce green H2 and high value-added chemical inputs. Studies on the role of morphological and electronic properties of materials in process efficiency will be presented, along with challenges to be overcome for possible large-scale applications.

Organic solar cells: Advanced nanoscale characterization towards biodegradable photovoltaics

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The study of organic solar cells (OSCs) is intriguing from a fundamental point of view because of the short lifetime of excitons (strongly-correlated electron-hole pairs) in these devices. While the origin of short exciton lifetime is still open, it is now clear it is linked to strong electron-phonon coupling. The photoactive layers of OSCs is made by polymers, small organic molecules, or their combination. To date, photoconversion efficiencies (PCEs) approaching 20% have been reported for organic photovoltaics [1] by modulating the exciton recombination processes, which allows for enhanced electron-hole separation. Our talk will review the photophysics of OSCs, with a focus on the contributions from our group in their characterization with advanced superresolution optical tools based on scanning probe microscopies and scanning near-field optical microscopy (SNOM). SNOM is a powerful nano-optical technique capable of achieving nanometer-scale optical resolution beyond the diffraction limit by using evanescent waves, which is uniquely poised to be integrated into AFM and STM probes and may be unique nanoimaging tools [2] for mapping the photoconversion efficency [3] and photocarrier mobility,[4] of nanostructured photovoltaics, such as OSCs. In the last part of our talk, we will present our ongoing efforts towards biodegradable and green OSCs entirely fabricated from aqueous solutions and using poly[2-(3-thienyl)ethyloxy-4-butylsulfonate]-sodium (PTEBS, a water soluble organic polymer) as a photoactive material. These are among the best organic photovoltaics obtained to date (up to 3% PCE) from water-based solutions, which highlights the importance of advanced nanoscale characterization tools in designing novel organic photovoltaic architectures.

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Plasma synthesis of oxide materials for photonics, energy and water treatment

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Innovation in materials science and engineering resides in our ability to control the structure of materials at the nanoscale in order to design advanced materials with outstanding functional properties (electrical, optical, magnetic, photocatalytic, etc.). One of the most powerful means to arrange matter at the nanoscale is to use laser produced plasmas due to their exceptional ability to provide simultaneously ions and neutral atoms with various energies in a non-equilibrium environment. Moreover, the possibility to perform growth in a reactive environment such as oxygen or to operate in a double-beam configuration offers an additional flexibility to control the stoichiometry of oxide materials, the dopant content and the surface quality. In this presentation, we will focus on the use of pulsed laser deposition for the growth of various oxide materials in the form of thin films, including undoped and doped vanadium dioxide and titanium oxide. They are exploited for the development of the next generation of photonic and energy devices, or for advanced environmental applications such as water treatment.

Theoretical insight into hematite as a photoelectrode for water splitting

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By using a combination of atomistic simulations and continuum modeling, we have analysed the properties of the iron oxide hematite for photoelectrocatalytic water splitting. The overpotential of the reaction is calculated from surface chemistry by means of density functional theory. Atomistic simulations also provide an estimate of the Helmholtz capacitance. Doping and nanostructuring have a profound impact on the distribution of electric fields at the oxide/electrolyte interface. At high doping, the width of the space charge layer is reduced, and substantial part of the potential drop is located in the Helmholtz layer; nanostructuring counterbalances some of these effects. Signatures of this behaviour can be recognised in electrochemical measurements. I will discuss how this work could lead to a better interpretation of experiments, and what future directions of investigation are.

The polymorphous nature of halide perovskites

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Many halide perovskites exhibit a cubic crystal structure (Pm-3m) at elevated temperatures but transition to lower symmetry structures such as orthorhombic or tetragonal at lower temperatures. Recent theoretical findings have cast doubts upon the cubic structure, as it may exhibit negative phonon modes, unusual band gap trends, and incomplete alignment with PDF measurements. In this context, we propose the concept of polymorphous structures, suggesting that the cubic structure emerges as a result of temporal and spatial averaging of lower symmetry structures. To substantiate this idea, we will employ ab initio and molecular dynamics simulations.

Ab Initio Investigation of Cathode Materials for Rechargeable Zinc Ion Batteries

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Zinc-ion batteries (ZIBs) employing aqueous electrolytes have emerged as one of the most promising alternatives to lithium-ion batteries (LIBS). Nonetheless, the development of ZIBs is hindered by the scarcity of cathode materials with suitable electrochemical properties. In this work, we investigate the properties of ZnV2O4 (ZVO), ZnV2S4 (ZVS) and ZnV2Se4 (ZVSe) compounds as cathode materials, focusing on their electrochemical performance and potential applications in ZIBs. The study was conducted within the density functional theory framework, where the structural, electronic, electrochemical, and spectroscopic properties of ZVS, ZVO, and ZVSe are investigated both with and without zinc deficiency. Our findings reveal that these compounds exhibit similar magnetic properties since vanadium exhibits the same oxidation state in all three compounds, yet they display distinct electronic and electrochemical properties. On average, ZVS stands out as the most promising candidate for ZIBs cathodes, followed by ZVO. ZVSe, in turn, shows lower electrochemical performance. Our theoretical results align closely with available experimental data, providing valuable insights for the advancement of high-performance cathode materials in zinc-ion battery technology.

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A Model for the Sputter Deposition of Si Films with Ta Nanoparticle Scaffolds

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Si-based nanocomposites are interesting as anodes of Li-ion batteries due to the high lithium storage capacity of Si combined with the need of controlling its large volume change during lithiation/delithiation and reducing growth of solid-electrolyte interphases. This scenario recently motivated the fabrication of films with sputter deposited a-Si layers (~30nm each) intercalated with scaffolds of Ta nanoparticles (NPs) of average diameter 3nm, which showed mechanical and electrochemical properties much superior than those of continuous Si films [1].

Here we introduce a deposition model that reproduces several morphological features of these hybrid films. The model is defined in a simple cubic lattice, the discretized Ta NPs aggregate with a ballistic deposition mechanism (first contact), and the transient mobility of Si atoms after they land on the film surface is represented by a sequence of G hops to neighboring points with probabilities dependent on local bond energies. Kinetic Monte Carlo simulations performed with several model parameters show the radial coating of the NPs by the Si atoms and show a larger surface roughness than the same model with pure Si, in agreement with results of SEM and AFM of Ref. [1]. The effective porosity ~20% of the hybrid films [1] is obtained in the simulations with $G\sim10^4$ and a hop probability factor ~0.1 (~0.3) for each first (second) neighbor, which implies that Si atoms thermalize on the film surface with a diffusion length of a few tens of nanometers. When the simulations are performed with the same Si/Ta stoichiometry but with smaller or larger mass in each layer/scaffold pair, the resulting porosity is the same or smaller, showing that the model also captures the optimal deposition conditions of the experimental work.

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Analysis of hysteretic behavior in hybrid and inorganic perovskites

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In consideration of the diversity of materials studied for application as the active layer in the field of photovoltaic devices, perovskites exhibit notable characteristics such as flexible films, ionic conduction, and high conversion efficiency. The advancement in the performance of perovskite photovoltaic devices has not always been accompanied by a fundamental understanding of their electronic and physicochemical properties, which can modulate the photovoltaic parameters. Hysteresis can lead to erroneous estimates of device efficiency, raising questions about its reliability during usage. Although numerous theories have been proposed to elucidate the underlying causes of hysteresis, its origin is a highly debated topic to date. Given this, we seek to understand the origin of hysteresis in perovskites, facing several hypotheses such as variation in chemical formula, where the choice of composition can result in a polarized structure; synthesis parameters that allow us to control thickness and grains, aiming to minimize electrical traps that are directly associated with the capacitive effect or charge storage; and the electrical measurement process, where the electrical response obtained by current detectors evaluates the interaction of charge carriers with the network. Variations in the thickness of the film and the volume of anti-solvent, used to initiate crystallization, have an impact on polarization, thereby affecting the intensity of hysteresis. Furthermore, the formation of larger grains in perovskite had a double impact. On the one hand, it intensifies the capacitive effect, which can be disadvantageous in terms of electrical performance. On the other hand, larger grains can also improve efficiency in photovoltaic devices. The energy loss in a material is a function of frequency and depends on the electronic transitions of the defects present. When the rate of variation of the applied potential is compatible with the relaxation time of the defects, losses are reduced due to the decrease in the ability of these defects to trap charge carriers. Therefore, there is a trade-off to be considered between the capacitive effect and efficiency in photovoltaic devices when optimizing grain in perovskite.

Application of $BiVO_4$ for reducing the overpotential of hematite photoelectrodes for solar hydrogen production

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The current demand for clean energy alternatives makes green hydrogen an important energy carrier to meet the world's energy needs. Hematite (α-Fe_2O_3) is a promising photoanode material, with a suitable band gap (2.2 eV), excellent PEC stability, and natural abundance. However, although the maximum theoretical photoconversion efficiency of hematite is close to 12%, the short hole diffusion length and slow carrier mobility reduce its efficiency and cause an overpotential in the photoanodes.1 Heterojunctions were the best way to improve the charge separation and prolong the charge carrier lifetime. In this work, heterojunctions of $Fe_2O_3/BiVO_4$ based on α-Fe_2O_3 nanorods covered with $BiVO_4$ microstructures deposited via electrodeposition. α-Fe_2O_3 photoanodes are produced hydrothermally, by reacting in a 1.5:1 ratio of $FeCl_3$ and urea for 5 h under 100°C and thermally treated under N_2 atmosphere under 750°C (10 min). The photoanodes show the alpha phase of hematite (α-Fe_2O_3), with a main peak at 35.9° referring to the plane (110) and nanorod morphology observed by SEM. The $BiVO_4$ nanostructures were produced through the formation of BiOI via electrodeposition and converted to $BiVO_4$ through solid-state reactions at 550°C. The coating of Fe_2O_3 with $BiVO_4$ microstructures provides an increase in photocurrent from 1.11 $mA.cm^{-2}$ (α-Fe_2O_3) to 1.30 $mA.cm^{-2}$ (Fe_2O_3/BiVO4). The facilitation in electron extraction is observed when reducing the OCP, going from 0.388 to 0.314 V vs. RHE. The photoelectrodes present a significant reduction in electron transfer resistance, going from 58.2 kΩ (α-Fe_2O_3) to 2.79 kΩ ($Fe_2O_3/BiVO_4$), indicating interfacial improvement in electronic transfer between the electrolyte and the heterojunction. In this way, the heterojunction formation proves to be effective in reducing the overpotential of α-Fe_2O_3, improving the performance of the electrodes. [1] Carminati, S. A. et al., J Catal., 2019, 372, 109−118.

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Bismuth vanadate synthesis for biogas photoelectrocatalysis

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Biogas is a gaseous mixture formed through the anaerobic fermentation of organic matter, predominantly comprising methane, nitrogen, and carbon dioxide. In the waste management domain, sewage treatment emerges as a significant biogas source due to its high organic load content. However, the overproduction of these gases raises considerable environmental, economic, and social concerns. Consequently, numerous studies and technologies have been proposed to effectively manage biogas emissions. Among these approaches, photoelectrochemistry stands out for its capability to convert biogas components into more valuable substances like methanol and ethanol [1-2]. This research focuses on investigating the synthesis of bismuth vanadate semiconductor, employing ammonium metavanadate and bismuth nitrate as precursor materials. The resulting product underwent thorough characterization utilizing various chemical analysis techniques such as FTIR, Raman spectroscopy, XRD, and TEM, confirming its monoclinic crystalline nature. Subsequently, this synthed material was immobilized onto an electrode using the drop-coating method, and its photocurrent response was evaluated in conjunction with gas application. These experimental trials underscored the material's promising potential in photoelectrocatalytic applications, thereby facilitating its utilization in processes aimed at converting biogas into higher-value products.

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C60/organic self-assemble monolayer for electron transport layer applied in perovskite solar cell

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C60-self-assemble monolayers (C60-SAMs) are one of the few materials used in n-i-p devices as electron transporting layers that can substantially reduce the presence of hysteresis. C60-SAM provides efficient electron extraction and higher mobility compared to metal oxides such as SnO2, TiO2; the common electron transport layers (ETLs) applied in n-i-p photovoltaic devices. It can be deposited at low temperatures, being compatible with flexible devices [1]. In this work, we demonstrate an efficient planar n-i-p perovskite solar cell with 18% power conversion efficiency, by simply depositing C60-SAM directly on the conductive substrate at low temperature. Apart from the higher power conversion efficiency, the cells present a high fill factor value, reaching 80%, showing a lifetime of ~1000 hours under artificial illumination.

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Cellulose nanofibers as a reactive template for nanometric oxide synthesis

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Cellulose is one of the most available biopolymer and can be used as raw material for functionalized nanocellulose fibers, usually applied as adsorbent for metals or metallic complexes in aqueous solutions or as additive for enhancement of mechanical properties in composites [1,2]. More recently, some reports from literature suggest the possibility of using the nanofibers also as a reactive template for nano materials synthesis, for example, alloys [3] or spinel oxides [4], which are associated with technological applications of significant value, such as in the branches of energy storage and transport, or heterogeneous catalysis. The present work explores the use of carboxylated nanocellulose fibers (TCNF) for synthesis of two spinel oxides, Fe2ZnO4 and Fe2CoO4. After exposing the nanofibers to aqueous metallic solutions, stimulating cationic adsorption, the generated solid phase is separated through vaccum filtration process and thermal treated under air atmosphere at 500oC for 2 h. After presenting some characterization results regarding morphology and chemical composition of the sample, some data regarding the application of the mentioned spinels are presented, Fe2ZnO4 as a supercacitor and Fe2CoO4 as catalyst for H2 generation from NaBH4 aqueous solutions.

Chemical synthesis of nickel nanoparticles embedded in graphitic carbon nitride as HER electrocatalyst for water splitting systems

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Water splitting electrolysis is a promising pathway to meet the global demand for clean and renewable energy. Electrocatalysts play a critical role in water splitting technologies and thus represent a key component to achieve highly efficient H2 production [1]. However, platinum group metals (PMG) are commonly used as catalysts in these technologies, which implies high costs and makes large-scale commercialization difficult. Transition metal-based catalysts are an appealing option to replace PGM catalysts because of their low-cost, high efficiency and long stability [2]. Nickel nanoparticles (Ni-NPs) have demonstrated excellent catalytic activity for hydrogen evolution reaction (HER) [3]. In this work, Ni-NPs for HER were embedded in graphitic carbon nitride (GCN) supports by using chemical methods. The morphology and structure of chemically produced were evaluated using scanning electron microscope (SEM). Electrochemical impedance spectroscopy (EIS) and cyclovoltammetry (CV) were employed to understand electrochemical activity of the HER electrode. The results reveal the catalytic activity of Ni-NP embedded in GCN and the reaction rate for HER compared to pristine GCN by controlling the particle , enlarging the active sites, and boosting charge transfer properties, and compare the

catalytic efficiency for the manufacturing route selected. This contribution provides a cheaper and stable HER electrocatalyst that can be used in water splitting systems for efficient hydrogen generation.

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Dark TiOx Thin Films

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Currently, humanity's challenges go in the development of materials that act in environmental preservation and remediation. In this context, TiO2 has been reported as a promising material in decreasing carbon emission and treating environmental pollutants. However, its high bandgap value restricts the production of electron pair efficiency to the ultraviolet region. A strategy that has been used to decrease the band gap energy of TiO2, increasing its efficiency in the visible spectrum, is the creation of intermediate states with the inclusion of defects. Because it is highly absorbent in the visible light region, the material has been called dark or black TiO2. The technique of producing thin films by sputtering is suitable for producing sub-stoichiometric films with defects, ideal for producing dark TiO2. A high base pressure of 5x10-5 mbar was shown to be necessary for the inclusion of hydroxyl groups for both hydrogenation and oxygen reduction. Dark TiO2 films have a band gap energy value of 1.42 eV, 50% lower than anatase TiO2 of 3.02 eV. The dark films showed high efficiency of photogeneration of electric current in the visible spectrum range, presenting great potential for applications in sectors of light converting devices, such as photovoltaics or photocatalytic, both technologies that are promising to help reduce carbon emissions to zero.

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Deposition of P-type Iron-manganese cocatalysts on BiVO4 via Magnetron sputtering to Engineer Heterojunctions for Enhanced Photocatalytic Oxygen Evolution

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Bismuth vanadate (BiVO4) is a well-known n-type semiconductor that has been used as a potential candidate for converting solar energy into chemical fuels in photocatalysis and photoelectrochemical (PEC) setups. However, it is prone to high charge recombination due to short hole diffusion length and electron-hole recombination. Many strategies have been developed to suppress charge recombination. Site-selective cocatalysts have been used as a strong candidate to suppress charge recombination and improve the photocatalytic response of BiVO4. In this research work, we deposited p-type FeMnOx cocatalyst on pure and W doped BiVO4 via magnetron sputtering to induce a p-n heterojunction and suppress charge recombination on BiVO4. All the samples were characterized using XRD, SEM, Raman, UV-vis, XPS, and HRTEM. The photocatalytic activity of the prepared samples was tested for oxygen evolution in the photocatalysis setup under solar radiation conditions (1.5G) for 3 h. After the deposition of FeMnOx cocatalyst, the photocatalytic O2 evolution boosted from 93 to 143 µmol for pure and 160 to 181 µmol for the W doped BiVO4 which was attributed to the formation of p-n junctions that led to the development of the built-in electric field, thereby increasing the charge transfer and suppressing the charge recombination. Furthermore, the BiVO4 film was constructed by RF magnetron sputtering using a 100% oxygen atmosphere, producing a photocurrent density of 1.05 mA/cm2.

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Direct recycling of $Li_xNi_{0.5}Mn_{0.3}Co_{0.2}O_2$ cathodes from scrap and end-of-life LIBs using relithiation process

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Recycling processes of discarded lithium-ion batteries (LIBs) have been developed to recover valuable chemical compounds from these batteries for secondary uses, as well as resynthesizing their cathode material using indirect many-step or direct, short-loop recycling processes to be used as cathodes of fresh batteries. The reason for extracting compounds from the cathode of discarded LIBs is that they are composed of high-value and critical minerals such as Li, Co, Ni, and Mn. The $LiNi_xMn_zCo_xO_2$ (NMC) cathodes from end-of-life (EoL) LIBs contain around 15 to 20% fewer lithium ions than found in the cathodes of fresh batteries. It has been challenging to return these EoL batteries by processing the recovered NMC materials in a simple and few-step process, turning them electrochemically active again to be reused in a new cell. This work describes a direct recycling route for discarded NMC532 batteries using a low-cost and facile relithiation process applied to their cathodes. The cathode materials from pouch cell batteries in EoL and from scraps supplied by the manufacturer were extracted by delamination of the aluminum collectors in a NaOH solution and by mechanical scraping. The recovered powder was analyzed using ICP-OES, XRD, CHNS, TGA-MS, FTIR, and PSA techniques. Solid state relithiation of the cathode material was carried out with LiOH as a lithium source at 700 °C. The above techniques also analyzed the reaction products, and a button half-cell was employed to evaluate the relithiated cathode electrochemical performance.

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Efficient photoelectrochemical hydrogen generation from glycerol using Morphology-Controlled TiO_2 nanostructures

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The production of hydrogen via photoelectrochemistry and the increase in technology readiness level of the photoelectrocatalytic strategy is associated with improved performance of semiconductors. In this work, we present the use of hydrothermal strategies to produce hierarchical TiO_2 structures (nanoribbons/spherullites) with rutile single crystalline phase. The resulting photoanode exhibits photoelectrochemical (PEC) water-splitting performance, achieving a photocurrent density of 0.14 $mAcm^{-2}$ at 1.23 V RHE (pH 7, Na_2SO_4 0.5 M). Using the hydrothermal synthesis, controlling the concentration of Cl^- and Sn^{4+}, a high-efficiency system with a rutile crystalline phase was obtained. Using glycerol as hole-scavenger, promoting the photo(electro)reforming, the prepared photoanodes obtained current densities of 1.54 $mAcm^{-2}$ (V vs. RHE, 83 % of Jabs theoretical) with 0.81 % of applied bias photon-to-current efficiency (ABPE) and photoelectrochemical hydrogen generation of 2.2 $mLH_2cm^{-2}h^{-1}$, under 1 Sun (AM 1.5G filter, 100 $mWcm^{-2}$) and long time stability, demonstrating sustained operation for 12 hours. These remarkable results are attributed to the controlled formation of single rutile phase and hierarchical morphology and expands possibilities for performance gains and process scaling.

Enhanced Electrochemical CO_2 Reduction to Hydrocarbons on Polybenzimidazole-Modified Copper Electrodes

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Electrochemical reduction of CO_2 to carbon-based fuels and feedstock is one of the most important strategies for mitigating climate change. Metallic copper (Cu) is unique among electrocatalysts, since it produces hydrocarbons and alcohols via electrochemical CO_2 reduction reaction (ECO_2RR). However, Cu electrocatalysts have some drawbacks, such as lack of selectivity, long-term stability, and the generation of hydrogen gas (H_2) through competitive hydrogen evolution reaction (HER). One strategy for improving Cu activity and selectivity towards ECO_2RR is its coating with organic additives. Herein, a facile procedure was used to coat Cu electrocatalysts with polybenzimidazole (PBI). This strategy reduced the HER and increased the activity and stability of the electrode for ECO_2RR. PBI stabilizes the atoms on surface defects through chemical coordination, thereby inhibiting copper's dynamic behavior (dissolution) during operation. The chemical modification of Cu with PBI reduced the HER from 42% to 18% of Faradaic Efficiency (FE) of H_2, while also improving the selectivity towards CH_4 and C_2H_4 on ECO2RR when compared to pristine Cu. We achieved ca. FE = 50% for CH_4 and 15% for C_2H_4 on CuPBI, compared to FE = 37% for CH4 and 8% for C_2H_4 on pristine Cu, at -1.2V vs. RHE. Furthermore, CuPBI is more stable than pure Cu in long-term experiments. After 18 h of ECO2RR, pure Cu retains ~30% of its maximum activity in producing C_2H_4, while CuPBI retains ~66%. Cu maintains ~40% of CH_4 production, while CuPBI maintains ~60% over the same period. These findings offer promising directions for improving the stability of active Cu sites for ECO_2RR, as well as developing more robust electrocatalysts required for effective CO_2 electrolysis in real-world settings.

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Enhanced Electrochemical Reduction of CO2 into HCOOH on 2D-SnO2 gas diffusion electrodes

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CO2 emissions are considered one of the main causes of climate change, which makes it necessary to take measures to mitigate it. The electrochemical CO2 reduction into chemical feedstocks comes as an alternative to overcome this problem. However, this process faces several challenges such as, the low activity, selectivity and stability of the catalysts, in addition to the low solubility of CO_2 in aqueous electrolyte resulting in current densities below 30 $mA.cm^{-2}$. In this sense, the use of gaseous diffusion electrodes in an electrochemical flow cell eliminates the need to solubilize CO_2 in an aqueous electrolyte, achieving current densities greater than 200 $mA.cm^{-2}$.[2] Therefore, the present work seeks to investigate the effect of different SnO2 synthesis routes on its physicochemical properties and electrochemical activity in reducing CO_2 to HCOOH. Two materials were synthed by a hydrothermal route at different pH and the respective gas diffusion electrodes were prepared via spray-coating. The characterization techniques demonstrated that both materials presented a tetragonal crystalline structure in the rutile phase of SnO_2 and were free of impurities. The samples presented nanosheet and nanosphere morphologies for SnO_2-NS and SnO_2-NP, respectively. The synthed materials showed good efficiency in reducing CO_2 to HCOOH using an electrochemical flow cell, the SnO_2-NS sample presented an F.E. (~90%) higher than the SnO_2-NP sample. The SnO_2-NS sample under optimized conditions presented an F.E. 98% with current density greater than 220 $mA.cm^{-2}$. In this way, it can be observed that the morphology of SnO_2 affects its performance in the electrochemical reduction of CO_2.

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Fast microwave calcination of $Na_{2/3}Ni_{1/3}Mn_{2/3}O_2$ as cathode material for sodium-ion batteries

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For an expansion of sustainable technologies, the efficient storage of energy from renewable sources, requires greater investment in research and innovation in infrastructure, in which rechargeable batteries are key technologies in the energy transition.
Sodium ion batteries (BIS), are ideal alternatives for energy storage in large-scale systems. The advantages of BIS are that sodium is an abundant resource and cathode materials can be manufactured with only low-cost transition metals and non-metals.
The benefits of calcination by microwave irradiation to prepare P2–$Na_{2/3}Ni_{1/3}Mn_{2/3}O_2$ cathode materials for sodium-ion batteries have been evidenced.
FEG-SEM images revealed that microwave calcination provides a homogeneous distribution of elements, while X-ray diffraction patterns showed well-crystallized samples. The good kinetic response evidenced by the electrode material prepared at the fast-heating ramp (20 °C min^{-1} and 2 h) when cycled at high rates was confirmed by cyclic voltammetry and impedance spectroscopy.
In summary, microwave calcination, as a replacement for conventional annealing, is evidenced to be a cheap and reliable method to prepare low-cost and well-performing P2–$Na_{2/3}Ni_{1/3}Mn_{2/3}O_2$ layered oxides as cathode materials for sodium-ion batteries.

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Flexible Lithium Ion Microbatteries

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Rechargeable lithium-ion batteries are present in the most diverse electrical and electronic equipment, driven by their high energy density in small volumes and weights. Flexible electronics has grown alongside other technologies such as implantable devices and technology of things, so lithium-ion batteries can also fill this gap as a power source. Conventional methods of producing lithium ion batteries use rigid systems, in addition to containing liquid electrolytes that reduce the safety of the devices. An alternative in the production of lithium ion batteries is the manufacture of thin film electrodes using physical techniques such as sputtering. Among the advantages of this process, the lack of addition of ligands and electronic conductors stands out, which promotes an increase in specific energy. With the aim of producing high charge capacity films with large electroactive area and high interfacial diffusion electrode electrolyte on a flexible substrate, thin films of ternary lithiated transition metal oxide (Ni, Mn and Co) was investigated and optimized. As an optimization methodology, was used a factorial design of experiments with 4 variables (power, pressure, thickness and percentage of O2) at two levels and additional central point. In the optimized deposition conditions via factorial planning, it resulted in a charge capacity 50% greater than the best commercial electrodes currently used. This opens a window of possibilities for increasing charge capacity for both flexible devices and rigid batteries for conventional devices.

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Grain boundary-controlled lithiation of Li-solid solution systems for lithium metal batteries

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Lattice defects often dominate the properties in a material [1], and yet their role on the lithiation behaviour of anodes is still unclear. Here, we developed an in-situ micro-diffusion couple inside a focused ion beam – scanning electron microscope to target grain boundaries. Micro-pillars from nanocrystalline and <100> single crystal Ag were manufactured and contacted with metallic Li, causing spontaneous lithiation. The diffusion process is interrupted by cooling the stage at a desired reaction state; atom probe tomography and transmission electron microscopy were then combined to reveal the distribution of Li at the near-atomic scale. We observe that lithiation takes place primarily at high angle grain boundaries, whereas low angle boundaries and coherent twin boundaries do not offer a fast diffusion path for Li. Even in the absence of an externally applied potential, >93.8 at.% Li regions nucleate within Ag grain boundaries. Kinetic effects dictate the lithiation, and the resulting microstructure cannot be accounted on the basis of equilibrium thermodynamics alone. Contrastingly, <100> Ag micropillars only exhibit Li plating at the surface, without Li alloying in the bulk. This study showcases that grain and grain boundary character are key parameters to engineer for optimizing the lithiation kinetics of solid solution forming electrodes.

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Harnessing the Power of Cu-Doped SrTiO3: Tailoring Photocatalytic Performance for Sustainable CO2 Reduction

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Artificial photosynthesis, a promising strategy to produce a clean fuel, aims to mimic nature process of converting sunlight, water, and CO2 into energy. Despite advancements, current photocatalysts face challenges like inefficient charge separation, recombination, and limited product selectivity. SrTiO3, a well-established perovskite photocatalyst, offers state-of-the-art water splitting and CO2 reduction performance. However, the insufficient optical absorption hinders its efficiency owing to the high bandgap. Doping SrTiO3 with Cu has shown enhanced redox potential and spatial charge separation. Optimizing the interaction between dissolved CO2 and the photocatalyst surface through modifications like doping or adjusting the reaction phase can significantly improve the overall efficiency of the photoreduction process. Therefore, the different reaction phases (solid-gas, solid-liquid, and solid-gas pressure) can significantly influence product formation rates and selectivity in CO2 reduction. Our study investigated CO2 reduction using SrTiO3 under various reaction phases, including solid-gas, solid-liquid, and solid-gas with pressure. We found that the solid-gas phase exhibited the highest selectivity and quantity of CO2 reduction products, surpassing solid-liquid and solid-gas with pressure by two and 1.5 times, respectively. While solid-gas with pressure demonstrated comparable production, further optimization is needed to achieve higher yields and selectivity. These results highlight the potential of SrTiO3 doped Cu photocatalysts for efficient CO2 reduction. Further optimization of parameters like reaction phase and temperature is crucial for maximizing performance and achieving practical applications. This aligns with Brazil's Nationally Determined Contribution (NDC) to reduce greenhouse gas emissions, paving the way for a sustainable fuel production method utilizing sunlight and CO2. Acknowledgment
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Life Extension Process for Springs (PN’s VD250 and VD280) used on Brazilian Air Force AMX A-1 Fighter Bomb support.

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Brazilian Air Force-FAB uses, since 1991, the Fighter-Bomber A-1 AMX, built by a bi-national joint venture between Brazil and Italy, operating more than 40 aircrafts during this period. Being a Fighter-Bomber aircraft, the AMX A-1 is capable of carrying a big variety of weapons, as well as fuel tanks used to increase its operational range. These items are mounted in the aircraft fuselage through the bomb supports, known as pylons. Inside the pylons mechanisms are used springs to avoid the vibration transfer between the aircraft and the pylons pads when theses last ones are detached. Due to the aircraft life time cycle is closing to its end, many spare parts are difficult to acquire, so FAB works actively to extend the life cycle of the items that reached its life time limit – TLV, by means of repair, tests and analysis, always maintaining its reliability and project objectives. In this regard, this paper presents the springs (PN VD280 – 15EA e PN VD250 – 24EA) life extension process, used on A-1 aircraft pylons. The process consists in the following method: cleaning, non-destructive inspection (NDI), physical measurement, load x displacement charts construction, result analysis and protective painting of the approved items. NDI didn’t show structural defects for any analyzed specimen. Physical measurements show variation for all analyzed specimen regarding unloaded length, step, wire diameter and external diameter, comparing to the project values. Three load x displacement charts were analyzed for each PN according to its constructive characteristics. For PN VD250, the analyzed charts were: 60mmx3,2Kgf; 50mmx7,2Kgf and 40mmx11,2Kgf, resulting in 20,83%, 20,83% and 12,5% respectively, according to project design tolerance, resulting on the approval of 17 items. For PN VD 280, the analyzed charts were: 35mmx9Kgf, 30mmx16,5Kgf and 25mmx24Kgf, resulting in 80%, 100% and 100%, respectively, according to project design tolerance, resulting on the approval of all items.

Materials and Processes for the Upscaling of Perovskite Solar Cells

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Perovskite solar cells (PSCs) are currently considered promising candidates for the next generation of photovoltaic devices. Considering the commercialization of these devices, not only achieving high power conversion efficiency and device stability is important, but other technological aspects related to their upscaling (selection of materials and processing conditions compatible with industrialization, for example) are also relevant matters. Some key issues that still need to be addressed include the fact that the high efficiencies of about 25% obtained for small cells have not yet been achieved for larger cells and modules, long-term stability, and the use of high-cost, or not abundant materials, toxic solvents and processes that are not scalable. Here, we will discuss four strategies employed by our team to assemble large-area PSCs (in 5 cm x 5 cm-d substrates), starting from lab-d cells (active area ~0.1 cm^2), and looking into the use of locally accessible materials. The first strategy includes substrate modification with metallic grids to enhance the charge extraction at the transparent conductive oxide electrode. [1] The second strategy involves replacing the often used spin-coating technique with the blade-coating technique (compatible with S2S and R2R lines) for the deposition of the perovskite layers and selective contacts. [2] The third strategy involves the use of low-cost, abundant inorganic materials, in replacement of imported expensive materials. Finally, the fourth strategy deals with the development of an encapsulation process at low temperature, since the perovskite layer might degrade if temperatures higher than 130 °C are used.

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Molecular Dynamics Simulations of Ionic Liquids Confined Into MXenes

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Two-dimensional (2D) transition metal carbides known as MXenes have been extensively investigated as electrode material of electrochemical devices, including supercapacitors. Here we present a detailed computational study of ionic liquids in contact with Ti3C2F2, both at planar surface and under confinement. The simulations employ an extension of the constant potential model (CPMχ) that can properly deal with materials composed of chemical elements with different electronegativities. The average partial charges of MXene atoms calculated with CPMχ are in excellent agreement with the ones obtained by DFT calculations. The differential capacitance and the charging mechanisms are thoroughly analyzed for two ionic liquids with a common cation, [EMIM][BF4] and [EMIM][NTf2]. By varying the MXene interlayer dimension, the best performance in terms of charge storage is obtained in electrodes with 12.6Å spacing, with outperformance of [EMIM][BF4]-based cells.

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OBTAINING NANOFIBERS BY COAXIAL ELECTROSPINNING OF P3HT:PCBM FOR ACTIVE LAYER OF BHJ TYPE SOLAR CELLS

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Electrospinning is a technique that allows nanofibers to be obtained by applying an electric field to a polymeric solution. However, the electrospinning of conductive polymers needs to be by coaxial electrospinning. This process consists of two nozzles that are aligned concentrically with the core layer and shell layer solutions [1]. In order to increase the photovoltaic parameters of BHJ-type solar cells and the thickness of the active layer of this device without exciton recombination [2], one of the alternatives is to add nanofibers of the donor polymer and acceptor material within the active layer. The objective of this work is to obtain nanofibers containing P3HT and PCBM from coaxial electrospinning and use them as the active layer of a BHJ-type solar cell. The polymer to be used as the shell layer is poly(methyl methacrylate), and the core layer consists of the P3HT polymer with PCBM. The parameters studied in the electrospinning process were the pump flow rate used in the core-shell layer solutions and the distance between the needle and collector. The flow rate of the core layer solution varied from 0.10 to 0.25 ml/h, while that of the shell layer solution was 0.5 ml/h and 1.0 ml/h. The applied voltage was 20 KV. The shell layer was removed by washing the nanofibers in acetone. Subsequently, the samples were dried in an oven at 70°C to eliminate the solvent. The morphology of the nanofibers was analyzed by SEM, TEM and fluorescence microscopy with the presence and absence of the shell layer. Furthermore, XRD, Raman, UV-vis, VC, FTIR and AFM-IR analysis of the nanofibers was carried out to verify the complete absence of the shell layer.
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Optimizing Tantalum Nitride Nanotube Synthesis via Design of Experiment for Enhanced H_2 Photogeneration

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Utilizing photocatalysts to harvest sunlight and drive photochemical reactions holds immense promise for producing solar fuels, particularly green hydrogen. Tantalum nitrides and oxynitrides present a suitable bandgap energy for efficient sunlight absorption (2.1 eV) [1]. Enhancing photoconversion efficiency is crucial for its applicability, with strategies like nanoscale engineering [2,3] able to minimize charge diffusion distance. In this work, we optimized the synthesis parameters of TaO_xN_y nanotubes (NTs) to maximize H_2 production by using design of experiments (DoE). The precursors, Ta_2O_5 NTs, were obtained by anodization followed by nitridation. By employing a central composite rotational design (CCRD), we explored the impact of nitridation temperature (ranging from 700 ºC to 1000 ºC), heating rate (1 to 20 ºC min^{-1}), and duration (1 to 3 hours). Samples with higher H_2 production rates were characterized with SEM-EDS, XRD, UV-Vis spectroscopy, and BET analysis of N_2 adsorption. Analysis of the CCRD revealed that the nitridation efficiency of Ta_2O_5 NTs is primarily influenced by nitridation time and temperature. The most efficient visible-light H_2 production sample was achieved by nitridation at 940 °C (5°C min^{-1}) for 85 min, yielding 1.5 µmol H_2 $h^{-1}g^{-1}$ of photocatalyst without any cocatalyst, further reaching 34.50 µmol H_2 $h^{-1}g^{-1}$ using Pt as a cocatalyst.

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Photovoltaic efficiency of transition metal dichalcogenides thin films by ab initio excited-state methods

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Transition metal dichalcogenides (TMDCs) have garnered significant interest in optoelectronics, owing to their scalability and thickness-dependent electrical and optical properties. In particular, thin films of TMDCs could be used in photovoltaic devices. In this work, we employ *ab initio* many-body perturbation theory within GW-BSE approach to accurately compute the optoelectronic properties of thin films of 2H-TMDCs composed of Mo, W, S, and Se [1]. Subsequently, we evaluate their photovoltaic performance including exciton recombination effects, and show this is a key ingredient. We obtain efficiencies of up to 29 % for a 200-nm thick film of WSe_2, thus providing an upper limit. We also include other phenomenological recombination mechanisms that could be present in current samples. This slightly reduces efficiencies, indicating that even with current synthesis technologies, there is still potential for further enhancement of TMDCs' performance in photovoltaic applications.

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Synthesis and photoelectrochemical applications of spinel Zinc Ferrite ($ZnFe_2O_4$) nanostructure and heterojunctions for Hydrogen production

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To satisfy the increased global energy demand, the actual challenge is developing green, clean, and renewable energy sources, especially solar energy conversion technologies [1]. Therefore, photoelectrochemical (PEC) technology is a promising tool for the conversion of solar energy into molecular hydrogen, an energy alternative environmental approaches and considered as substitute for fossil fuel [2]. In this context, this work proposes the design of photoelectrodes based on semiconductor materials for PEC water splitting to hydrogen generation. Spinel ferrites are promising semiconductor with an appropriate band gap (2.0 eV) and used as photoanode for solar water oxidation. $ZnFe_2O_4$ are produced by hydrothermal growth in stoichiometry proportion between of 1:2 of Fe^{3+}: Zn^{2+}, urea solution and NH_4F at 120°C in Teflon vessel. $ZnFe_2O_4$ was growth on FTO glass substrates and thermal treatment at 650°C. Have been explore the construction of heterojunctions with other nanostructures synthed, as $ZnFe_2O_4$/ZnO, $ZnFe_2O_4/Fe_2O_3$ and $ZnFe_2O_4$/ cobalt oxide with phosphate moiety, (Co-Pi). For pristine $ZnFe_2O_4$, was obtained a photocurrent of 0,6 $mAcm^{-2}$ and was obtained a significatively enhancement of photocurrent to 1,3 $mAcm^{-2}$ when is formed the heterojunction with Fe_2O_3. For $ZnFe_2O_4$/Co-Pi was obtained a reduction of the overpotential classic for iron-based materials and an enhancement to almost 100µA in photocurrent. The morphology of photoanodes is altered with the heterojunctions, from a flower-based structure for pristine $ZnFe_2O_4$ to coating and reformed the structure, verify by SEM images. It was approached structural, morphological and electrochemistry characterization for demonstrate the promising results of zinc ferrite and their modifications to construction of photoanodes and the use to hydrogen production.

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Synthesis of green ammonia from Cl-doped nano-Fe2O3: the role of interfacial segregation

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The utilization of solar-driven photoreduction for ammonia production presents a promising alternative to the energy-intensive Haber-Bosch method. The possibility of using solar light during this process offers a greener and more energy-efficient pathway. Among the materials used for this application, iron oxide emerges as a viable option due to its abundance and low toxicity. However, iron oxide also presents a low charge transfer, a short diffusion length, and a high electron-hole recombination rate [1]. Thus, one of the strategies to mitigate this problem is doping iron oxide with ions that can increase the recombination time of the electron-hole pair and consequently improve its photocatalytic performance. In this study, Fe2O3 and Cl-doped Fe2O3 nanoparticles were synthed using a modified polymeric precursor method [2]. The segregation of Cl ions at the interfaces of Fe2O3 was confirmed through selective lixiviation. Subsequent analysis using electrochemical impedance spectroscopy (EIS) revealed a significant reduction in electric resistivity in the doped samples, attributed to grain boundary segregation of Cl, facilitating electron and hole transport. Finally, the ammonia production using Fe2O3 and Cl-doped Fe2O3 nanoparticles were evaluated in a reactor under UV light.

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Towards Sustainable Hydrogen Production: Modification Strategies in the design of highly efficient Photoelectrodes

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Highly efficient photoelectrodes are essential for implementation of green hydrogen production systems via photoelectrochemical devices. Unfortunately, the classical semiconducting photoelectrodes have not achieved the efficiency, stability, and cost-effectiveness for industrial applications. In this study, we present a simple and economical method for synthesizing dual-modified hematite photoelectrodes. This approach allows for the bulk doping of one element and simultaneous interfacial engineering by a second modifier.[1,2] The synergy resulting from these dual modifications enhances charge carrier dynamics, thus improving photoelectrode efficiency and stability. This synergistic effect leads to a significant increase in photocurrent response, rising from 0.7 mA cm^{-2} for pristine hematite to 4.5 mA cm-2 at 1.23V and exceeding 6.0 mA cm^{-2} with a 300 mV overpotential under simulated sunlight illumination. Our findings highlight the promising potential of synergistic dual modification strategies in evolving photoelectrochemical water splitting devices toward practical industrial applications.

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Tracking the Halide Dynamics at Quantum Dot/Perovskite Interface for Solar Cells

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Perovskite solar cells (PSCs) hold great promise for the future of photovoltaic technology, but they encounter challenges related to environmental stability.[1] To tackle this issue, researchers propose using passivating nanomaterials such as perovskite quantum dots (QDs).[2] In this work, we found and investigated a halide exchange reaction occurring at the interface between QDs and bulk (3D) perovskites using in situ photoluminescence (in situ PL). By determining the activation energy for the interfacial bromide-to-iodide exchange, we discover its effectiveness in passivating film defects and grain boundaries. Incorporating QDs into solar cells introduces a new energy level alignment, which enhances hole extraction and impedes electron transfer, thereby reducing bimolecular charge carrier recombination and increasing conversion efficiency. Moreover, the interfacial halide composition remains stable under thermal stress, and the hydrophobicity of QDs' ligands prevents moisture penetration into the perovskite films. Thus, strategically integrating QDs enhances photovoltaic performance and holds promise for mitigating moisture and thermal-induced degradation.

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Unveiling the Influence of Alkaline Modifiers in CuO Synthesis on Its Photocatalytic Activity for CO_2 Reduction

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Aiming to contribute to the field of sustainable technologies to mitigate CO2 emissions, this research explores the enhancements of CuO photocatalysts synthed with different alkaline modifiers for CO2 photoreduction. The methodology focuses on altering the alkaline environment during synthesis to evaluate changes in the catalyst's surface chemistry and morphology, critical for enhancing CO2 conversion to valuable chemicals using solar energy. The chemical precipitation method utilized the NaOH, KOH, NH4OH, and monoethanolamine (MEA) as bases to examine their effects on the photocatalytic efficiency of CuO catalysts. The results reveal that all CuO samples maintained a monoclinic structure, but displayed significant differences in particle morphology and surface chemistry, influenced by the type of alkaline modifier used. Notably, the incorporation of MEA introduced nitrogen-containing functional groups to the surface of CuO, significantly enhancing its photocatalytic activity for CO2 reduction, with a marked increase in methane production. A synergistic effect was observed when MEA was combined with KOH, surpassing the performance of catalysts modified with a single base. This synergism between MEA and KOH led to enhanced particle nucleation and effective surface functionalization, optimizing the photocatalytic activity of CuO for CO2 reduction. In conclusion, the study underscores the critical role of alkaline modifiers in tailoring the synthesis of CuO photocatalysts for improved CO2 photoreduction. It demonstrates that by adjusting the synthesis parameters, specifically through the strategic use of alkaline modifiers, it is possible to enhance the photocatalytic efficiency of CuO significantly.

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3D Printing by Direct Ink Writing of $TiNb_2O_7$ Electrodes for Li-Ion Batteries

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The use of batteries for energy storage has been the subject of increasing debate, driving the search for new materials for this application. The aim is to achieve greater efficiency and storage capacity, as well as to reduce the dimensions of the devices. Among the materials, titanium oxide and niobium (NTO) such as $TiNb_2O_7$ stand out for their cycle stability and high theoretical capacity when applied as electrodes in lithium-ion batteries [1]. 3D printing is a suitable manufacturing technique for producing complex geometries in a cost-effective manner. Direct Ink Writing (DIW) is a relatively new variant of additive manufacturing that prints from fluids (inks). Printing ceramic components requires the formulation of inks composed of a resin medium with dispersion of oxide particles, and it is essential to adjust the rheological aspects in relation to the resin concentration and concentration of dispersed particles [2]. There is little information in the literature about formulations of NTO-based resins. Therefore, the objective of this work is to produce, optimize, and adjust the compositional characteristics of the NTO/resin ink, aiming for better printability and ensuring the production of electrodes with good compositional, dimensional, and geometric uniformity.

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Addressing the scale-up challenges present in nanostructured hematite photoelectrodes

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Green hydrogen's promise as a sustainable fuel has sparked global interest, urging the need to scale up efficient production methods, such as photoelectrochemical devices. Currently, photocurrent density measurements typically utilize geometric areas ranging from 0.1 to 2 cm^2, classifying them as laboratory scale. However, scaling up photoelectrodes often leads to a noticeable reduction in photocurrent response as the area increases. This study elucidates the challenges of transitioning a method from laboratory to demonstrative scale to expand the photoelectrode area to 200 cm^2 [1]. Hematite (α-Fe2O3) was chosen as the model material due to its cost-effectiveness and abundant availability in nature. To mitigate the drop in photocurrent, Hf4+ was introduced as an interface modifier to maintain efficiency. The incorporation of Hf4+ facilitated improvements in morphology, adhesion, and conductivity of the film, resulting in a homogeneous photocurrent of 1.6 $mAcm^{-2}$ at 1.45 V across an active area of 15.75 cm^2 [2]. **Acknowledgements:**
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Advancing Photovoltaic Electrolysis: Carbon-Based Electrodes for Sustainable Hydrogen Production

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In the realm of hydrogen production through photovoltaic electrolysis (PVEL), the pursuit of economically viable solutions has encountered a significant hurdle despite the inherent cleanliness of hybrid systems. Addressing this challenge calls for a pioneering exploration into novel materials for both photovoltaic panels and electrolysis cell electrodes. Thus unfolds the mission of this project: the development of composite carbon-based electrodes harnessing the synergies of iron oxide anchored on graphene and multi-walled carbon nanotubes (MWCNTs) to propel hydrogen generation via aqueous electrolysis under neutral conditions, buoyed by photovoltaic energy. Firstly, iron oxide nanoparticles (Fe3O4) were synthetized by ammonia solution precipitation, followed by their incorporation with graphene oxide (GO) and MWCNTs. Copper electrodes were modified by drop-casting using suspensions with different proportions of Fe3O4 nanoparticles, GO and MWCNTs. The modified electrodes were characterized by field emission scanning electron microscopy (FE-SEM), energy-dispersive X- ray spectroscopy (EDS) and chronoamperometry (CA). The FE-SEM images showed the characteristic morphology of the Fe3O4 nanoparticles, in which homogeneous particles were observed with a nanometric diameter. The EDS spectra showed the presence of carbon, oxygen, silicon, and iron in the Fe3O4 samples, corroborating with the elements present in the substrates and samples. The electrodes modified with FMWCNTs/Fe3O4 and FMWCNTs/Fe3O4/OG showed the formation of hydrogen gas around -1.3 V in chronoamperometry studies in phosphate buffer and citric acid solution. Through the integration of carbon-based composites modified with Fe3O4 nanoparticles, this study contributes to the development of environmentally friendly hybrid hydrogen production systems. Acknowledgments: Grant nº 2023/04842-8, São Paulo State Research Support Foundation (FAPESP).

Advancing Stable Gas Diffusion Electrodes with CuO Catalysts for Enhanced CO2 Electroreduction

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The escalating CO_2 levels in our atmosphere demand innovative, commercially viable solutions. The electrochemical CO_2 reduction process stands out, offering a path to convert this greenhouse gas into valuable fuels and chemicals. A pivotal component in making this technology effective is the development of catalysts that are not only efficient and selective but also demonstrate long-term stability. This study explores the utilization of copper oxide (CuO)-based catalysts, known for their simplicity and cost-effectiveness in synthesis, for CO_2 electroreduction. Following a chemical precipitation method, we synthesized these catalysts and conducted a comprehensive analysis of their composition and morphology. Techniques such as Fourier Transform Infrared Spectroscopy (FTIR), X-ray Diffraction (XRD), and X-ray Photoelectron Spectroscopy (XPS) were employed for compositional analysis, while Scanning Electron Microscopy (SEM) and Brunauer-Emmett-Teller (BET) analysis provided insights into the catalysts' structure and surface area. Electroreduction experiments were carried out at various potentials (-0.8 V, -1.0 V, and -1.2 V vs. RHE), with the resulting products analyzed through Gas Chromatography (GC) and Nuclear Magnetic Resonance (NMR). This allowed for the identification and quantification of the reaction outputs. The synthed material was confirmed to be copper oxide (JCPDF: 48-1548), featuring oval particles measuring approximately 163 nm in length by 103 nm. The experimentation revealed optimal conditions for electrode preparation, crucial for process stability. Notably, in final testing phases, the primary electrode consistently maintained current for 100 consecutive hours, underscoring the catalysts' potential for practical application in CO_2 reduction strategies.

Agro-industry waste-derived biochars applied as support for Pd nanoparticles to hydrogen production in acidic medium

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Energy transition is urgent and green hydrogen is an alternative for reducing carbon emissions. The sharp population growth, in addition to the increase in energy demand, brings with it an increase in waste generation, mainly from agro-industries. Thus, new possibilities for waste applications become essential. This study evaluates sugarcane bagasse (C_B) and rind (C_C), pine nut shells (C_P), and pequi peels (C_{PE}) biochars as supports for palladium (Pd) nanoparticles in the electrocatalysis of hydrogen evolution reaction (HER) in H_2SO_4 medium, with Vulcan XC-72R carbon black (C_V) used as a benchmark. The biochars were obtained in a muffle furnace, at 300 °C for 20 min, under air atmosphere [1]. Pd/C_X materials were synthed via borohydride reduction [2]. The C_X materials were characterized by Raman spectroscopy, CHN elemental analysis and BET surface area analysis; as Pd/C_X materials were by X-ray diffraction, scanning and transmission electron microscopies, and energy dispersive X-ray spectroscopy. Electrochemical studies involved cyclic and linear sweep voltammetries, electrochemical impedance spectroscopy, and chronopotentiometry. The results indicate the Volmer-Heyrovsky mechanism for all electrocatalysts in HER [3], with Pd/C_V and Pd/C_B yielding similar exchange current densities (j_0) of 1.97 mA cm^{-2} and 1.03 mA cm^{-2}, respectively. Both Pd/C_V and Pd/C_B electrodes exhibit high stability and faradaic efficiencies (94.7% and 93.4%, respectively) for HER. All materials proved to be active for HER, from which Pd/C_B stands out with similar activity to the Pd/C_V reference. In summary, our study highlights the potential of biomass waste-derived materials for applications in hydrogen energy.

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$Al_2W_3O_{12}$ from the low-positive thermal expansion ceramic to an efficient photocatalyst under low-power visible light

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The development of new materials for photocatalytic applications that are economically viable, easy to synthesize, industrially scalable and sensitive to visible light represents a great challenge. This study constitutes the first complete study of the photocatalytic properties and the mechanisms involved during the photodegradation of pollutants by the low-positive thermal expansion ceramic $Al_2W_3O_{12}$ under visible light radiation. $Al_2W_3O_{12}$ nanopowders were synthesized on a large scale *via* co-precipitation following a similar procedure to that reported by Henriques et al. [1]. Visible light sensitization was carried out through the introduction of oxygen vacancies by thermal treatment under different conditions. The crystalline structure, morphology, specific surface area, photocatalytic performance and physicochemical properties of $Al_2W_3O_{12}$ nanopowders were evaluated using various techniques. The photodegradation results highlighted the photocatalytic potential of the oxygen-deficient $Al_2W_3O_{12}$ nanopowders under low-power visible light radiation. It was found that the increased oxygen vacancies concentration was beneficial for the photocatalytic performance of $Al_2W_3O_{12}$ nanopowders due to the synergistic effect between the increase in sensitization to visible light of $Al_2W_3O_{12}$ ceramic and enhanced migration of photogenerated charge carriers, resulting in the efficient production of reactive oxygen species (ROS).

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Analysis of dc conductivity, a study using the impedance spectroscopy technique and theoretical-experimental simulation, using the EIS Sectrum Analyzer program, in BNV/MWCNT nanocomposites.

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This work, in addition to aiming to prepare a conductive polymer nanocomposite based on vulcanized natural rubber (BNV) as matrix and second phase multi-walled carbon nanotubes (MWCNT), also aims to create the composite to be applied as a piezoresistive sensor. The nanocomposite samples were produced in an open mixer with cylindrical rollers, in which 100 phr of BN was used as a reference, in which the quantity was kept fixed, as well as the vulcanizing agents (sulfur, zinc oxide, etc.) while varying concentrations. of MWCNT (from 1 to 7 phr). To evaluate the properties of the BNV/MWCNT conductive nanocomposite samples, electrical analyzes were carried out in the dc regime for conductive analyses.

With the BNV/MWCNT samples obtained in the form of films, they were subjected to the impedance spectroscopy technique, this technique studies the resistance or impedance that the material imposes on the passage of an alternating current (ac) that arises when an alternating electric field its applied. With the data obtained through impedance spectroscopy analysis, it was possible to simulate some parameters existing in each nanocomposite, loaded with different concentrations of MWCNT, using the EIS program. With the help of the program simulation, it was possible to find the different parameters that can be adopted to obtain the values obtained in impedance spectroscopy. In other words, it was possible to compare simulation data with in situ data.

It was observed that the samples become more capacitive as the concentration of MWCNT is increased inside the nanocomposite, resulting from the greater quantity of charge carriers trapped at the BNV/MWCNT interfaces.

Finally, the results obtained in this study indicate that it is possible to obtain significant data when comparing theoretical-experimental simulation. Therefore, the program is suitable for carrying out analysis of the parameters stipulated in the nanocomposite. Some of the applications of the obtained nanocomposite include antistatic blankets, piezoresistive sensors and electromagnetic radiation shielding devices.

Analysis of Photovoltaic Parameters in PM6/Y6/PCBM Devices with NitTPP and ZnTPP Addition

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Photovoltaic devices based on active layer structures composed of organic polymers, notably represented by the combination PM6/Y6/PCBM, have sparked considerable interest due to their potential in directly converting solar energy into electricity [1]. However, to optimize the performance of these devices, it becomes imperative to evaluate and understand the photovoltaic parameters that directly influence their efficiency [2]. In this context, the introduction of additives such as NitTPP and ZnTPP into the active layer has been investigated as a viable strategy to enhance photovoltaic properties [3]. This study primarily aims at a comprehensive evaluation of the photovoltaic parameters of devices incorporating the PM6/Y6/PCBM active layer, along with the addition of NitTPP and ZnTPP. Parameters such as energy conversion efficiency, short-circuit current (Isc), open-circuit voltage (Voc), fill factor (FF), and current density (Jsc) will be analyzed, aiming to understand the substantial impact of these additives on the intrinsic energy conversion properties of photovoltaic devices. The evaluation of photovoltaic parameters will be conducted through experimental procedures encompassing the acquisition of current-voltage (I-V) curves and the use of electrochemical impedance spectroscopy (EIS). It is anticipated that the inclusion of NitTPP and ZnTPP in the active layer of photovoltaic devices will provide substantial improvements in photovoltaic parameters, resulting in an increase in energy conversion efficiency. The proposed study aims to provide relevant contributions regarding the effects of incorporating NitTPP and ZnTPP into the active layer of PM6/Y6/PCBM-based photovoltaic devices.

Barocaloric effect evaluation in composite of thermoplastic elastomer, polyethylene and carbon nanotube

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The growing demand for refrigeration systems has substantially increased the search for technological innovations in this area. Systems that utilize the solid-state refrigerators can be based on the barocaloric effect, which is a mecanocaloric effect occurring from the application of a hydrostatic pressure over the material, and are one of those modern innovations. A plethora of materials have been tested for this effect, and elastomeric polymers have presented a great to giant barocaloric effect [1]. But, polymers tend to have thermal insulating properties, which makes the usage of this effect on a refrigeration system difficult. With that, this work aims to increase the thermal properties, derivative from the characteristics of the Carbon Nanotube (CNT)[2], and maintain a great barocaloric effect on a composite made of TPE, PE and CNT, thus having a potential use for refrigeration systems. The materials were made from the mixture of a pure TPE with a commercial composite of PE with 2% of CNT, using a counter-rotating twin-screw extrusion. Subsequently, the materials underwent compression molding into cylindrical geometries at 180°C. The materials were characterized by hardness (Shore D), a modulus of elasticity, thermal conductivity and barocaloric effect. The results suggest a promising material for application as a solid-state refrigerant. Acknowledgements: The Author thank the graduated program in Mechanical Engineer/ State University of Maringa (PEM/UEM). This work was supported by Núcleo de Apoio à Pesquisa e Inovação - Energia Zero Carbono (NAPI-EZC).

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$BiFeO_3/Ag_3PO_4$ heterostructures as photocatalysts for the degradation of norfloxacin antibiotic.

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Inadequate disposal of antibiotics is a serious environmental issue for water bodies. Norfloxacin (NOR) is an antibiotic used in urinary tract and gastroenteritis. Bismuth ferrite (BFO) is a multifunctional material, while Ag_3PO_4 is recognized for its photocatalytic activity, so we investigated the photocatalytic properties of heterostructures (HT) composed of BFO with 12, 24, and 48 wt% of Ag_3PO_4 (HT12, HT24 and HT48, respectively) for the degradation of NOR. The BFO particles were obtained by the sol-gel method, calcined at 600ºC for 3 hours in a hybrid microwave oven [1]. Ag_3PO_4 materials were synthed by co-precipitation [2]. A dispersion of BFO in propanol, Na_2HPO_4, and $AgNO_3$ were used as precursors. The BFO particles and HTs were characterized by XRD, SEM, and DRS-UV-Vis. The photocatalytic study was carried out of 10ppm NOR solution under UV light for 60 minutes (3.6 mW/cm^2). The results revealed the photocatalytic efficiency of the samples was proportional to the addition of Ag_3PO_4, with an increase of 37%, 36% and 33% for HT48, HT24 and HT12 compared to BFO. The degradation kinetics were modeled as a pseudo-first order reaction, with rate constants of 0.028, 0.027, 0.024, and 0.0096 min^{-1} for HT48, HT24, HT12 and BFO, respectively. The HT48 achieved the highest degradation of NOR and it has good recyclability compared to BFO. The kinetic analysis indicates a faster degradation rate for HT48, and it is more effective in removing the contaminating compound compared to the other samples.

$BiFeO_3$ photoelectrodes for photoelectrochemical water splitting: Sol-gel synthesis and effect of annealing temperature

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Our work is focused on investigating the performance of perovskite type bismuth ferrite nanoparticles (BiFeO3 or BFO) for photoelectrochemical (PEC) water splitting at different annealing temperatures. BFO powders were prepared by sol-gel synthesis and annealed at 400, 500, 600, 700, 800, and 900°C. By electrophoretic deposition, we produced thin films that exhibited strong adhesion to the fluorine-doped thin oxide (FTO)/glass substrate. These films displayed smooth surfaces and achieved satisfactory coverage. Structural, optical, and morphological properties were studied using XRD, UV-Vis, SEM/EDS, and PEC properties determined by linear sweep voltammetry, Mott-Schottky, and electrochemical impedance spectroscopy studies. Results showed the presence of hexagonal perovskite structures in all samples, but only samples heated to 500 and 600°C had a monophasic perovskite BFO with an average crystal of 40 nm. The samples exhibited a bandgap energy of approximately 2.4 eV and flat-band potentials ranging from around 0.35 to 0.6 V vs. RHE. They preserved primarily the BFO phase up to 800°C, accompanied by the emergence of a minor Bi2O3 phase. By 900°C, BFO transitioned to a secondary phase, with the predominant phase identified as Bi2Fe4O9. Best PEC water splitting performance was observed for photoelectrodes annealed at 600ºC (BFO600), exhibiting photocurrent densities of 1.53 µA/cm2 at 1.23 V vs. RHE under one sun illumination. Additionally, the BFO600 electrode showed the lowest charge transfer resistance at the semiconductor/electrolyte interface and the best ABPE efficiency when exposed to visible light. Although the photoelectrodes didn't show an impressive PEC activity, this work brings new knowledge for understanding BFO properties and their further modifications for different PEC applications.

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Biochars as support for Pd nanoparticles applied in the electrocatalysis of the oxygen reduction reaction

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As global energy demand rises, the need to diversify and decarbonize the energy matrix becomes increasingly evident. In order to reduce the reliance on fossil fuels and address environmental concerns, hydrogen (H_2) emerges as a promising clean and renewable energy vector. This study evaluates sugarcane bagasse (C_B) and rind (C_C), pine nut shells (C_P), and pequi peels (C_{PE}) chars as supports for palladium (Pd) nanoparticles in the electrocatalysis of the oxygen reduction reaction (ORR), one of the main bottlenecks of electrochemical H_2 energy conversion [1]. For comparison of the electrocatalytic activity, Vulcan XC-72R carbon black (C_V) was used as a reference. The characterization of the materials include Raman spectroscopy, CHN elemental analysis, BET surface area analysis, X-ray diffraction, scanning and transmission electron microscopies, and energy dispersive X-ray spectroscopy. Hydrodynamic voltammetry was performed to evaluate the ORR kinetics in 0.5 H_2SO_4 medium. Additionally, polarization and power density curves were obtained in a proton exchange membrane fuel cell (PEMFC), in room temperature. The findings indicate that Pd/C_{PE} and Pd/C_B exhibit comparable electrochemical kinetics to Pd/C_V. However, the biomass-derived materials show limited effectiveness due to the formation of H_2O_2, suggested by the Koutecký-Levich analysis [2], as later confirmed by their lower activity as cathodes in the PEMFC, when using Pt/C as anode. In summary, our study highlights the potential of exploring biomass waste-derived materials for electrochemical applications in hydrogen technology, contemplating waste management and also clean and renewable energy.

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Black Bismuth Vanadate Thin Films

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The expansion of light photo-converting devices relies on affordable and eco-friendly photoelectric materials. The metallic oxide BiVO4 shows potential, but its high band gap energy limits its efficiency in converting visible light into electricity. In this study, we aimed to darken BiVO4 to enhance its absorption of visible light and thereby improve its efficiency. Thin films of BiVO4-x were produced through RF Magnetron Sputtering, following a factorial experiment design exploring the relationship between RF power, thickness, pressure, and thermal treatment. Structural and morphological analysis, including estimation of the band gap energy through the Tauc methodology, revealed that the optimal experimental setup (100 W; 200 nm; 1.5x10-2 mbar, treated) resulted in films with increased light absorption, lower band gap energy, indicating higher photoconversion activity. These findings hold promise for the development of more efficient solar energy conversion devices suitable for optical applications.

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Carbon nanomaterials-based conducting polymer-matrix nanocomposites for energy storage

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The interest on the properties of conducting polymers (CP)-matrix nanocomposites is related to the possibility of the different applications of these materials, such as energy storage and conversion and membranes for liquid separation [1-2]. Our research group has been studying the properties of these materials for application in different areas. Our main goal is to use graphene oxide (GO) and carbon black with CP, as well as to study the effect of different CP:carbon nanomaterials composition ratios on its properties. The XRD, Raman and FTIR spectroscopic characterization confirmed the OG and polyaniline were obtained by the syntheses processes used. Our results have shown supercapacitors with specific capacitance values, normalized by the material mass, from around 200 up to 270 Fg -1.

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Characterization of Thin Films of GO and PEDOT:PSS Applied in Organic Photovoltaic Devices

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The exploration of alternative materials for charge transport in organic solar cells has attracted considerable interest [1]. An emerging solution involves using graphene oxide (GO) dispersed in water with poly(3,4-ethylenedioxythiophene) doped with polystyrene sulfonate (PEDOT:PSS) as the hole transport layer (HTL) or even as a potential replacement for indium-tin-oxide electrodes [2]. This study focuses on thoroughly examining these devices that utilize GO combined with PEDOT:PSS as both the HTL and electrode. The GO was synthed using the modified Hummer's method, and thin films were fabricated via the blade coating technique. Morphological analysis was conducted using scanning electron microscopy and atomic force microscopy, while optical properties were assessed through UV-visible spectroscopy and Fourier-transform infrared spectroscopy. These analyses aim to provide deeper insights into the performance of the GO with PEDOT:PSS solution for photovoltaic devices based on organic polymers.

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Comparative Evaluation of Thiophene and Thienothiophene as Electron-Donating Monomers in D-A Structure Photovoltaic Polymers

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Thiophene has been extensively used in novel photovoltaic polymers with a D-A (donor-acceptor) structure, serving as an electron-donating monomeric unit, owing to its cost-effectiveness and its ability to yield polymers with low bandgaps [1]. Thienothiophene, bearing a closely related structure to thiophene, was employed with the objective of enhancing conjugation within the polymer backbone, while aiming to enhance its favorable characteristics. In this study, three acceptor monomeric units (M1, M2, and M3) were chosen, each paired separately with thiophene (T) and thienothiophene (TT), to synthe D-A polymers, enabling a comparative assessment of the influence of the donor unit. For the acceptor monomers M1 and M2, the optical bandgap was found to be smaller in their combinations with TT donor. However, the synthesis reactions of the polymers produced with TT exhibited significantly lower yields compared to those synthed with T. The acceptor monomer M3 yielded polymers with the lowest optical bandgap value (1.27 eV), which remained consistent with both T and TT donors. Nevertheless, the polymer containing TT exhibited very poor solubility, posing challenges for its application in photovoltaic devices. Consequently, due to issues related to yield and solubility associated with TT, only polymers containing T donor were employed for device fabrication. Among these, the T-M3 polymer demonstrated the most promising performance, exhibiting an efficiency of 3.56% in devices assembled under atmospheric conditions, without the use of a glove box. The device efficiencies of the T-M1 and T-M2 polymers were 0.2% and 0.43%, respectively. In conclusion, for the acceptor monomers investigated in this study, polymers synthed with thiophene proved to be more promising than those synthed with thienothiophene.

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COMPARISON OF HIGH ENTROPY ALLOYS Ti35V35Nb20Cr5Mn5; Ti32V32Nb18Cr9Mn9 AND Ti27.5V27.5Nb20Cr12.5Mn12.5 IN AS-CAST AND HEAT-TREATED CONDITIONS FOR HYDROGEN STORAGE

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New energy sources are currently being explored around the world, seeking to reduce dependence on fossil fuels. Recently, hydrogen has been studied as a fuel with greater potential for this replacement. The problem surrounding this class of energy is precisely how this hydrogen is stored. The difficulties encountered when storing H2 in liquid and gaseous form result in high pressures and low efficiency. Therefore, materials are being developed that can store hydrogen in solid form, through metal hydrides. This work aims to develop High Entropy Alloys (HEA) of the TiVNbCrMn system for application in hydrogen storage and evaluate their hydrogenation and cycling potential. The design of the alloy compositions was carried out using the Thermo-Calc Software aiming at alloy compositions with, BCC (solid solution) and Laves as a second phase. The results obtained in the hydrogenation properties will be compared, correlating them with the microstructure and phases present in the HEA alloys designed and developed, in as-cast and heat-treated conditions. The compositions Ti35V35Nb20Cr5Mn5; Ti32V32Nb18Cr9Mn9 and Ti27.5V27.5Nb20Cr12.5Mn12.5 were produced by arc melting and characterized by X-ray diffraction (XRD) and scanning electron microscopy (SEM) techniques. The three alloys mentioned have different fractions of Laves phase, which directly affects the storage and cycling of hydrogen within the alloy structure. The results show absorption values in order of 3.5% wt. of hydrogen in the Ti27.5V27.5Nb20Cr12.5Mn12.5 alloy in the as-cast condition, but low kinetics was a recurring factor in the raw fusion alloys. As the compositions presented great absorption potential, the thermal treatments carried out showed that the best microstructural control and ideal proportions of Laves promoted improvements in the maximum absorption capacity and hydrogenation kinetics of the Ti35V35Nb20Cr5Mn5 Alloys; Ti32V32Nb18Cr9Mn9, despite having an incubation period upon activation.

Composite materials based on vulcanized natural rubber and magnetic particle dispersion.

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Composites are multiphase materials which are composed of at least two materials, to maintain the characteristics of each individual material. As a result of a variety of industrial and technological needs, composite materials have emerged as a preferred material since they can be tailored according to the desired applications and properties. Therefore, the present study aimed to obtain a flexible composite of vulcanized natural rubber (NRV) reinforced with magnetic particles (PM). Two-phase NRV/PM composites were prepared using a two-roll open mill, in which NR (100 phr), accelerators, and crosslinking agents were kept constant, and PM concentration was varied at 10, 20, and 30 phr. To evaluate the synergy between the two phases and their effect on the composites' final properties, thermal, mechanical, and electrical properties were studied for two-phase NRV/PM composite samples. Using rheometric analysis, it was possible to determine the ideal vulcanization time (t90), which varied between 4 and 5 minutes, indicating that the dispersion of PM influences the vulcanization parameters of the NRV matrix. Increasing the PM concentration also resulted in an increase in maximum torque. In the TG/DTG analysis, samples of the biphasic NRV/PM composite with different concentrations of PM displayed a thermal profile like pure BNV, that is, with a mass loss event between 300-450°C originating from structural degradation of the NRV. According to mechanical tests performed in tensile mode, PM dispersion in the NRV matrix led to an increase in stress at break while strain at break decreased. An analysis of ac electrical conductivity ($\sigma'(f)$) in the alternating electric field regime revealed that all samples exhibit frequency-dependent behavior, which is typical of disordered materials. Finally, the two-phase NRV/PM composite samples have the potential to be used as electromagnetic radiation shielding devices because of their good thermal and mechanical properties.

Composites of PDMS with incorporation of Graphene quantum dots applied as encapsulant of photovoltaic cells.

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Photovoltaic panels are covered by films (encapsulant) usually composed of Ethylene Vinyl Acetate (EVA) responsible for protecting cells against aging caused by ultraviolet (UV), heat, moisture [1]. However, some encapsulants present degradation earlier than established in the warranty of the modules. In this sense, several research searching for new encapsulating materials or even evaluating incorporation of nanomaterials to improve the encapsulant properties. Here, we propose to replace the EVA layers of photovoltaic modules with a new polymer composed of polydimethylsiloxane (PDMS) and graphene quantum dots to avoid aging process and degradation due to exposure to ultraviolet radiation without reducing the efficiency of modules and thus prolonging their service life. Graphene quantum Dots were acquired from Aldrich. The PDMS used will be Sylgard 184 in the proportion of 10 (base): 1 (curing agent) where the quantum Dots will be dispersed and then deposited on the solar cells by casting and cured in an oven at 100oC for 30 minutes. The photovoltaic cells were evaluated in a solar simulator comparing the power generation with and without polymeric coating and in UV-Vis spectroscopy to evaluating the change in the transmittance of the composites, proving the possibility of use the composite as encapsulants in photovoltaic cells.

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Composites of PDMS with incorporation of SiO_2 applied as encapsulant of photovoltaic cells

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Used in photovoltaic modules, the encapsulant is a protector film deposited on the solar cells that protects them against humidity, dust and UV radiation. The polymer ethylene vinyl acetate (EVA) is used on a large scale as an encapsulant, however it can present rapid degradation, reducing the efficiency of the photovoltaic modules.[1] Other polymers are studied to replace EVA, among them polydimethylsiloxane (PDMS) stands out for transparency and UV stability. Moreover, the addition of silica nanoparticles (SiO_2) has the potential to reinforce the polymer resistence.[2] This research presents a new encapsulant developed by PDMS and SiO_2 composites for application in photovoltaic panels as an alternative to EVA, with the goal to extend its service life. Laboratory tests were performed comparing pure PDMS with the addition of SiO_2 at concentrations of 1.5% to 5.7% (wt/wt%). The characterization was performed by exposing the cells with and without coating to a light source and measuring the energy generated, as well as analyzing light transmittance by UV-Vis spectroscopy. It was observed that lower proportions of SiO_2 do not significantly alter the transmittance (90% to 1.50% (wt/wt%) of SiO2) and can be used in composites. Regarding efficiency, the incorporation of SiO_2 showed no significant changes. In a next step, the service life of the composites will be tested by exposure to UV light in aging chamber.

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Conductive polycarbonate/carbon nanoparticle nanocomposites for the production of 3D printing filaments.

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The present work aimed to develop functional nanocomposites that use a polycarbonate matrix (PC) doped with carbon nanoparticles to produce 3D printing filaments and printed test specimens. Different carbon nanomaterials were used, such as black (NF), graphene nanoplatelets (GNP) and single-walled (SWCNT) and multi-walled carbon nanotubes (MWCNT). The final aim of the study is to produce bipolar plates by 3D printing, which will later be used in ethanol fuel cells. The materials were produced using a conical twin-screw mini-extruder, and different processing parameters and compositions were tested. The electrical conductivity of these composites was characterized using 2- and 4-point probe electrical impedance methods, indicating a considerable increase in conductivity with the use of nanoparticles. Besides this, the polymers also had the addition of acrylonitrile butadiene styrene (ABS), varying in percentage between 10-50%, in order to improve the mechanical properties and facilitate the filament production process.

Cooling with torsion: how shear stresses in Ni-Ti can drive future cooling devices

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Traditional cooling devices are based on vapor-compression systems, which use greenhouse gases and it is estimated to consume up to 30% of the total global electricity[1]. A promising alternative is solid-state cooling systems based on materials that present thermal and entropic responses when subjected to external stimuli variations (such as magnetic, electric or stress fields). These materials can convert energy from their respective fields into thermal energy in a process called i-caloric effect (i-CE). In past decades, many remarkable materials have shown promising i-CE, however, challenges such as the high costs of raw materials, the need for high-intensity fields, and even the use of unsustainable materials remain. Recently, i-CE materials that operate under stress field stimulus gained attention due to their variety, high i-CE, and ability to address some of the aforementioned challenges[2]. Most of these materials were studied under isotropic (barocaloric effect) or uniaxial stresses (elastocaloric effect). However, the application of shear stress (torsiocaloric effect) on i-CE materials is very recent with few studies reported in the past years. Nonetheless, the torsiocaloric effect is very promising due to its high i-CE achieved with low shear stresses[3]. In this work, we explored the shape memory alloy Ni-Ti under shear stress to understand its i-CE. Applying shear stress induced martensite-austenite transformation accompanied by the release/absorption of heat when the torsion was applied/removed. Our findings highlight the potential of Ni-Ti for cooling and heating applications based on the torsiocaloric effect. Ni-Ti could be a sustainable material with high cooling capacity, performing among the best i-CE materials studied so far.

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D-π-A azine/cobaloxime dyes for photocatalytic water splitting

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Fossil fuels remain the main source of energy used throughout the world, despite being associated with a high environmental impact. The decrease in discoveries of new oil sources, the growing energy demand and the global call for minimizing climate changes caused by human action make the search for sustainable energy sources urgent [1]. In this scenario, a promising alternative for the future of the global energy sector is the production of molecular hydrogen through the photocatalytic water splitting process [2,3]. A new series of push-pull type organic photosensitizers (1a-c), applicable to photocatalytic processes for molecular hydrogen production, were synthed, structurally characterized and subjected to preliminary theoretical evaluation of their electronic properties. Next, it is proposed to insert a fragment with photocatalytic properties, already described in the literature, a cobaloxime-type complex with a cobalt(III) metal center, into the electronic acceptor portion of substances 1a-c. This change aims to optimize the photocatalytic property of the previously obtained systems. Therefore, in this work three new photocatalysts (2a-c) were synthed with the insertion of the cobaloxime group. This step was confirmed using a single crystal XRD technique. All new substances are in the characterization phase and will have their photocatalytic efficiency evaluated.

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Defect engineering and bang gap control in perovskites films for silicon tandem solar cells application.

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The wide bandgap lead-halide perovskites (LHP) inorganic or hybrid organic-inorganic has become competitive candidates for tandem solar cells each of them with their own advantages and drawbacks [1]. However, ABX_3 perovskite compositions with single A, B, and X species have not delivered the desired high performance and stability. On the other hand, the mixed A-Site cation $FACsPbI_3$ composition despite their excellent humidity and chemical stability have shown residual stresses and cracks due its undesired morphology and phase [2]. Herein, we demonstrate strategies for obtaining high quality perovskite films with composition $FA_XCs_{1-X}Pb(I_xBr_{1-X})_3$. Several compositions and process parameters were explored for preparing films based on changes in solvents, processing additives and quenching approaches. The band gap control based on composition adjustment was performed, increasing the amount of bromine and maintaining the film quality for tandem solar cells applications. Compact, smooth and high quality perovskite films have been successfully obtained by gas quenching treatment on HTL layer coated ITO/glass substrates with increased environmental stability evaluated by spectroscopic techniques.

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Degradation of microplastics in photoeletrocatalytic processes with TiO_2 nanotubular structures.

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Pollution caused by micro and nanoplastics present in water bodies has reached alarming dimensions, causing environmental impacts of large proportions and damage to human health that is not yet fully understood [1]. The physical retention of these particles as a means of separation and treatment in effluents are measures that do not completely solve the problem, with great possibilities of starting new cycles of contamination [2]. In this work, undoped and doped TiO_2 samples were synthed by the anodizing process under different conditions to obtain the materials Al-TiO_2, N-TiO_2 and TiO_2 undoped with mixture of anatase and rutile phase. Samples were analyzed by XRD, SEM-EDS, XPS, Raman and UV-Vis spectroscopy. The different materials obtained were subjected to photoelectrocatalytic tests for the degradation of polyethylene microparticles suspended in aqueous sodium sulfate solution (1M), under simulated solar irradiation and application of a potential of 0.7 V for 6 h. Polymer degradation was monitored with total organic carbon (TOC) analysis of the solution obtained in each test. Although polyethylene presents greater resistance to degradation, due to the absence of functional groups that could facilitate the fragmentation of the molecular structure, an increase in the concentration of carbon dissolved in solution of up to 37% was observed, in relation to the value obtained in photolysis, being a strong indication of the occurrence of degradation of this polymer. In addition to the appearance of terminal functional groups observed in the FTIR spectra of the particles obtained after the photoelectrocatalytic test.

Keywords: TiO_2, photoeletrocatalysis, microplastic, degradation.

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Deposition and characterization processes for obtaining layes in solid oxid electrolyzer

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Green hydrogen has the potential to replace fuels that, when burned, emit polluting gases, such as natural gas, diesel, and kerosene [1]. These are responsible for significant CO_2 emissions, thus posing a challenge in limiting global warming. Among the available methods for producing Solid Oxide Electrolysis Cells (SOEC), there are three well-known techniques, i.e., spin coating, tape casting, and screen printing [2]. High-temperature SOECs are currently at the technology readiness level (TRL) 7, operating in the 600–900 °C range at less than 15 bar pressure, with 80 % efficiency and 2.99–7.02 USD/kg hydrogen cost [3]. In this context, these techniques will be employed in creating suspensions, which will be used to manufacture tapes and carry out layer depositions. The ultimate goal is to construct a SOEC, primarily composed of anode, cathode, and electrolyte, for green hydrogen production. Special attention will be given to the formation of the electrolyte from 8 mol% yttria-stabilized zirconia, as well as the electrodes from strontium-doped $LaMnO_3$, strontium-doped lanthanum cobalt ferrite, or lanthanum strontium cobaltite. Later, these layers will be investigated by X-ray diffraction and scanning electron microscopy. This approach aims to develop more sustainable technologies for H_2 production and contribute to greenhouse gas emission reduction, promoting a cleaner and ecologically healthier future.

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Design of technical ReOx/TiO2 catalyst for CO2 conversion into methanol in a pilot plant

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Methanol production from CO2 using a ReOx/TiO2 catalyst offers a promising solution to address the challenges of climate change. Methanol is a very important raw material in chemical industry, several other products can be obtained starting from methanol and it is also a very flexible liquid fuel [1]. The ReOx/TiO2 catalyst was successfully prepared on a laboratory scale with no additives and using water as solvent, as already reported by our group [2]. For large-scale catalyst production, the key challenge is to produce a structured catalyst (pellets) to maintain the catalyst activity even by using additives to improve the mechanical properties. The pellets have been prepared through extrusion method, from a paste composed by nanoparticles of different titania (P25, anatase and rutile), as support, with silica as a binder, obtaining pellets with diameter of 1 ± 0.2 mm and length of 4.1 ± 1.6 mm. Different Re contents were tested, from 0.5-5% (w/w) to evaluate catalytic performance for methanol production. Re content was validated using ICP OES. The different materials were characterized using TEM, XRD, BET surface area and XPS. Surface area remains unchanged before and after the addition of Re and after thermal treatment. The catalytic test revealed that the titania phase has a strong influence on the selectivity for methanol, with values for P25 of 67%, anatase of 80% and rutile of 30%. Methanol STY ranges from 0.3-0.8 mmol h-1g-1, for the different catalyst. The CO2 conversion increases with increasing Re content, however from 3-5% (w/w) a gradual loss of selectivity for methanol occurs and an increase in methane production is observed.

Developing Piezo-Photocatalysts for Industrial Effluent Degradation

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Water scarcity is a pressing global challenge due to limited usable water resources, which is vital for human survival. Industrial activities, particularly the release of organic compounds like dyes, contribute significantly to water pollution. Effective treatment of industrial effluents is therefore crucial for preserving both the environment and human health. This study focuses on developing heterogeneous piezo-photocatalysts for degrading organic compounds [1] and enhancing water treatment processes. In the present work we synthed nanostructured Bismuth Ferrite ($BiFeO_3$), a well-known magnetoelectric compound, by using the fast-firing sintering followed by high energy ball cryomilling protocol [2]. Additionally, heterojunctions with magnetic nanoparticles (Magnetite) were synthed to enhance the catalytic performance, by preventing charge recombination and allowed its magnetic recovering/filtration. Various techniques including scanning electron microscopy, ultrasonic waves, transmission electron microscopy, and X-ray diffraction analyze the physical, chemical, and structural properties. Future analyses will evaluate synthed catalysts efficiency in degrading organic compounds, analyzing its potential for advancing water treatment technologies.

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Development of an electrochemical capacitor based on carbon black/polyaniline/lignin electrodes

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Compared to batteries, electrochemical capacitors have low specific energy [1]. To mitigate this disadvantage of capacitors, this work aims to manufacture and optimize a prototype of a symmetric electrochemical capacitor (pseudocapacitor) whose electroactive material is a composite carbon black (CB)/polyaniline (PANI)/lignin (LIG)/paraffin (PAR) (low-cost materials and easy production). Charge storage occurs in a non-faradaic way (in the electrical double layer) and a faradaic way (involving redox processes); this is, therefore, a pseudocapacitor [2]. Preliminary tests using cyclic voltammetry in a three-electrode system in a 0.5 mol dm-3 H2SO4 medium using a composite electrodes formed by CB:PANI:LIG:PAR were evaluated in the following mass proportions: E1 (75:0:0:25), E2 (50:0:25:25), E3 (50:25:0:25) and E4 (50:20:5:25). It was observed that the specific charge that can be stored in these electrodes is much higher when PANI is present. Cyclic voltammetry data indicated that adding LIG confers greater chemical stability to PANI without compromising charge storage. These preliminary results showed the great potential of this composite material in the manufacture of an electrochemical pseudocapacitor.

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Development of catalyst supports based on sugarcane bagasse for the electrocatalysis of nitrogen cycle species.

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The presence of nitrite and nitrate in aquatic and terrestrial ecosystems causes environmental damage and has become a global problem that requires immediate and efficient solutions. Given this, new materials that can reduce environmental contaminants have been proposed. This work aimed to synthe and characterize catalyst supports based on sugar cane bagasse for use in the electrocatalysis of nitrogen cycle species. The supports were obtained by calcinating a previously washed and dried sugarcane bagasse sample under a controlled atmosphere and different temperature conditions. The supports prepared were modified with metallic platinum using the shake bake method to obtain the final catalysts. The materials were characterized by thermal analysis (TG-DTA/DSC), X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), and FTIR and Raman spectroscopies. The general electrochemical characterization of the materials and their catalytic activity towards nitrite and nitrate electroreduction reactions were evaluated using conventional techniques (CV, CA, RRDE) in acidic and alkaline aqueous solutions. The reaction mechanisms and the detection of intermediates were studied by online electrochemical mass spectrometry (OLEMS). Results showed that sugarcane bagasse-based supports display excellent conductivity and catalytic activities towards the reactions studied. This work contributed to developing efficient and inexpensive materials for the electrodegradation of these species, which can be applied to the electrochemical environmental remediation field.

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Development of Multi-cell Supercapacitor Devices Utilizing Optimized Polypyrrole Electrodes

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The evolution of supercapacitors has been a central focus in energy storage research, with polypyrrole (PPy) emerging as a promising material due to its high specific capacitance and stability. This work describes the use of electrodes made from an optimization of PPy synthesis and the subsequent construction of multi-cell supercapacitors with 2, 4 and 6 electrodes, with the aim of improving energy efficiency and storage capacity.

The synthesis of PPy was improved through direct polymerization techniques combined with a convective mass transport mechanism, in addition to the grinding of the metal substrate, favoring the modification of the material's morphological properties. The construction of the devices involved the manufacture of a multi-cell shell via 3D printing, which allowed the electrodes to be associated in parallel without the need for a separator.

The devices were electrochemically characterized by cyclic voltammetry (CV) and galvanostatic discharge (GCD). The results indicated that grinding the steel current collectors significantly improves the specific capacitance of the electrode. In addition, convection during the synthesis of the PPy films resulted in a more uniform distribution of the polymer and increased capacitance.

After the electrochemical synthesis of the polypyrrole electrodes, the devices were assembled with an aqueous electrolyte and characterized electrochemically. The cells with 4 and 6 electrodes were connected in parallel, forming a multilayer sandwich device. The supercapacitors with multiple PPy electrodes in parallel configurations showed an increase in capacitance and energy density. A comparison between devices with 2, 4 and 6 electrodes revealed that the 6-electrode device had approximately 7.25 times the capacitance of the 2-electrode device, indicating a substantial improvement in charge storage capacity. These results suggest that advanced configurations can significantly improve supercapacitor technology.

Development of polyvinylidene fluoride nanocomposites with the addition of carbon nanoparticles for the production of 3D printing conductive filaments.

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In this work, the main objective was the development of functional nanocomposites based on a polyvinylidene fluoride (PVDF) matrix combined with carbon black (NF), graphene nanoplatelets (GNP) and single-walled (SWCNT) and multi-walled carbon nanotubes (MWCNT). The composites were compounded and processed into conductive filaments using a conical twin-screw mini-extruder, in which different variables were tested, such as: the types of carbon nanoparticles and their concentrations (ranging between 10-30% for graphene and carbon black and around 1-5% for nanotubes); processing time (ranging from 0 to 10 minutes); and the rotation speed of the screws (from 100 to 300 RPM). Finally, the electrical conductivity of these composites was characterized using 2- and 4-point probe electrical impedance methods, indicating an increase in conductivity with the use of nanoparticles, going from a value of 10-12 S/cm of the pure polymer to values in the order of 100 S/cm for the nanocomposite.

Eco-Friendly Organic Semiconductive Nanoparticles as Active Layers of Organic Solar Cells

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With the increasing global energy consumption and the decreasing fossil resources for energy production, the need for development of clean and renewable energy sources has become urgent. Among the many energy production technologies, the Organic Photovoltaic Devices (OPVs) have become one of the most promising technologies due to their lightweight, scalability, flexibility and low-cost. One of the biggest challenges to overcome in the OPVs manufacturing process in addition to the complex layers morphology control is that the best performing materials use organic, toxic and flammable solvents. These toxic solvents unnecessarily increase the environmental impact of the future OPV technologies. With the nanoparticulation of those inks we can obtain water based polymer nanoparticle conductive inks, which can be used for further application in organic electronics, such as in OPVs. The aim of this study is to produce and analyze the possibilities of applications of donor and donor:acceptor nanoparticle inks as active layers for OSCs. This study also compared the use of both fullerene and non-fullerene acceptors in the nanoparticle solutions used for the active layers. With the slot die, blade coating and spin coating techniques, homogeneous films were obtained in glass and acetate substrates and the samples were used for optical, morphological, electric and chemical analysis, showing potential of the polymer nanoparticles to be used as active layers. The OPVs produced were analyzed using the open circuit voltage (Voc) and the short circuit current density (Jsc) parameters. Stability studies were also made using an weathering simulation chamber following the ISOS-L-2 protocol, comparing organic solvents and the water-based nanoparticle inks, showing that the nanoparticle inks are more stable than the organic solvent ones. Therefore this study demonstrates the possibility of obtaining flexible water based organic photovoltaics.

Effect of 3D Printing Orientation on the Electrical Properties of Test Specimens Fabricated by the Fused Filament Fabrication Technique

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Fuel cells are a promising technology to compose a set of solutions that can advantageously replace combustion engines in automotive vehicles. Among the various challenges present, we highlight two in particular: the weight of the components and processability. The first will have a direct impact on energy autonomy, while the second impacts the ability to produce shapes that are convenient both from the point of view of chemical kinetics (channel format) and the cost associated with the operations necessary for manufacturing.In this study, commercial conductive ABS (Acrylonitrile Butadiene Styrene) filaments were used for 3D printing test specimens to investigate the effect of printing angle on electrical properties. The study varied the printing angle from 0°, 45°, 90°, and ±45°, as well as the angle of the fabricated parts at 0°, 45°, and 90°. The Van der Pauw method was used for resistivity measurement.Furthermore, the effect of heat treatment during and after printing was evaluated. The results indicate that heat treatment during printing promotes a significant increase in the conductivity of printed parts, followed by the influence of the printing angle.

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Effect of curing agent on protonic conductive properties of polymeric membranes based on a semi-interpenetrating polymeric network

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Protonic Exchange Membrane Fuel Cells (PEMFC) are a promising alternative for electric vehicles. The Nafion® membrane (polymeric solid electrolyte, PSE) is a market leader used in these devices and has a phase separation in the nanoscale, giving rise to a morphology of hydrophobic and hydrophilic domains. Few studies have used semi-interpenetrating polymer network systems (SIPN) as a base for PSE. This work aims to compare the effect of the curing agent on SIPN membrane conduction properties. The synthesis employed bisphenol A (DGEBA) and the curing agents DDS (Diamino Diphenil Sulfona, SIPND) and Teta (Trietilenotetramine) in the presence of polyethyleneimine (PEI), which varied from 33 to 50 % (m/m) concerning the total mass [1]. All samples formed membranes by casting, with high dimensional, thermal, and electrochemical stability. FTIR, RMN, and AFM characterized the samples. Electrochemical impedance spectroscopy (EIS) employed frequencies from 10 mHz to 1 MHz, between 20 and 80 °C, with steel electrodes. The membranes were studied after immersion (24 h) in an H_3PO_4 20 % aqueous solution. The band's disappearance at 905 cm^{-1} (FTIR) indicates the opening of the epoxy ring in the network formation reaction, which RMN confirmed. AFM observed that the hydrophilic nanometric domains (PEI), homogeneously dispersed by the epoxidic and hydrophobic matrix, are lower for the TETA than for DDS. It is an effect expected, as cure agent molecules have different strategically chosen structures to infer nanostructural changes in SIPN. EIS spectra (Nyquist) present a capacitive-resistive behavior, characteristic of low resistance values ionic membranes. The samples showed conductivity (σ) thermoactivated with maximum values reached at 80 °C, $SIPN_{T50} = 1.04 \times 10^{-3}$ and $SIPN_{D50} = 8.79 \times 10^{-2}\ \Omega^{-1}cm^{-1}$ (triplicate averages).

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Effect of Different Fluorides in the MXenes' synthesis

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MXenes are 2D compounds that hold enormous potential for several technological applications, particularly in energy conversion and storage [1]. Despite their potential uses, producing these materials with high quality, i.e. contamination-free and defect-free lamellas efficiently exfoliated and delaminated, is a challenging task. Moreover, it is essential to develop environmentally friendly routes of exfoliation and delamination of the precursor MAX phase to obtain MXenes with adequate properties since the classical routes involve the use of concentrated fluoridric acid solutions. In this study, we investigated new synthesis protocols for producing the Ti3C2Tx MXene from the Ti3AlC2 MAX phase. The HF etchant was replaced by HCl and LiF solution. Further, we proposed the the substitution of LiF by other fluorides, NaF and KF. To analyse the effect of the synthesis protocol on the MXene produced, an extensive set of characterizations was performed through XRD, SEM-EDS, XPS, and TEM. In addition, the electrochemical properties of the obtained MXenes were characterized by electrochemical impedance spectroscopy and Cyclic Voltammetry. The obtained results indicated that all routes produced MXenes with good structural features. Concerning the electrochemical properties, a higher capacitance was obtained for the MXenes exfoliated with LiF. The obtained results allowed to better understand the play rolled by different types of fluorides on the synthesis and features of the final 2D compound.

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Effect of Severe Plastic Deformation on the Electrochemical Hydrogenation of a β Titanium Alloy

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Metal hydrides are promising materials for hydrogen storage applications such as solid-state tanks and Ni-MH batteries due to their high volumetric storage capacities. To enhance the hydriding / dehydriding properties of hydride forming alloys, severe plastic deformation routes have been investigated in the literature In the present work, we investigated the effect of Severe Plastic Deformation (SPD) through the Equal Channel Angular Pressing (ECAP) technique on the microstructure and electrochemical properties of the Ti-29Nb-13Ta-4Mo alloy (β Titanium alloy). The ECAP processing was carried out varying the number of passes and the obtained samples were characterized by Confocal Scanning Laser Microscopy (CSLM), Scanning Electron Microscopy (SEM), and X-ray Diffraction (XRD). The effect of ECAP processing on the electrochemical hydrogenation and dehydrogenation was analyzed by galvanostatic cycles of charge and discharge in alkaline. The interplay between ECAP processing, microstructure and electrochemical properties of the alloy is discussed.

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Effects of the Rheological Parameters for Mxenes and Graphene nanofluids under temperature variation

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Nanofluids are composed of a dispersed fraction of nanostructures in a base fluid to enhance the base fluid characteristics such as thermal conductivity, and tribology aspects. However, the addition of nanostructures in a fluid might affect flow characteristics and rheological properties. This work considered graphene nanostructures, obtained from a commercial source and synthed Mxenes dispersed in a PAG oil as base fluid. Mxenes is a 2D nanostructure with a high potential for enhancement of conventional applications. In this work, a 3D MAX phase, Ti3AlC2, was submitted to a chemical etching through an agitation process with LiF and HCl to obtain the 2D Mxenes, Ti3C2Tx. The nanofluids were prepared through the 2-step method with 0.1%wt. and 0.5%wt., considering a stirring process and sonication bath for 30 minutes. The characterization of graphene and Mxenes nanostructures was made through SEM and TEM images, and XRD patterns. For the verification of nanofluid stability and in-fluid nanostructure distribution, the Zeta potential and dynamic light scattering were used, respectively. A rotational rheometer was used for the measurements of viscosity and flow curves in the temperature range of 20ºC to 60ºC. The viscosity and flow curves were plotted for 30 seconds considering a shear rate range of 0 to 1000s-1. The results showed that Mxenes nanofluid tends to have a smaller viscosity than graphene nanofluid for the shear rates below 200 s-1. For the temperature of 20°C, the graphene nanofluid showed a lower viscosity than Mxenes for shear rates below 200 s-1. The Mxenes nanofluid showed a more enhanced flow curve than graphene nanofluid for shear rates above 200s-1. Graphene and Mxenes showed a pseudoplastic behavior for the shear rate range from 0 to 200s-1 in the analyzed temperature range from 20°C to 60°C. At shear rates above 200s-1s, a Newtonian behavior was noticed for Mxenes and graphene nanofluids for temperatures above 30°C.

Effects of the Tribological Parameters for Mxenes and Graphene nanofluids in a reciprocating system

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Nanofluids are dispersions of nanoparticles into a base fluid to enhance the properties of the base fluid. Over the last few years, graphene has been proposed as a 2D nanostructure to enhance the base fluid properties. However, the emergence of another 2D nanostructure, Mxenes, has been considered to improve the tribological, thermal, and rheological properties. This work considered comparing tribological characteristics between Mxenes and graphene nanofluids with 0.1%wt. and 0.5%wt. For the nanofluid preparation, it was considered commercial graphene nanostructure and synthed Mxenes nanostructures. Mxenes are 2D nanostructures obtained from the MAX phase (3D nanostructure) through chemical etching. The 3D MAX phase, Ti3AlC2, was mixed with a certain amount of HCl and LiF under a centrifugation process, thus a washing process was performed to obtain the lamellar 2D Mxenes, Ti3C3Tx. Thus, the 2D nanostructures were characterized through SEM and TEM images and XRD patterns. The nanofluids were prepared using the 2-step method by dispersing the Mxenes and Graphene in PAG oil through stirring and sonication processes. The nanofluid stability and the nanostructure of nanofluids were measured through Zeta potential and Dynamic Light scattering analyses, respectively. A nanofluid film of 2-4µl was poured over a flat aluminum surface, thus a setup with an iron sphere positioned in a nanotribometer performed a reciprocating movement over the flat surface generating a wear track of 2mm length. After the reciprocating process, the roughness and wear volume were evaluated by measuring the wear track characteristics using a confocal microscope. The results showed that higher mass fractions of graphene and Mxenes tend to generate smaller wear track volumes and smoother roughness parameters. The Mxenes nanofluid produced smaller wear track volumes than graphene nanofluids at the same mass fraction.

Electrical conductivity in epoxy-carbon nanocomposites, for fuel cell application

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One of the emerging technologies, with a potential for automotive applications, is fuel cells. This type of technology can generate electrical energy through chemical reactions fed by hydrogen or a liquid fuel, such as ethanol or methanol. One of the most promising types of fuel cell is based on ionic polymeric membranes. This kind of cell has many components, including bipolar plates, which must be electrically conductive. This work focuses on the development and characterization of electrically conductive polymeric nanocomposites based on epoxy, carbon nanoparticles and carbon fiber, aiming at fuel cell applications. The composites were produced with different filler concentrations using high energy dispersing devices and a hydraulic hot press. The electrical, chemical and mechanical properties of the samples were then evaluated.

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Electrocatalysis on molybdenum nanodots anchored in graphene oxide with selectively controlled properties.

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Ammonia is essential for modern society and emerges as a possible hydrogen carrier in a future hydrogen-based energy infrastructure. The Haber-Bosch process is the main method for ammonia production, which is energetically costly and polluting. The electroreduction of nitrogen to ammonia at ambient temperature and pressure, using electrical energy from renewable sources, arises as a clean and economical alternative. Electrocatalysis can foster efficient and sustainable nitrogen-to-ammonia conversion. Literature shows that Mo-based materials display a promising conversion efficiency and maximum currents towards nitrogen reduction reaction (NRR). These materials can be anchored on graphene oxide (GO) and its variations (rGO) to improve catalytic activity by modulating the surface oxygenated groups with systematical variation of synthesis parameters. Samples were characterized by XRD, TG, DSC, FTIR, Raman spectroscopy, SEM, and NMR. The electrochemical characterization was carried out in an acidic medium with cyclic voltammetry (CV) and chronoamperometry (CA). The results confirmed the possibility of establishing selective control of surface oxygenated species of rGO. Molybdenum nanodots showed a crystallite of c.a. 11 nm and were anchored to the graphene-based supports. Composites prepared showed differences in catalytic activities towards HER and NRR depending on the metal-support interaction caused by the presence of different surface groups. The study allowed elucidation of the relationships between material properties, catalytic activity, and the reactions mechanisms, which is essential to improve the technology for electroconverting nitrogen to ammonia through efficient and sustainable routes.

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Electrochemical characterization of the ZnO-CNT structure: impact of carbon nanotubes on the (photo)electrochemical properties of zinc oxide

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Zinc oxide demonstrates a broad range of technological uses such as electronics, solar cells, sensing, catalysis, and biomedical applications. Similarly, carbon nanotubes (CNT), are also investigated in the electronics and energy storage areas because of their conducting properties [1]. In this sense, this work aims to incorporate carbon nanotubes into the zinc oxide matrix to be used as an electrochemical sensor for ascorbic acid, due to its high surface area and conductivity properties [2]. Cyclic voltammetry (CV) from 0 to +1.0V (scan rate = 20 mVs^{-1}), chronoamperometry at +1.0V for 300 s, and electrochemical impedance spectroscopy from 100 kHz to 0.05 Hz were used for electrochemical characterization. Through CV, we observed a linear increase in the photocurrent increasing the ZnO layers, reaching a maximum at 4 layers. Sodium sulfate 0.1mol L^{-1} was used as an electrolyte solution, and aliquots of 1mmol L^{-1} ascorbic acid solution were added to the Na_2SO_4 during sensor construction. The results indicated that the incorporation of CNTs into the zinc oxide was successful, with cyclic voltammetry showing a linear increase in current upon UV light exposure up to a 4-layer ZnO. Electrochemical impedance spectroscopy results showed that adding ascorbic acid resulted in a linear decrease in charge transfer resistance, demonstrating higher sensitivity for the carbon nanotube-modified electrodes. A sensitivity comparison was done using the slope of the graphic Z' vs. concentration of ascorbic acid, on 0.1 Hz because the better correlation coefficient of EIS is in range of 1 to 0.1 Hz, resulting in 1048.72 Ω μmol^{-1} L for ZnO modified with CNTs and 613.76 Ω μmol^{-1} L for ZnO. This gain in sensitivity helps detect acid ascorbic in lower concentrations than pure ZnO.

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Enhanced H_2O_2 Production via Carbon-Nitride Doped MnO_2 Electrocatalysts

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Manganese Dioxide (MnO_2) is widely used in constructing cathodic electrodes for fuel cells, which is achieved by manipulating its physicochemical characteristics controlling its , shape, composition, and structure to maximize its performance and efficiency. Studies conducted by researchers have shown the impact of the morphology and structure of MnO_2 nanowires on the Oxygen Reduction Reaction (ORR), promoting pathways for continuous current flow with shortened diffusion length and high surface area, thereby facilitating a $3e^-$ mechanism in ORR. Compared to MnO_2, carbon materials represent promising alternative electrocatalysts for the electrochemical production of hydrogen peroxide (H_2O_2). They demonstrate significant electrocatalytic activity and selectivity improvements when a heteroatom is associated with the mesoporous carbon structure. These materials also benefit from their high surface area and favorable mass transport. In this context, our study has adopted strategies to dope nitride-carbon (CN) to enhance selectivity in the electrochemical production of H_2O_2. Preliminary results have shown increased production of this product with higher CN to MnO_2 nanowire ratios. Furthermore, a notable improvement in the onset potential (E_0) was observed, where the value obtained for MnO_2 was -0,13 V vs Ag/AgCl, while for the synthed electrocatalysts it was less than -0,105 V vs Ag/AgCl. Such a result indicates that the synergy between these materials reduces the activation energy required to initiate the reduction reaction of O_2 molecules, thereby contributing to the electrocatalytic efficiency in H_2O_2 production.

Enhanced Oxygen Reduction Reaction with Hydrothermally Synthesized Mn_3O_4

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Oxygen reduction reactions (ORR) are very important for technological and environmental advancement, enabling the development of more effective and sustainable energy solutions. Mn_3O_4 is an excellent candidate for this. The work aims to synthe Mn_3O_4 in a simple manner and under mild conditions of pressure and temperature. The oxide synthesis was carried out in a hydrothermal system utilizing an autoclave with a 100 mL Teflon cup. This will contain 10 mL of $KMnO_4$ 0,2 mol L^{-1}, 4 mL of EDTA 0,5 mol L^{-1}, and be filled to 75 % of the volume with ultrapure water. The mixture was heated in an oven at 180°C for 4 hours and then allowed to cool to room temperature. After cooling, the precipitate was filtered and washed 12 times with water and absolute ethanol and dried in the oven at 60 °C for 6 hours. After drying it was placed in a tube furnace in an inert atmosphere, heated at a rate of 10 °C per minute till 600 °C, and maintained for 1 hour [1],[2]. Characterization was performed using X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), Dynamic Light Scattering (DLS). XRD exhibits that oxides pre-thermal treatment have a mixture of phases of Mn_3O_4 (60%), MnOOH (28%), and MnCO3 (12%). After thermal treatment, there was an increase in the Mn_3O_4 phase (88%) and the emergence of another phase, Mn_4O_4 (12%). The thermal treatment converted all MnOOH into Mn_3O_4. The results from DLS showed that the particles have a very narrow distribution, with s ranging from 400 to 600 nm after thermal treatment. Cyclic voltammetry shows that the electrodes presented higher current values when oxygen was bubbled into the solution, with current increasement of 100% for pre-thermal treatment and 80% for post-thermal treatment oxides.

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Enhanced stability of $CsPbI_3$ solar absorber by mixed halide and bismuth dopping

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In recent years, notable advancements have been made in harnessing $CsPbI_3$ as a semiconductor within the realm of photovoltaics. Its remarkable photoelectric characteristics and solution processability render $CsPbI_3$ solar cells highly promising for large-scale industrial deployment, owing to their cost-effectiveness and impressive photoelectric conversion efficiency [1]. Nonetheless, the stability concern, particularly in high-moisture environments and under light exposure, poses significant hurdles to its further progression [2]. In this work, we explored various approaches to enhance the stability of $CsPbI_3$ perovskite films aiming its utilization as top absorber in tandem Si-perovskite solar cells. Particularly in this study, we prepared modified $CsPbI_3$ films on various charge transport layers, whose stability is augmented through the incorporation of bromide and bismuth in different amounts into the precursor solution. The films obtained via spin coating exhibit morphology, after thermal annealing, characterized by grains exceeding one micrometer. Additionally, with the perovskite films exhibited notable stability of the black-phase comparatively to the pristine $CsPbI_3$.

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Enhancing Hydrogen Evolution from NaBH4 Using K7HNb6O19 Decorated with Bimetallic Pt-Co Nanoparticles Supported

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It is crucial to seek clean and sustainable energy sources due to environmental concerns about fossil fuels[1]. Hydrogen (H2) is a viable energy alternative to fossil fuels, due to its high energy density and the unique production of water vapor during its conversion into electricity. However, production and storage are challenges for its industrialization [2]. Solid state hydrogen storage, such as NaBH4, is an attractive alternative, but requires catalysts for its hydrolysis at room temperature and atmospheric pressure. Noble metal nanoparticles (NPs) act as catalysts, but agglomeration reduces efficiency and may leach into medium. The use of supports can maximize the efficiency of nanocatalysts, generating synergistic effects with NPs. In this study, a polyoxoniobate, K7HNb6O19, decorated with bimetallic Pt-Co NPs was used as a catalyst in the hydrogen reaction. K7HNb6O19 was produced by hydrothermal method. The material was characterized by Scanning Electron Microscopy (SEM), showing a plate-shaped morphology. Energy-dispersive X-ray spectroscopy (EDS) confirmed the presence of Nb, K, O. H2 evolution assays were conducted using 10 mg of the support. Different reaction parameters were evaluated, including the assessment of monometallic (Pd, Pt, Ni, Co) and bimetallic nanoparticles, as well as nanoparticle dosage. The experiments were carried out at a controlled temperature of 28.4 °C. The best results were 0.05 mmol of the bimetallic composition Co-Pt (8:2), NaBH4 0.05 mmol L-1. The hydrogen evolution rate (HER) found was 14507.56 mL min-1 g-1. Given the results comparable to those in the literature, polyoxoniobates seem a promising alternative to facilitate the evolution of H2 from NaBH4

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Enhancing Hydrogen Storage Properties through Alloy Design: A Study of High-Entropy Alloys derived from Ti21Zr21FexNiyVz (x, y, z = 0 to 58 at%) system

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High-entropy alloys (HEAs) are gaining increasing recognition for their superior properties compared to traditional alloys [1]. In hydrogen storage applications, this class of materials holds significant promise as metallic hydride [2]. This study aims to investigate alloy design methods and evaluate the hydrogen storage properties of four HEAs with varying proportions of C14 Laves and BCC phases: Ti21Zr21Fe41Ni17 (denoted as V0), Ti21Zr21V4.8Fe29.6Ni23.6 (V5), Ti21Zr21V10.4Fe17.4Ni30.2 (V10), and Ti21Zr21V14Fe4.3Ni39.7 (V14). Through the CAPLHAD method, which relies on semi-empirical models and computational thermodynamic calculations, the insertion of V into the V0 alloy was analysed to increase the quantities of BCC phases. A ternary diagram was developed, keeping fixed amounts of Ti and Zr while varying the proportions of V, Fe, and Ni from 0 to 58% at an equilibrium temperature of 1000°C. From these results, theoretical biphasic C14 and BCC alloys were identified, leading to the selection of the three alloys V5, V10, and V14, with theoretical C14/BCC proportions of 0.65/0.35, 0.35/0.65, and 0/100, respectively. The HEAs were synthed via arc melting and subjected to structural and microstructural analyses using XRD and SEM. These techniques, coupled with Rietveld analysis, revealed that the proportions of C14 and BCC phases partially agreed with CALPHAD predictions. Regarding the hydrogen storage kinetics, the findings indicated that as the amount of V increased, reversibility decreased, absorption capacity at room temperature enhanced, and kinetics sped up. Further PCT analysis will be conducted to assess thermodynamic properties during hydrogen storage.

Enhancing the Magnetic Anisotropy of NdFeB thin films through grain boundary diffusion with dysprosium layers grown by sputtering

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The manufacturing of NdFeB (neodymium-iron-boron) magnets is prominent due to their robust magnetic properties, essential for applications in electric motors, wind turbines, Hard Disk Drives (HDDs), Magnetic Resonance Imaging (MRI), microelectromechanical systems (MEMS) among others. These magnets possess high uniaxial magnetocrystalline anisotropy (MA), which diminishes at operational temperatures ranging from 80 to 220°C [1-3]. To counteract this degradation, the addition of rare earth elements (REEs) like Praseodymium (Pr), Terbium (Tb), Cerium (Ce), Lanthanum (La) and in special dysprosium (Dy) is necessary. This study investigates the influence of Dy on the magnetic properties of NdFeB through the mechanism of grain boundary diffusion (GBD) in multilayers of NdFeb;Dy [1-3]. We employed magnetron sputtering to fabricate multilayer thin films of NdFeB/Dy with alternating layer thicknesses of 50, 25, and 12.5 nm and layer repetitions of 1, 2, and 4. The structure of the samples was Si/Ta/[Dy(t)/NdFeB(t)]N/Ta, where all layers were deposited at 600°C, except for the 50 nm thick Ta layers which were deposited at room temperature. This high temperature deposition promotes the formation of the Nd2Fe14B phase, known for its high uniaxial anisotropy along the c-axis. Our findings, supported by X-ray diffraction and magnetometry, indicate significant enhancements in magnetic anisotropy along the c-axis due to Dy interdiffusion at the interfaces and percolation at the NdFeB grain boundaries, compared to a reference sample without Dy [3]. The broad peaks in X-ray diffraction patterns confirm the polycrystalline nature of the films, which is attributed to the interfacial and GBD processes, resulting in increased coercivity and magnetization. The hysteresis loops revealed a competitive magnetic coupling between the Nd/Fe phases enhanced by Dy interdiffusion, leading to varied coercive fields. Understanding these processes is essential for advancing the development of high-pe

Evaluation of Different Morphologies of Ag2WO4 for Hydrogen Production from Formic Acid

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The continuous pursuit of cleaner fuels has been driving the development of functional materials capable of catalysing reactions for hydrogen gas production, such as formic acid dehydrogenation.[1] On that matter, nanomaterials can be adopted for the fabrication of highly selective and cost-effective heterogeneous catalysts. Therefore, this project proposes the synthesis of the semiconductor Ag_2WO_4 in three different morphologies (rod, cube and nano) and evaluate their performance in dehydrogenation of formic acid using an open burette system. Each morphology will undergo distinct synthesis methodologies, with the aim of achieving different s and morphologies. The structural characterization of the materials will be conducted using X-ray Diffraction, Raman Spectroscopy, and UV-Vis Spectrophotometry, while morphological analyses will be determined through Scanning Electron Microscopy. In summary, the pre-established parameters will be optimized to achieve the highest H_2 production rate.

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Evaluation of different supports in Cu-catalysts used in the reverse water gas shift (RWGS)

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As climate change worsens, reducing greenhouse gases, especially CO_2, gains more attention. One solution is converting CO_2 into valuable chemicals through the Reverse Water Gas Shift (RWGS) reaction [1]. This produces syngas, used in various chemicals like methanol, dimethyl ether, Fischer-Tropsch fuels, and ammonia. Yet, a key challenge is developing stable catalysts with high CO selectivity. This study aims to synthe copper catalysts using titanate nanotubes and zeolites as support. Copper shows promise due to its activity and selectivity in CO_2 reactions [2]. Cupper titanate nanotubes (Cu-TNT) were prepared from sodium titanate nanotubes via impregnation with copper solution. MCM-22 zeolite was synthed from silica based on rice husk ash (RHA) and then impregnated with copper solution, named Cu-MCM22. Characterization involved microscopy (SEM and TEM), spectroscopy (FTIR and Raman), X-ray diffraction, and nitrogen adsorption/desorption isotherms. Catalytic tests for RWGS will be conducted at 450-700°C in a fixed-bed reactor, evaluating temperature, gas hourly space velocity (GHSV), and reaction time. The findings of this study will bring valuable insights for the enhancement of catalysts aimed at the conversion of carbon dioxide.

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Exploring different parameters of solvents as electrolyte to enhance the performance of Li-O2 batteries

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Global focus on rapid economic growth and sustainable energy sources is increasing. Wind and solar energy show promise, but their intermittent nature poses challenges due to resource availability. Electrochemical storage, especially lithium batteries, is essential for powering electric vehicles and storing renewable energy. For instance, the Li−O2 battery stands out for its ability to deliver significantly higher energy density (3500 Wh kg−1) compared to conventional Li−ion batteries, reducing the necessity for heavy metal oxide cathodes. Despite its advantages, air components can unchain unwanted reactions that negatively impact the performance of the Li-O2 battery. As a result, researchers are actively exploring ways to improve its efficiency. The electrolyte relies on the Li-O2 battery's behavior, acting as a bridge for transporting Li+ ions. Key factors for optimal performance include low viscosity and high ionic conductivity for desired rate capability. In this study we evaluate different properties of electrolyte as viscosity, density, and ionic conductivity for 1M LiTFSi (Lithium bis(trifluoromethanesulfonyl)imide) in acetonitrile and DMSO (dimethylsulfoxide) solvents in different ratios 0:100, 25:75, 50:50, 75:25, 100:0, and the rate capability of the Li2O2 batteries. a 1M LiTFSi solution with 100% DMSO has higher viscosity and lower ionic conductivity compared to other electrolytes. This is likely due to the molecular structure, which may be more flexible and less compact, affecting ion transport and electrolyte wettability, thus impacting ORR reactions, as demonstrated by various researchers.

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Exploring Hybrid Solar Cells: Integrating Ferroelectric Oxides and Organic Polymers

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In recent years, there has been a growing interest in the research exploring the potential of combining different materials for hybrid solar cells. This interest stems from the prospect of leveraging the positive characteristics of multiple materials to enhance photovoltaic conversion response [1] . Ferrolectric oxides, such as $BiFeO_3$, have garned attention due to their low cost production and mainly for the bandgap exceed photoresponses induced by their built-in electric field [2]. Organic solar cells are prized for their flexibility, lightweight nature, and cost-effective production, making them an intriguing partner for hybridization [3]. In this study, we conduct an electrical, optical and structural characterization of ferroelectric oxides and organic materials for photovoltaic devices production and exploring the chalenges to produce a hybrid Organic/ferroelectric oxide device. The thin films are prepared using blade coater from the materials solution. The electrical properties were measured using metalic contacts with the active layers in sanduich struture under room and low (liquid nitrogen) temperature. The morphology was exploited using scanning electron microscopy and AFM. The optical properties involves UV-vis and RAMAN spectroscopy.

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Exploring New Variants of Polymer D18: Comparative Study of Terpolymer Containing Thiophene or Hexylthiophene in D18 Composition for Organic Solar Cells Fabrication

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In recent years, the development of new semiconductor polymer structures has enabled the creation of high-performance organic solar cells. Particularly noteworthy is the D18 polymer, based on units containing fused benzodithiophene and benzothiadiazole rings, which has shown energy conversion efficiencies (PCE) of 18% [1] and 19% in binary and ternary cells [2], respectively. Since then, this polymer has been under investigation by many researchers. One of the challenges for the widespread application of semiconductor polymers is their solubility in green solvents, such as O-Xylene. Despite being the most efficient conjugated polymer discovered to date, D18 has poor solubility, which hinders its use in large-scale device fabrication. Recently, Lu et al. reported the preparation of the terpolymer donor OPz11 by adding 5% ester-substituted thiadiazole (E-Tz) acceptor units to the D18 polymer to adjust energy levels, molecular aggregation, and phase separation. Considering the idea of making a promising polymer, such as D18, feasible for large-scale device fabrication, this study was conducted by adding 5% thiophene (P2) and 5% hexylthiophene (P3) to the D18 polymer and evaluating its molecular weight, energy levels, PCE, and solubility, comparing these results with traditional D18 (P1).

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Exploring the impact of magnetic field on the synthesis of nanostructured spinel ferrites for green energy applications

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Harvesting sunlight to drive photochemical reactions using semiconductors as photocatalysts is a promising approach for green fuel production, such as producing H_2. Spinel ferrites have been extensively applied in electronic devices, sensors, and batteries, among others. Nevertheless, their potential as photocatalysts remains largely unexplored. These materials are considered low-cost, abundant, non-toxic, and present interesting electronic and optical properties [1]. Particularly, $NiFe_2O_4$ presents an optimal bandgap of 1.5 – 2.1 eV. The incorporation of elements such as Zn, can modify the bandgap of $NiFe_2O_4$ and optimize its electronic properties for photocatalysis by changing the octahedral (O_h) and tetrahedral (T_d) occupation by different metal ions within the lattice. In this work, Zn-doped $NiFe_2O_4$ nanoparticles were obtained by a surfactant-assisted co-precipitation route [2], varying synthesis parameters such as the nature of the precursor, reaction time, and calcination temperature. Moreover, by applying a magnetic field (MF) during synthesis [3], we aim to induce different occupancies of the T_d and O_h sites in the structure, therefore modifying the bandgap energy of these materials, as well as modifying the of the particles, thus changing the magnetic properties, and provide oriented morphologies. Sample characterization was performed by XRD, XPS, SEM, and UV-Vis and Mössbauer spectroscopy.

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Exploring the potential of MXenes additive in transport layers of perovskite solar cells

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A novel class of two-dimensional transition metal carbides and nitrides (MXene) has been explored due to their unique properties, including high electrical conductivity, transmittance, and hydrophilicity [1]. MXenes ($M_{n+1}X_nT_x$) have been used as a viable solution for enhancing the efficiency and stability of perovskite solar cells (PSCs) [2]. In this study, we exfoliated and characterized two different MXenes composites ($Ti_3C_2T_x$ and V_4AlC_3) and analyzed the effects when added to the transport layer of the PSCs. The Minimally Intensive Layer Delamination (MILD) route was used to exfoliate the precursor MAX phase to obtain the MXene phase. Afterward, the MXenes were incorporated into the transport layer in the regular mesoporous n-i-p (Nb_2O_5/TiO_2) architecture of perovskite ($Cs_{0.17}FA_{0.83}Pb(I_{0.83}Br_{0.17})_3$) solar cell. Advanced characterization techniques were performed to investigate the structural features of MXene compounds and their correlation with desired transport properties. The results indicate that incorporating low concentrations of MXene leads to improved photovoltaic performance. Additionally, CELIV analysis revealed an enhanced photogenerated charge carrier extraction density and mobility. Furthermore, investigation of transient photovoltage (TPV) and impedance reveals prolonged charge recombination times in devices containing MXenes. These findings underscore the potential of MXenes as additives in PSCs, offering insights into their structural-functional relationships and paving the way for enhanced solar cell technologies.

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Fabrication of Fully Printable Flexible Large Area MicroSupercapacitors

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In recent decades, microsupercapacitor devices have garnered considerable attention as promising technological solutions across various domains, including wearable electronics, portable storage units, and medical devices. Renowned for its diminutive dimensions, rapid energy storage, and swift discharge capabilities, microsupercapacitor offers a compelling alternative to traditional energy storage systems. This study focused on the development of a processable ink comprising poly(3,4-ethylenedioxythiophene):polystyrene sulfonate and carbon nanotubes, tailored for printable application and scalable processes. Our research showcases the fabrication of microsupercapacitors using this ink on large areas through a combination of doctor blade and laser-scribed techniques, both readily adaptable to process production lines. Electrochemical performance of the devices was evaluated in terms of different designs and optimization processes. Leveraging straightforward and scalable methodologies, we produced flexible devices exhibiting remarkable electrochemical performance, reaching a high capacitance of 212.4 mF.cm^{-2}, energy and power densities of 16.6 µW.h.cm^{-2} and 318.7 µW.cm^{-2}, respectively. Besides a low internal resistance of 22 Ohms. Furthermore, a stability assessment revealed strong capacitive retention, with 80% of the initial capacitance retained after 5,000 charge-discharge cycles, alongside a minimal leakage current of 40 µA. The versatile manufacturing approach in this study underscores its efficacy in yielding high-performance microsupercapacitor devices.

Facile synthesis of polypyrrole-gold nanoparticles composite electrodes for enhanced quasi-solid-state supercapacitor

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Conducting polymers, such as polypyrrole, exhibit pseudocapacitive behavior and offer distinct advantages including low cost, lightweight construction, and flexibility. However, further advancements in polypyrrole electrodes are needed to enhance charge transfer processes and device lifespan in supercapacitor applications. Composite materials of polypyrrole with gold nanoparticles show promise in addressing these challenges and improving supercapacitor performance. Additionally, integrating a gel as an electrolyte improves application feasibility by preventing solution leaks and acting as a separator, enhancing system efficiency and stability. This study proposes a fast synthesis of gold nanoparticles directly on polypyrrole electrodes, using the polymer as a reducing agent with minimal overoxidation risk. Polypyrrole electrodes were synthed via potentiostatic deposition on a stainless steel mesh with a charge control of 300 mC/cm^2. Gold nanoparticles were subsequently incorporated into the polymer by exposing the electrode to a HAuCl4 solution under stirring for 30 seconds. The electrolyte gel was prepared from a 2% (w/v) sodium alginate dispersion with Na2SO4 and CaCl2 additions to achieve appropriate gel viscosity. Initial tests indicated complete permeation of the gel electrolyte into the polymeric electrode within 24 hours. Cyclic voltammetry, electrochemical impedance spectroscopy, and galvanostatic charge-discharge curves were conducted to analyze the effects of gold nanoparticles on the polypyrrole electrode. While cyclic voltammetry results showed no significant differences, impedance measurements demonstrated a notable decrease in charge transfer resistance with gold nanoparticle presence. Additionally, charge-discharge curves exhibited lower ohmic drop and extended charge-discharge time. Overall, findings suggest that gold nanoparticles enhance polymer properties for supercapacitor application, with minimal polymer overoxidation.

Fe Surface-Modified TiO2 Photocatalysts: Synthesis, Characterization and CO_2 Photoreduction properties

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CO2 photoreduction is regarded as a crucial approach to mitigate CO2 emissions into the atmosphere, particularly through the generation of hydrocarbon fuels from CO2 [1]. Although TiO2 – anatase exhibits favorable properties for CO2 photoreduction applications, there is still a need to enhance its characteristics, such as optical absorption capability and electron-hole pair separation [1]. Thus, the aim of this study was to investigate the synthesis of Fe surface-modified TiO2 and its performance in CO2 photoreduction. Various TiO2 morphologies were prepared using the oxidant peroxo method followed by hydrothermal treatment at different pH values (6, 8, and 10) [2]. The samples were decorated with Fe in different proportions of 0.2, 0.8, and 1.6% by mass relative to TiO2 [3]. XRD and Raman analyses confirmed the presence of the TiO2 – anatase phase in all obtained samples. UV-Vis DRS analyses revealed enhanced optical absorption capacity in the presence of Fe. SEM and HRTEM analyses demonstrated the formation of TiO2 nanoparticles with different morphologies. XPS analysis and STEM combined with EDX confirmed the existence of Fe species on the nanoparticle surfaces. The sample synthed at pH 8 with 1.6% Fe exhibited superior CH4 production performance under UVC radiation, likely attributed to efficient electron transfer facilitated by the presence of Fe species on the sample surface.

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Film deposition methodology influence on CsPbBr3 PSCs hysteretic behavior

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Perovskite-type materials have excelled in the energy conversion field due to their exponential increase in efficiencies in recent years, being considered a potentially cost-effective alternative for the photovoltaic sector. Despite the various advantages, the technology still has limitations, such as stability and difficulty in scaling. Some challenges for scalability are related to the difficult of keeping materials properties along all device's, connected to film uniformity, which in turn is connected to crystallinity properties, impacting on charge carriers transport and extraction, and consequently on hysteretic behavior. Hysteretic behavior on PSCs is one of the technology obstacles for the achievement of practical application and in their commercialization pathway. [1] Deposition methodology present a detaching influence on film uniformity, consequently impacting hysteretic behavior. In order to evaluate the film deposition methodology influence on devices energy conversion performance and on hysteresis, deposition methodology such as direct deposition, spin coating, blade coating and screen printing have been used. To deal with stability limitations of the materials, the inorganic perovskite CsPbBr3 had been chosen as composition for the evaluation. Perovskite nanocrystals (LARP synthetized) produced paste had been used for deposition, being used TiO2 as electron transport layer (ETL), and carbon as counter electrode. The study showed the film deposition influence on devices photovoltaic parameters, as well as how deposition can influence on film properties and consequently on hysteretic behavior.

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Flexible carbon fiber improves power density and mechanical stability for application in redox flow batteries

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Due to the current focus on manufacturing safer and bioinspired batteries, organic and organometallic compounds have been proposed as active compounds in energy storage devices. Nevertheless, to achieve a better performance in a redox flow battery (RFB), it is necessary to understand the carbon electrode surfaces, as the electrochemical charge transfer reactions occur at the electrode. Thus, there is much to be improved in the chemical and electrochemical stability of the electrodes, as they rapidly degrade after several charge and discharge cycles, significantly restricting their long-term use. Based on this, we studied the conventional SGL 39AA electrode and proposed the application of a flexible carbon fiber never used in an RFB, the Delpho electrode. Studies show that the Delpho electrode has a higher current and power density and is more robust than the SGL 39AA. Furthermore, Raman measurements confirm the Delpho electrode functionalization sustained by the ratio of the intensity of D- and G- bands (I_D/I_G). In line with the Raman measurements, X-ray photoelectron spectroscopy (XPS) displays a rise in the atomic ratio of oxygen to carbon (O/C), confirming functionalization by organic functional groups. The images obtained by scanning electron microscopy (SEM) serve as a support to confirm the structural and chemical surface characterization. In addition, compared with those produced with SGL 39AA, larger power densities were obtained using the Delpho electrode. In summary, we strictly propose that the Delpho electrode is a promising electrode for application in an RFB that does not degrade after charge and discharge cycles and provides a higher power density.

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Friendlier Perovskite Film Deposition For Photovoltaic Application

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Metal halide perovskite materials have attracted attention due to their rapid development as energy converters, due to their great properties. About the devices using these materials, the perovskite solar cells, they had a phenomenal development, which generated significant increase in energy conversion efficiency, having additional advantages. However, the technology still has limitations [1], such as toxicity and scaling difficulty, and some of the possibilities to overcome these limitations are the improvement of the materials properties [2], as well as the obtainment of isolated materials (not grown directly on substrate as films). Colloidal crystals synthesis is an interesting way of obtaining materials, as well as a way to control obtained materials properties, improving perspectives of scaling processes keeping materials properties along all device's extension. In our work we seek to treat limitations related to PSCs technology by developing materials with desired properties, evaluating materials deposition methods to increase scalability, and conversion response, as well as reducing toxicity. We proposed the environmentally friendlier perovskite NCs synthesis investigating compositions based on lead partial substitution on CsPbBr3 perovskite, obtained by LARP procedure, as well as the application of produced materials as films, for device assembly. Crystals obtained were used for paste production and films were deposited by blade coating. Films were evaluated considering crystalline structure, morphology, optical and conversion energy properties. High uniform films were obtained using prepared material, as well as interesting conversion energy responses, being obtained by an easy an scalable deposition methodology and lead poor perovskite materials. <div>Acknowledgements:
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Giant barocaloric effect in vegetable oils, submitted to moderate pressures

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Search for greater energy efficiency in cooling systems has driven the development of innovative technologies. In this context, there has been a significant increase in the search for new materials that exhibit the barocaloric (BC) effect. We can highlight for example the colossal barocaloric effect discovered in the higher n-alkanes [1] (adiabatic temperature changes for eicosane (C20H42) are 38 K up to 218 MPa and predicted colossal isothermal entropy changes are higher than 900 J kg-1K-1). Another important discovery was the mechanocaloric compressive effect on cork (tensions up to 218 MPa with giant values of temperature change of up to 13.6 K and entropy change up to 101.3 J kg-1 K-1) because it is a natural, renewable and sustainable material. Driven by these discoveries, mainly the manifestation of the mechanocaloric compressive effect (which is the general case of the barocaloric effect, characterized by with the application of a hydrostatic pressure) in natural materials, this work aimed to investigate the BC in canola oil and sunflower oil, which are commercially available, highly processed, low cost material in addition to being a natural, renewable and sustainable material. To measure the BC effect, 2.5ml of the oil was used, placed in a cavity with a diameter of 12 mm. The BC effect was measured directly using homemade equipment, where the temperature variation of the specimens was measured after a compression and decompression procedure. Through these measurements, a maximum temperature variation of ~15.8 K at a pressure of 218 MPa at 323 K for canola oil and ~16.0 K at a pressure of 218 MPa at 323 K for sunflower oil, presenting values comparable to those observed in the literature. The two investigated oils have the potential to be applied in cooling systems using the BC effect principle. References:
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HIGH PERFORMANCE OF NANOSTRUCTURED ALKALINE-NIOBATE HOLLOW SPHERES OVER WATER-SPLITTING PHOTOCATALYSIS

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The limited resources and the harmful effects of fossil fuels on the environment are worldwide concerns, and their replacement by eco-friendly alternatives is highly desirable. Water has been considered a promising source of alternative energy due to being inexpensive, innocuous, and abundant. The core of water-splitting technology is a series of electrochemical processes involving hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) at the cathode and the anode of an electrolytic cell. Among the ferroelectric materials based on perovskite structure, alkaline niobates have been investigated as an eco-friendly alternative due to their excellent properties1,2. In this work, we investigate the photoelectric activity of K0.5Na0.5NbO3 (KNN) in water-splitting photocatalysis. Hollow-structured KNN spheres, were synthed using the same procedure reported by our research group1,2. The electro- and photoelectrocatalisys of KNN in water showed a better performance under light irradiation. The irradiation sensitivity of the niobate contributed to lower overpotentials and higher current flows.

Hybrid material from pyrolyzed fabric and gold nanoparticles for application in supercapacitor electrodes

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In recent years, there has been a noticeable increase in textile industry production, which has consequently led to a significant rise in waste generation. Faced with this scenario, this work was conducted with the purpose of exploring the use of textile waste as a basis for conversion into conductive materials, thus adding value to a material that would otherwise be discarded. To achieve this goal, the process of pyrolysis at high temperatures and in a controlled reducing atmosphere was employed. This method resulted in the formation of a product with a graphitic structure, confirmed through analytical techniques such as Fourier-transform infrared spectroscopy (FTIR), Raman spectroscopy, X-ray diffraction (XRD), and transmission electron microscopy (TEM). The electrical resistance found in this material was measured at 174 Ω, although its direct application as an electrode did not yield satisfactory results. In search of improvements, gold nanoparticles (AuNPs) were incorporated into the pyrolyzed fabric, synthed by two different methods. The use of pyrrole as a reducing agent, leading to the reduction of gold ions and the concomitant oxidation of pyrrole, yielded interesting results, with the formation of gold nanoparticles stabilized by polypyrrole. This addition was made with the intention of adding conductivity to the material, reducing electrical resistance, achieving a resistance of 66 Ω for AuNPs reduced with pyrrole, as well as increasing capacitive current and incorporating faradaic current into the material. The study explored possible modifications of the pyrolyzed fabric aiming at its application in electrochemical devices, especially in supercapacitors. This research not only contributes to the search for sustainable solutions in textile waste management but also explores new possibilities in the production of conductive materials with potential applications in advanced electrochemical technologies.

Hydrogen Evolution from NaBH4 Utilizing Platinum-Doped Manganese Tungstate Catalyst

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The shift to cleaner, more sustainable energy sources is urgent due to the environmental damage caused by fossil fuels. Solid hydrogen storage, such as NaBH4, is a promising solution, enabling the safe and efficient storage of this clean energy. Therefore, the use of catalysts such as platinum nanoparticles-doped manganese tungstate (PtNPs-MnWO4) becomes necessary, offering significant advantages due to their high catalytic activity and chemical stability [1]. This work describes the hydrogen evolution from sodium borohydride in a wet route using PtNPs-MnWO4. MnWO4 was obtained by microwave synthesis, as described by Siqueira and Dias [2], and then doped with platinum nanoparticles by chemical reduction using NaBH4. The materials were characterized by FTIR, XRD, showing the presence of MnWO4 and platinum in the materials. The generated H2 was measured by the water displacement method in a burette. The following parameters were evaluated: (i) NaBH4 concentration (0.23, 0.33, 0.40, 0.50 mol L-1), (ii) platinum nanoparticles amount (0.025, 0.050, 0.075, 0.100 mmol), (iii) NaOH concentration (0, 0.010, 0.050, 0.100, 0.200 mol L-1), and (iv) temperature (20, 30, 40, 50 °C). From these parameters, the hydrogen generation rate (HGR) and activation energy (Ea) were obtained. As a result of this optimization, it was observed that using (i) 0.500 mol L-1 NaBH4, (ii) 0.025 mmol platinum, (iii) absence of NaOH, and a temperature of 30 °C, an HGR of 5579.96 mL min-1 g-1, with an activation energy of 8.10 kJ mol-1. Given the excellent performance obtained, similar to what is described in the literature, it can be concluded that PtNPs-MnWO4 appears as a promising option to promote H2 production from NaBH4.

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Hydrogen generation from a sodium borohydride under hydrolytic conditions with Ni/ZrO2 catalyst

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Hydrogen generation from the hydrolysis of sodium borohydride (NaBH4) solution has drawn much attention since early 2000s, due to its high theoretical hydrogen storage capacity (10.8 wt%) and potentially safe operation. Recently, many catalysts have been developed for H2 generation by NaBH4 hydrolysis. ZrO2 emerges as a promising catalyst support, promoter, with versatile properties and mild hydrophilic nature. ZrO2 interacts with metals and/or other oxides, potentially influencing CO2 adsorption and activation. Therefore, here we report the eco-friendly synthesis of ZrO2-based catalysts for hydrogen production. The Ni/ZrO2 compounds were obtained at 180 ºC by hydrothermal method and characterized using X-ray diffraction (XRD), UV-visible absorption and Fourier Transform Infrared (FTIR) spectroscopy. Four parameters were investigated in the hydrolysis process: Ni concentration, temperature, crystalline structure and catalyst concentration. The crystalline phase obtained at 200 °C was confirmed with powder X-ray diffraction and the transition from tetragonal to monoclinic of crystalline structure occurs with pH value of synthesis. The Ni/ZrO2 nanocatalyst presented a maximum hydrogen generation rate of 6 L. min−1 using 6 wt% NaBH4–4 wt% NaOH (25 °C), which is much higher than those of without catalyst. The hydrogen generation rate increased with experimental temperature. The activation energy for the hydrolysis reaction was observed to be 31 kJ mol−1.

Impact of O2 Pressure on Niobium Oxide Film Growth via DC Sputtering: Photocatalytic Potential for Solar H2 Generation

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Currently, the search for carbon-free energy sources is a major global challenge. Molecular hydrogen (H2) stands out as a viable alternative due to its efficiency and environmental sustainability. To ensure that hydrogen production is truly beneficial, it needs to be clean, efficient and economically viable, which has motivated several research groups around the world. The photoelectrochemical production (PEC) of hydrogen, using sunlight in the water oxidation reaction process, appears as a promising approach. However, technical challenges such as increasing the absorption of semiconductors in the visible region and reducing the recombination of electron-hole pairs need to be overcome. This study investigates niobium oxide (Nb2O5) as a photoelectrode for H2 production by PEC processes. Nb2O5 films were deposited on different substrates and the influence of oxygen partial pressure on the properties of the films was examined. The samples were characterized by X-ray diffraction, Raman scattering, scanning electron microscopy (SEM) and mechanical profilometry measurements. The photoelectrochemical potential of the samples was evaluated by electrochemical impedance spectroscopy (EIS) and Mott-Schottky measurements.

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Incorporation of ZnO nanoparticles on a PDMS encapsulant to improve photovoltaic modules' thermal stability

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To safeguard photovoltaic modules from potential threats like humidity, dust, UV radiation, and biological activity, a protective layer known as encapsulant is applied to the structure [1]. Consequently, extensive research efforts are underway to develop improved encapsulants. Some studies focus on harnessing the unique properties of nanomaterials, such as zinc oxide (ZnO) nanoparticles. Notably, ZnO nanoparticles have demonstrated enhanced UV resistance in various applications, including wood, food, and polymers [2], suggesting their potential in protective coatings. This research introduces a novel polymer comprising polydimethylsiloxane (PDMS) and ZnO nanoparticles as an alternative to Ethylene Vinyl Acetate (EVA) for encapsulating photovoltaic modules, thereby extending their lifespan. Laboratory analyses were conducted by comparing pure PDMS with PDMS incorporating varying concentrations of nano ZnO (2.5% – 7.0% (wt/wt %)). Results from these experiments indicate that ZnO nanoparticles alter the thermal curve, preventing PDMS from decomposing into simpler chemical structures [3]. The film containing ZnO nanoparticles shifts the pique of thermal degradation, an advance of 5,426% in the encapsulant thermal resistance. Consequently, the proposed encapsulant not only preserves the superior qualities of PDMS but also leverages the beneficial properties of zinc oxide nanoparticles, presenting a more robust solution for photovoltaic modules.

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Influence of Electrolytes Plasma Activation on the TiO_2 Nanotubes Properties Growth by Anodization

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Titania (TiO_2) obtains unique physical and chemical properties, making it a widely studied oxide material. The synthesis of TiO_2 Nanotubes (TNT) is a process produced by anodizing metallic titanium through electrochemical anodization and is extensively studied due to its large surface area, chemical stability, and self-organization, which can be used for photoelectrochemical water decomposition and in the process of obtaining green hydrogen [1,2]. Studies with plasma show that Liquid Activation by Plasma aims to improve properties and increase chemical species in the activated liquid [3]. This research aims to compare structures and the alteration of properties of TNT samples and the effects of the electrolytes plasma activation. For the production process of TiO_2 nanotubes by anodization, a titanium plate was used as the anode, a copper plate was used as the cathode, and the electrolyte used was a solution of $C_2H_6O_2$, H_2O, and NH_4F all at room temperature. The plasma activation process was carried out in the electrolyte with atmospheric air plasma at 4 L/min for 10 minutes, where each sample had a stage of the electrolyte activated: a) Entire solution, b) H_2O, c) NH_4F, d) $C_2H_6O_2$. Preliminary characterizations indicate that the samples exhibit variations in the morphological structures of TiO_2 nanotubes caused by atmospheric plasma activation.

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Influence of Oxygen Flow Variation on the Photocatalytic Efficiency of WOx Thin Films in the Degradation of Methylene Blue

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The contamination of water sources by organic pollutants, such as dyes used in the textile industry, poses serious risks to human and animal health. In response, heterogeneous photocatalysis has emerged as an efficient solution for degrading these persistent contaminants [1,2]. In this context, tungsten oxide (WO_x) thin films have proven to be an effective photocatalyst due to their stability, low cost, and suitable optical and electronic properties [3]. This work aims to synthe and characterize WO_x thin films, as well as to evaluate their photocatalytic efficacy in the photodegradation of methylene blue. WO_x films were deposited on pre-cleaned Si (100) and glass substrates using a dual sputtering technique with a 100 mm tungsten target of 99.9% purity. To induce variations in the WO_x stoichiometry, the oxygen flow was adjusted between 0 and 10 sccm during the deposition process. This adjustment was characterized by a gradual increase in oxygen flow over 60 minutes, starting at specific values of 2, 4, 6, and 8 sccm, and increasing up to the limit of 10 sccm, resulting in the creation of six different samples. After deposition, the samples underwent thermal treatment at 450°C for two hours to ensure crystallinity, followed by characterization through mechanical profilometry, Raman spectroscopy, contact angle test, FEG/EDS SEM, and XRD. Additionally, photodegradation measurements of methylene blue were conducted using a solar simulator.

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Influence of PZT thickness on Ferromagnetic, Ferroelectric and magnetoelectric coupling properties in PZT/CFO thin film heterostructures grown by RF-Sputtering

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In recent decades, the high-tech industry has increasingly sought multifunctional materials[1]. In this context, materials that present magnetoelectric coupling have sparked the interest of researchers and industry in the development of new disruptive technologies, such as data storage, volatile and non-volatile memories (MERAM), solar energy conversion and medicine [1-3]. In this work, a systematic study was carried out to determine the influence of the thickness of the $Pb(Zr_{0.2}Ti_{0.8})O_3$ (PZT) layer, grown on a 250 nm layer of $CoFe_2O_4$ (CFO), on the structural, microstructural, ferroelectric, ferromagnetic and magnetoelectric coupling properties. Through this study, the evolution of PZT from a paraelectric state to a Ferroelectric state was observed due to the thickness and microstructural characteristics. Analyzing the results obtained from X-ray diffraction (XRD) measurements, it was possible to determine an increase of approx. 4% in the lattice parameter of the PZT layer in relation to the thickness of this layer. For the CFO layer, it was observed, from XRD measurements, that this layer starts from a tensile to compressive strain, relating this effect to the change in the easy axis magnetization and other magnetic properties such as saturation magnetization, coercive field and remanent magnetization. Finally, it was possible to relate the magnetoelectric coupling with the evolution of the ferroelectricity of the heterostructure.

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Influence of Topography on the Efficiency of DSSCs

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Dye-sensitized solar cells (DSSCs) are promising in the new generation of solar cells, composed of four components: semiconductor oxide film (electrode), dye, redox electrolyte, and counter electrode. The most commonly used semiconductor is TiO_2, responsible for the transport of the photo-generated electron upon light absorption, as well as adsorbing dye molecules [1]. Among its notable physical and chemical properties are chemical stability, transparency in the visible region, and good charge transfer [2]. However, attempts aim to improve these properties to increase the energy conversion efficiency (η), either through synthesis or deposition methods [1]. This work focuses on optimizing the η of DSSCs by controlling the topography of TiO_2 films, especially their thickness, area, and porosity. Depositions were performed on FTO via electrophoresis with potential difference rates (DDP) of (1.5 and 3.0V), deposition time (1, 2, 4, 8, 16 min), and temperatures (450, 500, and 650 °C) in sintering of (1 and 2 h), enabling the obtainment of tailored thicknesses and roughnesses. We will study the correlation of the optical, electrical, and topographical properties of the films aiming at an increase in η, using the following characterizations: Scanning Electron Microscopy, White Light Interferometry with Scanning, X-Ray Diffraction, UV-Vis Spectroscopy and Three-Point Resistivity Measurement. Efficiency will be determined thought IxV measurement, using Solar Simulator. Preliminary adhesion tests indicate, through the adhesive tape procedure, that the best sintering results are achieved in a time of 2 hours at 450°C, valid for different DDP and deposition times.

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Influence of visible radiation on the electrodeposition of bismuth oxide precursor for $BiVO_4$ photoelectrodes aiming green hydrogen production

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Green Hydrogen is produced without CO_2 emissions using renewable energy sources, typically through water electrolysis or splitting. $BiVO_4$ is one of the primary materials under study as a photoanode, given its bandgap of 2.4 eV and valence band suitable for water oxidation. This work investigates the influence of incident visible radiation during the $BiVO_4$ synthesis electrodeposition step. Photoanodes were synthed in two steps [1]: 1) Electrodeposition of a Bi_2O_3 oxide in dark/illuminated conditions. The radiation source was a 15W white LED. Chronoamperometry electrodeposited films at 2.57 V vs. Hg_2Cl_2 (3M) for 90 minutes, using a solution of Bi, H_3CCOOH, and HNO_3 pH = 0.44, with FTO as the working electrode, Hg_2Cl_2 (3M) as the reference electrode, and stainless steel as the counter electrode. A black box protected the cell from external light sources. 2) Thermal treatment (500°C, 2 h) of the electrodeposited film in the presence of an NH_4VO_3 solution drop cast on the electrode surface. The chronoamperometric profile differed considerably during the electrodeposition step in dark/illuminated conditions. Bi_2O_3 is photoactive, and currents are higher when the material is electrodeposited in white light, possibly changing the material's morphology and the amount of deposited material. In the second step, vanadium and oxygen atoms are incorporated into the crystal lattice of the precursor film, generating BiVO4. The final photoanode photocurrent was measured using a Xenon Illuminator with solar matching filters per ASTM E927-19 in 1M Na_2SO_4 solution. The photoanodes showed activity in the reaction of water electrolysis.

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In the search of optimal dopant combinations in hematite for efficient solar water oxidation reaction

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State-of-the-art approaches to mitigate charge separation and transport drawbacks in hematite photoanodes for efficient green hydrogen production involve the incorporation of one or multiple elements into its structure [1]. However, a rational consideration on how to combine the positive effects of dopants in multi-modified materials without weakening their individual benefits is needed. Here, a polymeric precursor solution method that simultaneously induces bulk doping and interfacial segregation was used in the search of an ideal couple of dopants toward highly efficient hematite photoanodes. Trivalent cations (Al^{3+}, Ga^{3+}, Y^{3+}, La^{3+}) were chosen to act as bulk dopants, inducing changes in the Fe^{3+} chemical environment to reduce polaronic effects and improve electronic mobility. Pentavalent modifiers (Nb^{5+}, Ta^{5+}) were incorporated into hematite to segregate at grain boundaries and enhance conductivity at interfaces. The photoanode modified with Y^{3+} and Ta^{5+} achieved a 57% overall efficiency, a significant improvement over pristine hematite (10%). Conversely, combining Ga^{3+} and Nb^{5+} led to a material with 21% overall efficiency, similar to niobium single-modified photoanode (22%). These results emphasize that careful nanostructure engineering must guide the search for an ideal material, and that only chemical compatible dopant combinations can provide efficient solar energy conversion.

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Investigating the Influence of Topography of TiO_2 Films on Electrolyte Diffusion in DSSCs

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The increase in research into photovoltaic cells, especially dye-sensitized solar cells (DSSCs), has led to a notable improvement in power conversion efficiency (η), reaching around 7 to 11% [1,3]. In the structure of a DSSC, there are different layers of components: FTO with semiconductor film (photoanode), sensitizer (dye), electrolyte [3] and FTO counter electrode with inert conductive film. The photoanode material, as TiO_2, must posses interesting properties in charge transport and recombination [3]. To achieve the economic viability of DSSCs, it is still necessary to overcome some challenges, for example, durability, stability, the increase in system's η, among others [2]. Therefore, aiming to improve the electrochemical properties of DSSCs, this work focuses on analyzing the topographic influence on the electrolyte diffusion process near the TiO_2 film surface. To achieve this, TiO_2 films will be synthed and deposited by electrophoresis with varying time, temperature and potential difference. The characterization techniques used during the research will be cyclic voltammetry to obtain the diffusion coefficient, impedance spectroscopy, which aims to analyze the electrolyte diffusion current, and then correlate this data with the topography, obtained through White Light Interferometry measurements (WLI). Finally, the aim is to correlate these measures with the efficiencies of the DSSCs. It is expected that, through the improvement of depositions and analysis of the films, it will be possible to optimize the electrochemical properties, increasing the η and that comparing the measured physical quantities will lead to a greater understanding of the influence of topography on the diffusion process.

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Investigation of a safe coating composition for energetic particles using simple coacervation

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Composite solid propellants are a class of propellants widely used in rocket propulsion. They consist of a polymeric matrix that incorporates particles of an oxidizer and other components of the formulation. Ammonium dinitramide (ADN) has been studied as a substitute for ammonium perchlorate (AP) due to its high energy density and its non-contribution to smoke formation during combustion [1]. However, the high hygroscopicity of this salt limits its use, making it essential to develop processing techniques to isolate it from moisture. One technique used for this purpose is simple coacervation coating, which occurs in a liquid medium. In this process, part of a coating substance migrates to the surface of the system, part agglomerates around nuclei (immiscible phase in the liquid medium), and part becomes solvated according to the polarities and affinities of the established composition [2]. In this context, the objective of this work was to evaluate the replacement of the liquid medium of a known coating system, replacing n-hexane, a toxic and volatile substance, with liquid vaseline, which at the system temperature (50ºC) operates outside the flammability region. For this, 100 mL of polymeric solutions composed of hydroxyl-terminated liquid polybutadiene (HTPB) in liquid vaseline, at various concentrations, were tested to identify the formation of coating on 1g of particles (500-425 µm), with 15 minutes for system stabilization and 2 hours of curing, promoted by the insertion of the curing agent diphenylmethane diisocyanate (MDI). Polyurethane coatings were obtained on ADN particles, intact and without agglomeration, establishing a safe and efficient composition within a range of diameters applicable to composite solid propellants.

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Investigation of CuO_2/WO_3-x Heterostructures for H_2 Generation by Photoelectrochemical Processes

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The photoelectrochemical (PEC) production of H_2 fuel through the water oxidation reaction (WOR) process is a potential technique for solving the energy shortage and environmental pollution crises[1]. Studies show that models to improve the overall applicability of converting solar energy into H_2 in PEC devices mainly include: improving light absorption by engineering the morphology of the semiconductor absorber layer [2]. Due to their wide range of applications, including catalysis and energy storage, metal oxides such as CuO_2 and WO_3-x are considered promising materials because of their distinct properties [3]. With the aim of collaborating with the real development of this innovation, this project is dedicated to studying CuO_2 and WO_3-x heterostructures, with the aim of using them as photoelectrodes in the generation of molecular H_2 via PEC processes. The CuO_2/WO_3-x films were deposited on FTO substrates using the DC magnetron sputtering technique. First, CuO_2 films were deposited with O_2 and Ar flows of 25 sccm and 5 sccm, respectively, at a pressure of $3x10^{-3}$ torr using different DC powers: 40w, 60w, 80w and 100w. Next, a WO_3-x film was deposited, keeping the O_2 and Ar flow at 10sccm and 10sccm respectively, pressure at $3x10^{-3}$ torr and DC power at 150w constant in the chamber. The samples were then heat-treated at 450 ºC for 2 hours at a rate of 5 ºC per minute. The samples were characterized by X-ray diffraction, Raman scattering, SEM and mechanical profilometry measurements. The photoelectrochemical potential of the samples was evaluated by electrochemical impedance spectroscopy (EIS) and Mott-Schottky measurements.

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Investigation of the Electrocatalytic Properties of 2D Bismuth Sulfide for Alkaline Hydrogen Evolution Reaction Using First-principles Calculations

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Cathodic hydrogen evolution reactions (HER) in acidic medium are generally 2-3 orders of magnitude more efficient when compared to alkaline media[1]. Nonetheless, the harsh conditions of the former play a major role in electrode degradation. On the other hand, alkaline HER offers a greater range of possible materials acting as catalysts including abundant metal compounds found as mineral as in the case of Bismuth (III) sulfide (Bi2S3) (mineral bismuthinite). In this work, we employ first-principles calculation based on DFT and the Computational Hydrogen Electrode (CHE) model[2] to investigate the catalytic properties of two-dimensional (Bi2S3). Our results show that Bi2S3 (001) surface binds H weakly for the acidic conditions (pH = 0 and U = 0 vs. Standard Hydrogen Electrode - SHE) with the best free-energy variation found at the S sites. Bader charge analysis reveals that stronger binding of S sites is related to the larger charge donation from S sites, which draw electrons from neighboring sites. Applying linear corrections for pH and U according to the CHE model reveals that the activity of S sites can reach the optimum for alkaline conditions (pH > 7) for U = -0.8 V vs. SHE, in agreement with experimental results. Furthermore, H2O adsorption on 2D Bi2S3 is found to be more energetic favorable, while OH adsorption is weak therefore favoring the hydrogen evolution. These results provide an atomistic understanding of the catalytic properties of 2D Bi2S3 supporting experimental findings.

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Investigation of the microstructure role in the NiO nanoparticles magnetism

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NiO is an antiferromagnetic (AFM) material in the bulk configuration below the Néel temperature TN=523 K. In this work, we studied the magnetic properties evolution of NiO nanoparticles (NPs) as a function of their microstructure. It is a primary attempt to quantify nanostructure details as the synthesis temperature changes and it affects the long-range magnetic exchange. We synthed NiO NPs using the Ni(OH)2 decomposition method at different temperatures (250ºC-700ºC). We collected transmission electron microscopy (TEM) images to determine the average particle s from 3 to 87 nm. An X-ray profile analysis (XPA) provided further (micro)structural details by combining a Rietveld refinement with a Convolutional Multiple Whole Profile (CMWP) fitting tool of the powder diffraction data [2]. We fitted the diffraction patterns by assuming that the defect structure arose from a distribution of dislocations, stacking faults, and crystalline s (coherent domains). Preliminary magnetization data using a PPMF-Evercoll II magnetometer revealed a ferromagnetic long-range order, which increases for smaller particles, coexisting with the AFM one. Also, there are shifts of the MxH curves (hysteresis loops) for T<220K, signing an AFM-FM interface interaction (exchange bias). We may confirm that the NiO magnetic moment increases together with the exchange bias effect for smaller NPs, and both effects are related to the increased defect density and smaller particle . The unit cell parameters also increased for smaller particles, which appears to determine the Ni-O-Ni superexchange.
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Investigation of WO3 and TiO2 Heterojunctions Applied as Photoelectrodes in Solar Energy Conversion to Hydrogen Fuel

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The use of molecular hydrogen (H2) as fuel is preferable to petroleum derivatives due to its higher energy efficiency and environmentally sustainable nature, as its combustion does not produce harmful pollutants. This helps reduce air pollution and combat climate change, making it a viable alternative for energy transition towards a more sustainable, low-carbon system. Many research groups worldwide are focused on developing techniques to produce H2 as fuel, with special emphasis on photoelectrochemical (PEC) production via the water oxidation reaction (WOA) using sunlight. However, there are challenges to overcome before this technology can be widely adopted, such as expanding the spectral absorption range of semiconductors to include the visible region and reducing the recombination rate of electron-hole pairs generated by light. This study aims to advance the technology by investigating TiO2/WO3-x heterojunctions for use as a photoelectrode in H2 production via PEC processes. The TiO2/WO3-x films were deposited on glass, Si(100), and FTO substrates using DC magnetron sputtering. Initially, WO3-x films were deposited with O2 and Ar flow rates of 10 sccm and 10 sccm, respectively, at a pressure of 3x10^-3 torr and DC power of 300w. To evaluate the influence of WO3 thickness on the PEC properties of the photoelectrode, films with different deposition times were prepared, ranging from 60 min to 5 min. A second TiO2 film was then deposited with O2 and Ar flow rates of 2 sccm and 10 sccm, respectively, at a pressure of 3x10^-3 torr, DC power of 150w, and a deposition time of 30 min. After growth, the films were thermally treated at 450 °C for 2h under a pressure of 1x10^-2 torr. The samples were characterized by X-ray diffraction, Raman scattering, SEM, and mechanical profilometry.Reference [1] M. Boundellal, PowertoGas:Renewable Hydrogen Economy for the Energy Transition, 2018:p. 211. doi:10.1515/9783110559811-201. [2] P. Chatterje, et al., Energy Convers. 261 (2022).

Large barocaloric effect on Graphene Oxide/Thermoplastic Elastomer composite

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The pursuit of enhanced energy efficiency in cooling systems has led to the exploration of innovative technologies, with solid-state cooling utilizing mechanocaloric effects emerging as a promising alternative to traditional refrigeration methods. Despite its significant potential, only a limited number of materials have been investigated as barocaloric refrigerants. The barocaloric effect, responsive to hydrostatic pressure applied to the material, presents a particular avenue for exploration. This study focuses on assessing the barocaloric effect in a composite material comprising thermoplastic elastomer (TPE) filled with graphene oxide (GO). The TPE and its GO/TPE composite were processed using counter-rotating twin-screw extrusion at 60 RPM, maintaining a constant temperature of 190°C. Subsequently, the materials underwent compression molding into cylindrical geometries at 180°C. For the pure TPE, measurements yielded a hardness (Shore D) of 16.5, a modulus of elasticity of 14.69 MPa, and a thermal conductivity of 0.15 W m-1 K-1. The evaluation of the barocaloric effect was conducted under a pressure of 218 MPa (at 333K), resulting in a temperature variation of 15 K. Similar measurements were carried out for the GO/TPE composite, revealing a large barocaloric effect without the occurrence of a phase transition [1,2], thus suggesting a promising material for application as a solid-state refrigerant.

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Laser induced graphene-cobalt oxide composite synthetized and supported on stainless steel mesh: An electrode for efficient alkaline electrolysis

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The CO_2 laser induced graphene and its composites received a lot of attention of the materials science community after its first publication in 2014. Due to a number of advantages front conventional synthesis methodologies, such as low cost and energy consumption, scalability, reproducibility and low time scale, this technique is desirable for a variety of applications, such as: Energy storage and conversion, sensors and flexible electronics [1]. This study aims in the production of high active area catalytic surface for oxygen evolution reaction (OER) provided by the laser ablation of a mixture of polyimide (PI)/cobalt chloride salt supported on a 1 cm² stainless steel (SS) mesh for a low resistivity composite electrode. The methodology consists of two simple steps: 1 – Impregnation of the SS mesh with a liquid solution of PI/N-Methylpyrrolidone/$CoCl_2$ and 2 – laser ablation of the dried mixture for the obtention of the composite SS-LIG-CoO electrode. Different PI/NMP/$CoCl_2$ proportions were tested to obtain the best condition in terms of surface coverage and good electric contact between the active material and the SS current collector. XRD, Raman spectroscopy and scanning electron microscopy were used to characterize the materials. The electrochemical characterizations were conducted in a three-electrode cylindrical cell and KOH 1 mol.L^{-1} as the electrolyte solution. It was observed a ten-fold increase in the capacitive current and a nine-fold decrease in the Rct values of the composite electrode when compared with the SS mesh, due to the high area porous catalytic material LIG-CoO. The SS-LIG-CoO electrode achieved an overpotential at 10 mA.cm^{-2} of 313 mV, overcoming the SS mesh's of 400 mV. This study points a direction to large scale, high efficiency and low-cost catalytic electrodes production for alkaline water electrolysis.

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Lignin and cellulose from Pinus elliottii barks for carbon xerogel

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Agro-forestry wastes offer great potential as raw materials for the production of high-value compounds, as these biomasses are rich in polyphenolic compounds and polysaccharides. For instance, barks from cut trees are mainly destined for energy production, even though they represent up to 14% (v/v) in Pinus spp [1]. In this work, we used lignin and cellulosic pulp obtained from a Pinus elliottii bark biorefinery as raw materials. Lignin was produced using soda pulping and precipitated with sulfuric acid. The cellulosic pulp was obtained from bleached soda pulp and mechanically defibrillated to produce nanofibrillated cellulose. A lignin-cellulose (75/25) suspension with 7% solid content was prepared using a magnetic stirrer. Then the mixture was placed in a mold dipped in liquid nitrogen bath, freeze-dried, and carbonized in a tubular oven under nitrogen atmosphere at 1000ºC for 1 h [2]. Then, the mixture was placed in a mold dipped in a liquid nitrogen bath, freeze-dried, and carbonized in a tubular oven under a nitrogen atmosphere at 1000°C for 1 h [2]. As a result, a sponge-like material was obtained after the carbonization of the lignin-cellulose xerogel. The resulting material presented a high surface area measured through BET analysis, as well as excellent electrical conductivity, proving to be an excellent material for use in devices such as supercapacitors or detection platforms for sensors.

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Luminescent Tb-doped Lu_2O_3 nanocubes obtained by microwave-assisted thermolysis of different precursors.

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The search of new efficient luminescence materials for application in a variety of fields is becoming very intense nowadays. The luminescence materials are present in the modern life in almost every electronic device and illuminated ambient. In the nanoparticle form it can find medical applications such as bioimaging and photodynamic therapy. However, rare Earth based nanoparticles are usually difficult to obtain by simple, one step methodology. Besides, to control the and morphology the synthetic approach can become expensive and time consuming. Microwave-assisted heating is a powerful tool to synthe luminescent materials due to the fast nature of the dieletric energy-to-heat conversion. Moreover, microwave irradiation of solid materials can increase the ionic diffusion, increasing the rate of reaction. The fast, volumetric microwave-assisted heating contribute to obtain high quality materials in a fraction of time compared to conventional heating methods. In this work, two different precursors are subjected to microwave-assisted heating to induce the ligand thermolysis to obtain $Lu_2O_3:Tb^{3+}$ nanoparticles. The thermolysis of $Lu_{0.99}Tb_{0.01}$TMA complexes (TMA: Trimelitic) acid leads to well formed nanocubes when heated in resistive furnaces. However, the microwave-assisted method yields $Lu_2O_3:Tb^{3+}$ nanocubes in mere 20 minutes, with controlled morphology and excellent optical properties. The precursor complex can be fully degraded after 10 minutes due to the use of activated Fe_3O_4 magnetite susceptor that induces the heating and promote oxygen-rich atmosphere necessary to degrade organic moieties. During the thermolysis using the $Lu_{0.99}Tb_{0.01}(NO_3)_3$ complex in granular carbon susceptor, it was observed that the formation of nanocubes was not as uniform as that obtained with the TMA precursor within the same 20-minute timeframe, when making a direct comparison between the samples.

Manufacturing of a Photo-Electrolyzer for large scale production of green Hydrogen.

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The production of green hydrogen is a highly promising mechanism in terms of its capacity to substantially reduce the damages caused by the greenhouse effect. Advanced semiconductor materials, such as Bismuth Vanadate (BiVO4), are widely used to provide an effective photocatalytic process, leading to the projection of new horizons for the advancement of this technology. Specializing in this research field, the LAPNano research group, coordinated by Professor Renato Vitalino Gonçalves, after a series of published articles, theses, and scientific initiations developed in the area, now presents a promising opportunity to produce hydrogen using large-scale photoreactors, aiming to achieve a production with a high level of market interest. This objective can be achieved through the meticulous study of materials engineering together with manufacturing processes, making use of tools that allow the appropriate prototyping of mechanical and electrical system designs, with the intention of manufacturing a "Photo-Electrolyzer'', combining the advances of basic with applied science [1].

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Maximizing artificial photosynthesis potential through optimized $ZnFe_2O_4$ thin films with $NiFe_x$ co-catalysts

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Rising global temperatures and environmental crises have driven the search for sustainable energy solutions, focusing on reducing greenhouse gas emissions, particularly green hydrogen, produced from water using a photoelectrochemical (PEC) system [1]. Recently, the focus on using zinc ferrite ($ZnFe_2O_4$) as a photoelectrode for H_2 production has significantly increased [2]. These materials are abundant, low-cost, non-toxic, and present good chemical stability, being emerging candidates for this application [3]. To optimize the efficiency of zinc ferrite, it is crucial to obtain this material in a way that reduces the recombination rate of electron-hole pairs and improves charge transport and separation. The addition of co-catalysts, such as $NiFe_x$ (Nickel-Iron) nanoparticles, can increase this efficiency, making the process more viable on a large scale [2]. In this study, $ZnFe_2O_4$ thin films were synthesized by initially obtaining β-FeOOH nanotubes onto FTO substrates with further deposition of Zinc by dripping a Zinc solution onto the films, with subsequent calcination. Moreover, we employed a thermal treatment in a reducing atmosphere (H_2) to induce oxygen vacancies aiming to control the deposition of co-catalysts. $NiFe_x$ co-catalysts were deposited by magnetron sputtering process to improve the efficiency of the material, using different deposition times. The films characterization was performed by XRD, UV-Vis spectroscopy, XPS and SEM analysis, as well as LSV. By evaluating the photocurrent density of the samples, we can estimate the potential to generate H_2.

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Mechanochemical synthesis of Ag NPs into ZIF8 structure for ammonia electrosynthesis using water in salt electrolyte

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Ammonia electrosynthesis offers an alternative pathway to the energy-intensive Haber-Bosch process under ambient conditions [1]. However, several challenges are associated with the electrochemical process, such as, parallel reactions as Hydrogen Evolution Reaction (HER) which competes with N2 reduction. Based on this, the design of catalysts is important to avoid HER. In this study, a hybrid catalytic material based on ZIF8 hosting Ag nanoparticles (NPs) was synthed by mechanochemical synthesis using a ball milling. The material was fully characterized by several techniques such as, PXRD, BET, UV/VIS DRS, ICP-OES and TEM, giving Ag@ZIF8. The TEM images reveal that the Ag NPs are into ZIF-8 matrix. The Ag@ZIF8 material was applied for N2 to yield NH3. The ZIF8 matrix [2], act both as a matrix for Ag NPs and as a water blocker, preventing HER. The catalytic properties of Ag@ZIF8 were tested in a non-conventional electrolyte, a water-in-salt electrolyte (WISE) [3] of lithium bis(trifluoromethanesulfonyl)imide (LiTFSI), in which the salt concentration superpass the amounts of water. Experiments were carried out under different WISE concentrations, 15 mol kg-1 and 12 mol kg-1. Controlled potential electrolysis under N2 atmosphere, revealed that the NH3 yield rate is strongly dependent of WISE concentration. At WISE 15 mol kg-1 the NH3 achieved was 23,65 µmol h-1g -1 RHE and FE 73,82 %, while at WISE 12 mol kg-1 the values obtained were 65,65 µmol h-1g -1 and FE 38,4 %. Additionally, experiments under light exposure are underway to investigate if in these conditions the effect of localized surface plasmon resonance (LSPR) of Ag NPs may enhance the NH3 production.

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Mesoporous Carbon Nitrides for Sorption and Photodegradation of Organic Pollutants

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The remediation of pollutants promoted by systems that are cheap and viable remains an important challenge in the field of catalysis. Carbon nitrides applied in photocatalytic systems are a promising class of materials for promoting advanced oxidative processes, with several studies demonstrating their potential in removing contaminants. Mesoporous Carbon Nitrides (mpg-CN) offers advantages such as high surface area and chemical stability,m rendering them resilient in harsh environments and reactive processes. Photocatalysis can provide a milder route (low pressures and temperature) in pollutants photodegradation. In this work, we synthed the mpg-CN and tested its activity against the sorption and photodegradation of three emerging contaminants: Rifampicin, Tetracycline and Bisphenol - A. Firstly, a certain amount of a precursor (cyanamide) and mesoporous silica (to shape the material) were together and stirred at 60º until the water completely evaporated. Afterwards, the material was treated in a muffle furnace, followed by washing with hydrofluoric acid, and dried in an oven. A certain amount of the catalyst was added to a vial, followed by 2 mL of the contaminant solution, then powered by a violet LED (410 nm) to simulate sunlight. Characterizations such as FT-IR, XRD and DRS were carried out first to understand the characteristics of the material. More advanced techniques such as TEM, SEM and BET were applied. Under microscopy, the material was close to that found in the literature, where its mesoporous form was confirmed in the scan. Then, the BET technique proved that the material had micropores, with pores varying in different sizes (nm), explaining the reason for the high sorption activity towards contaminants. Against the 3 substrates, nearly 100% of removal was observed after 4h of light radiation. In reuse tests, the catalyst proved to be quite resistant, with removal activities of 80% activity in the fourth reuse of the material.

Metal Single Atoms for Methane Conversion to Valuable Compounds

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Due to its environmental issues and vast reserves, selective methane oxidation to valuable compounds is of paramount importance. Recently, photocatalytic routes have demonstrated to be a viable and mild pathway to drive this reaction. However, controlling C-H activation to avoid overoxidation to CO2 molecules is the biggest challenge in this field. Single atoms have shown significant activity in producing oxygenated compounds from methane, especially when supported by carbon nitrides. Crystalline carbon nitrides with poly(heptazine imide) (PHI) structures can efficiently stabilize metal single atoms and emulate reaction mechanisms from homogeneous complexes.[1] In this study, we evaluate the activity of different metal single-atoms materials for photocatalytic methane oxidation. We observe that Fe-PHI photocatalysts possess high efficiency in producing formic acid from methane using O2 as an oxidant. Moreover, methane oxidation reactions carried out on acidic media improve significantly the HCOOH production, with a yield of 1980 µmol/g. This study expands the applicability of crystalline carbon nitrides for CH4 valorization.

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Microwave-Assisted Production of Anatase TiO_2 Nanoparticles: A Green Route for Improved Photocatalysis

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Titanium dioxide (TiO_2) nanoparticles are versatile materials used in various fields such as solar energy, coatings, and catalysis due to their unique properties such as photocatalytic activity, UV absorption, self-cleaning capability, and tunable characteristics [1,2]. This research aims to fabricate titanium dioxide nanoparticles through an environmentally sustainable approach, using a microwave-assisted method to augment photocatalytic efficacy. This methodology involves the reaction of titanium tetrachloride ($TiCl_4$) in an aqueous medium, pH adjustment to induce the anatase phase and microwave irradiation. The produced nanoparticles were characterized by transmission electron microscopy (TEM), X-ray diffraction, N_2 adsorption/desorption, thermogravimetric analysis, Raman spectroscopy, Fourier transformed infrared spectroscopy (FTIR) and UV-vis diffuse reflectance spectroscopy. The results confirmed desired properties such as thermal stability, a band gap of approximately 3.14 eV, anatase phase nanoparticles and a crystallite of around 14 nm. The results for the photocatalytic activity demonstrate its similar performance compared to the commercial TiO_2, Degussa P25. This environmentally-friendly method provides a promising pathway for producing TiO_2 nanoparticles with customized properties suitable for a wide range of applications.

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Modification of ZnO gas-diffusion-electrodes for enhanced electrochemical CO_2 reduction: Optimization of operational conditions and mechanism investigation

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The excessive emission of greenhouse gases to atmosphere, is one of the main causes of climate change, resulting in the devastation of essential natural ecosystems.[1] Therefore, the development of new catalysts based on low-cost materials with high activity, stability, and selectivity for the electrochemical CO_2 reduction, is of great importance in upgrading greenhouse gases to valuable fuels and feedstocks.[2] In this work, a ZnO catalyst were developed using the hydrothermal method, followed by it's functionalization with amine groups from monoethanolamine to improve its catalytic performance in the reduction of CO_2 to CO. It's observed that electrodes prepared with ZnO modified with amine groups exhibited the highest performance in the electrochemical conversion of CO_2 to CO when used in an electrochemical flow cell. Under optimized conditions, it was achieved a current density of -130 mA cm^{-2}, with a faradaic efficiency exceeding 80% at -1.2 V vs RHE. The SEM results revealed diffuse morphologies between the particles, suggesting that the presence of monoethanolamine played a significant role in altering the morphology of the ZnO. The XPS results confirmed the presence of nitrogen, related to amine groups, on the modified ZnO samples. We investigated the mechanism of CO_2 reduction using in situ FTIR spectroscopy, at potentials above -0.8 V vs RHE, there was consumption CO_2 at 2343 cm_{-1} and formation of the CO_2^- intermediate at 1668 cm^{-1}. Additionally, we confirmed the adsorption of CO_2 on the catalyst surface by detecting bidentate CO_2 at 1378 cm^{-1}. Consequently, the catalyst exhibited a remarkable CO^2 adsorption capability, making it promising for CO_2 reduction in the production of valuable chemical products.

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Modification of ZnO@ZnS photoelectrodes through the insertion of nanotubes titanium.

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The growing search for new technologies in order to meet the world's energy needs, motivated mainly by high population growth and associated with industrial development, highlights the use of efficient devices to modify the current energy scenario, aiming to mitigate the negative environmental effects generated by sector, at the same time being able to meet the progressive expansion of electrical demand. Therefore, the search for the development of new photovoltaic cells has been the object of study focusing on improving the conversion of solar energy into electrical energy through the photovoltaic effect.

The study by Flores (2016) and Fernandes (2020) on a core@shell ZnO@ZnS system managed to show that the compound is a decorated system, that is, ZnS nanoparticles decorate hexagonal ZnO nanorods. The system has interesting optical properties to be used as a photoelectrode in photovoltaic cells [1,2]. Therefore, the results obtained for the ZnO@ZnS system under certain synthesis conditions allow the investigation of new research perspectives, such as the modification of photoelectrodes [3].

In this sense, the present study investigated the creation of a Grätzel electrochemical photovoltaic cell, of the core@shell (decorated) ZnO@ZnS type with the insertion of titanium nanotubes (NTT) for modifying the photoelectrodes. The modification of the ZnO@ZnS system with NTT occurs through two synthetic routes, through the microwave-assisted hydrothermal method (HAM) and through a chemical route, with the aim of analyzing possible positive increases in photoactive parameters, through changes on the optical and electrical properties of the compound.

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Molecular dynamics simulations of sodium-based electrolytes confined between carbon electrodes for dual carbon batteries

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The energy demand is ever-growing in current days. The use of sustainable and green energy sources (solar, wind, and tidal energies) is increasing, but these energy sources have drawbacks due to their intrinsic intermittency. Therefore, there is a need to store energy when the sun is not shining or when the wind is not blowing. Li-ion batteries are already well developed, but the natural occurrence of lithium is less compared to sodium, which is more spread throughout the Earth's crust [1]. Many efforts have been made to develop efficient and cheaper Na-ion batteries [2]. Here, we performed molecular dynamics simulations of sodium-based electrolytes, comprised of sodium salts in carbonate solvents [3], to investigate transport properties and local structure characterization of the electrolytes in the bulk. Additionally, molecular simulations of the electrolytes confined in porous carbon electrodes were also performed to investigate the electrical properties of the electrochemical cells and the structuring of ions inside the nanopores of the electrodes under applied voltage. Despite its high viscosity, NaPF6-based electrolyte allows for similar charges accumulated on the electrodes compared to NaTFSI. With the strong Na-carbonate interactions, solvent molecules are dragged into the electrode upon the filling of the negative electrode by Na+ cations.

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Molecular sieves synthesized from metallurgical slag as catalysts to the conversion of nocive gas from automotive combustion

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Molecular sieves synthed from the slag copper artifact industry were applied as heterogeneous catalysts for converting harmful gases from automobile combustion (NOx). The future objective is to enable other materials to be active in the NOx reduction process and not precious metals (Rh, Pd, and Pt)[1]. Among the materials synthed from slag, some showed exceptional performance in converting harmful gases at low temperatures, the results obtained indicate a 50% greater conversion capacity compared to the materials currently used. On the other hand, materials were obtained that showed greater activity in converting harmful gases at high temperatures, achieving a 100% NOx conversion rate.

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Nanocellulose and carbon nanotubes modified with bismuth sulfate based nanocomposites development for efficient hydrogen storage

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Hydrogen appears in the current market as an alternative source of energy to fossil fuels, since when burned it releases only hot steam and water, in addition to presenting itself as an abundant and stable element. Even with all the advantages, the use of hydrogen as an energy source still limited by the lack of viable and effective designs for storage. Thus, the present project presents the development of a nanocomposite based on nanocellulose, carbon nanotubes and bismuth sulfide and to materialize this approach, the synthesis of bismuth sulfide anchored in carbon nanotubes uses the hydrothermal method, resulting in Bi2S3-FMWCNT. In addition, FMWCNT/NC and Bi2S3-FMWCNT/NC nanocomposites were obtained by wet impregnation technique. Subsequently, the nanocomposites are subjected to electrochemical laboratory analysis by MEV-FEG, EDS, FTIR and EIS, being evaluated in relation to their performance in the electrochemical storage of hydrogen, through methods such as cyclic voltammetry, charge/discharge, and electrochemical impedance. These analyses make it possible to determine the specific capacitance (Fg^{-1}) and the specific hydrogen discharge capacity ($mAh\ g^{-1}$). MEV studies for the synthed material (Bi2S3-FMWCNT) showed a bismuth flowers. The copper electrodes modified with FMWCNT/NC and Bi2S3-FMWCNT/NC showed promising results in cyclic voltammetry tests in alkaline media. The cyclic voltammograms of the modified electrodes showed redox peaks in smaller potential windows, reaching capacitive currents close to 8 and 10 mA. The unmodified copper electrode presented anodic and cathodic currents below 6 mA. Therefore, the modification of copper electrodes with FMWCNT/NC and Bi2S3-FMWCNT/NC generated an increase in the capacitive currents and highlighted the capacity to electrochemically store hydrogen. Acknowledgements: This project was made possible by São Paulo Research Foundation (FAPESP), N.º 2023/06161-8.

Nanocomposites based on UiO-66/MoS2/FMWCNT for electrochemical hydrogen storage

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Hydrogen stands out as a possible and promising energy solution. Its clean production from renewable sources and the potential to reduce air pollution emissions make it an ideal candidate for driving the energy transition. However, efficient, and safe hydrogen storage remains a challenge. The objective of this work was to study the use of nanocomposites based on UiO-66/MoS2/FMWCNT for the electrochemical storage of hydrogen. These porous materials can enable safe and effective electrochemical hydrogen adsorption, along with the added benefit of electrochemical storage. Initially, FMWCNT was decorated with molybdenum, and then MoS2/FMWCNT was formed by mixing an L-cysteine solution in an ultrasonic bath for 12 hours. UiO-66 was added to a MoS2/FMWCNT suspension, and the mixture was subjected to an ultrasonic bath for 12 hours. The SEM-FEG images showed the characteristic morphology of FMWCNT, and there was no change in morphology after the formation of MoS2/FMWCNT. It was clear that the samples had changed after UiO-66 was added; the UiO-66 nanoparticles were well spread out and tangled up in the FMWCNT threads. The electrochemical hydrogen storage capacity of the prepared compounds was investigated using cyclic voltammetry and galvanostatic charge and discharge methods in a three-electrode system in an alkaline medium (6M, KOH). The discharge capacities for FMWCNT, FMWCNT/MoS2, and UiO-66/FMWCNT/MoS2 nanocomposites were 808 mAh/g (2.96% by mass), 1435 mAh/g (5.26%), and 2050 mAh/g (7.51%), respectively. UiO-66/MoS2/FMWCNT represents a promising approach to improving electrochemical hydrogen storage capabilities, highlighting continued advancement in the search for effective materials to drive the transition to a more sustainable and clean hydrogen economy.

Nanoparticles of titanium-niobium mixed oxides for green hydrogen production

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The rise in emissions of toxic gases, a consequence of industrialization processes and the subsequent burning of fossil fuels, has exacerbated global climate change, which is becoming increasingly evident. Governments and environmental agencies have been warning about the dangers of global warming, thereby driving the pursuit of sustainable solutions [1]. In this context, green hydrogen emerges as a promising alternative gaining prominence due to its production from renewable resources, and its utilization entails no emission of toxic gases into the environment. This type of hydrogen is produced through the process of water electrolysis, and the equipment responsible for this process is known as electrolyzers. One of the most promising electrolyzers for green hydrogen production is the polymeric electrolyte membrane (PEM) electrolyzer, albeit with a high value added. The high production cost of this equipment is justified due to the elevated cost of some materials comprising it, such as catalysts which are made of noble metals with limited availability (platinum, iridium oxide, and ruthenium oxide) [2]. One possible solution to this significant challenge lies in the production of materials with similar efficiency to those currently used. Titanium-niobium mixed oxides (TNOs) possess suitable properties for application as catalysts in PEM electrolyzers. Despite their promise, TNOs still require research to optimize their efficiency and stability [3]. This study aims to produce a catalytic paint comprising ceramic nanoparticles of mixed titanium-niobium oxides doped with graphene. The structural, morphological, and electrochemical properties of the produced material will be assessed and characterized for PEM applications.

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Niobium-based plasmonic photocatalysts for water splitting and rhodamine 6G dye degradation

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Photochemical water splitting is a promising sustainable technology to directly produce hydrogen and oxygen from water in the presence of a photocatalyst and solar energy [1]. The hydrogen produced by this technology is clean and can be used either directly as a fuel or in chemical processes via CO2 hydrogenation to produce sustainable aviation fuels (SAF) [2]. However, solar energy conversion efficient photocatalysts are still challenging and must be improved. This work combined a spiky-shaped niobium oxide (Nb2O5) and plasmonic metallic noble metal nanoparticles (NPs) to achieve a synergic photocatalytic and optical response. For this purpose, the spiky-nanostructured Nb2O5 (NbSN) was prepared using the hydrothermal method [3]. Then, the Nb2O5 surface was decorated with Au/Pt, Au, and Pt NPs, producing NbSN-AuPt, NbSN-Au, and NbSN-Pt materials, respectively. TEM images of the NbSN-AuPt catalyst showed the Nb2O5 spiky with 70 nm of in and decorated with the Au/Pt NPs. XRD patterns exhibited the presence of both Nb2O5 and the metallic NP crystalline phases. Firstly, the photocatalytic efficiency of the materials was investigated towards rhodamine 6G dye degradation. Then, water splitting tests were carried out in a homemade 50 mL septum-sealed glass reactor, using 0.8 g of catalyst and 20% v/v of CH3OH/H2O. The reactor was irradiated with a green LED (532 nm) for 2h, and the gas product was analyzed by a micro-GC Agilent 990. NbNS and NbSN-Au were active in dye degradation under green-led irradiation. However, NbSN-Au showed higher photocatalytic degradation performance. NbSN-AuPt catalyst showed H2 formation compared to NbSN-Pt. These results are associated with the plasmonic band due to the presence of Au NPs, which enhance light absorbance in the visible region. The materials are promising photocatalysts and showed great potential to develop solar-driven photochemical water-splitting processes.
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Ni-YSZ anodes synthetized by spray drying for MS-SOFCs.

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Metal-supported Solid Oxide Fuel Cells (MS-SOFC) are promising energy conversion devices due to their higher electrical efficiency, mechanical robustness, and reduced ohmic losses. These cells comprise a porous metallic support, an anode, an electrolyte, and a cathode, where the nano-structured anode is responsible for catalytic oxidation of the fuel and electricity generation. The cermet Ni-8YSZ is one of the state-of-the-art composites for MS-SOFC anodes with high power density [1]. In this study, the synthesis of Ni-8YSZ 60:40 %wt was performed using spray drying and thermally induced congruent crystallization techniques. In the initial stage, amorphous microspheres were obtained, which were subsequently treated at 800°C for 2 hours in a reducing atmosphere of H2:N2 (5:95) or synthetic air to form nano-microstructured materials. XRD results indicate the presence of Ni° and NiO crystal s of 81 nm and 63 nm, respectively, and the 8YSZ with 27 nm. SEM images show the formation of spongy structures with an average pore diameter of 2.2 µm, where Ni and 8YSZ nanoparticles are mutually dispersed. These materials will be tested as base anodes for MS-SOFCs due to their catalytic activity and electronic conductivity from Ni°, ionic conductivity from 8YSZ, high density of triple-phase boundaries (TPBs) [2], and pores that facilitate fuel diffusion.
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Operational challenges in a photoelectrochemical cell for quantification of gaseous products from solar water-splitting

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This work details the design and operational challenges of a photoelectrochemical (PEC) cell designed for in-line analysis of gaseous products, named the Submarine Cell. Tailored for monitoring oxygen and hydrogen evolution during PEC water splitting at a laboratory scale, the design emphas user-friendliness and high sensitivity to detect minimal gas evolution rates. Recent reports have demonstrated the device's hydrogen detection capability at the micro-mole scale [µM][1]. Achieving hermeticity in the device poses a central and complex challenge due to electrode interfacing complexities while ensuring electrical connections. Furthermore, the cell offers stability for prolonged experiments, including characterizations exceeding 24 hours with continuous gas evolution. Internally, a magnetically rotated helix disturbs the electrolyte to disperse gas bubbles, preventing passivation of the photoelectrode surface during prolonged measurements. The Submarine Cell is also equipped with temperature and pressure sensors for real-time monitoring. This cell utilizes SLA 3D printing for manufacturing, using resins with high mechanical and chemical resistance for nearly all components. This fabrication method not only reduces costs but also facilitates the development of innovative architectures and allows configuration adjustments to meet various PEC analysis requirements.

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Optimization and High-Performance Photoelectrochemical $BiVO_4/NiFeO_x$ Photoanode Fabricated via Sputtering

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The high consumption and its low production in renewable energy by several techniques poses a significant threat to future worldwide. Many attempts have been undertaken to discover, generate, and employ renewable energy sources as alternatives to fossil fuels, which have significantly deteriorated the environment. The development of an effective, affordable, and decentralized system for H_2 and O_2 generation by water splitting such as source of energy production remains a critical need, energy efficiency and particularly to treat advancing the oxygen evolution reaction (OER) relevant concentrations.In this study, a self-standing electrode composed of an engineered interface of $BiVO_4/NiFeO_x$ (n-p type) was prepared on fluorine-doped tin oxide (FTO) substrate using magnetron sputtering deposition technique. By systematically adjusting the atmosphere of the deposition process, we controlled the formation of oxygen vacancies within the $BiVO_4$ structure to enhance photoelectrochemical activity. The layers of $BiVO_4$ and $NiFeO_x$ were characterized photochemically and electrochemically to identify their light harvesting and electron transfer capacities. The activity of the $BiVO_4/NiFeO_x$ electrode for water splitting was evaluated under photoelectrochemical (PEC) conditions. The PEC measurements at 1.23 V vs RHE under constant AM 1.5G illumination (100mW/cm^2) exhibited outstanding a high current density, around 1.6 mA cm^{-2} for bare $BiVO_4$ and increasing up to 2 times for $BiVO_4/NiFeO_x$ heterostructure. For assessing structural properties, XRD, SEM, Raman spectroscopy were utilized, while XPS technique was employed for determining oxygen vacancies. These findings underscore the importance of a rational design approach for produce $BiVO_4$ photoanodes applied to water splitting, highlighting the significant role of vacancies and the magnetron sputtering.

Optimizing Platinum Deposition: Laser-Induced Graphene Electrodes for Sustainable Hydrogen Production

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Clean energy production technologies, such as green hydrogen, are being sought and developed to meet global energy demands and promote sustainable development [1]. Platinum is the most well-known metal for its high electrocatalytic activity in the hydrogen evolution reaction (HER) [2]. The objective of this study is to identify the best experimental condition for platinum deposition on a laser-induced graphene (LIG) electrode applied to HER. The LIG was CO_2 laser printed at a power of 5 W with a speed of 90 $mm.s^{-1}$ on a commercial polyimide tape [3], while platinum (Pt) was deposited by sputtering with a fixed current of 40 mA varying deposition times between 10 to 50 s. Scanning Electron Microscopy (SEM) images showed that the pores of LIG were not fully covered by Pt and all films exhibited uniformity, with an average resistance of 30.1 ± 4.5 Ω. Energy Dispersive Spectroscopy (EDS) characterization showed an estimated percentage increase of Pt with deposition time. Through cyclic voltammetry, the reversibility of the system was noted. Without Pt, linear voltammetry at η=10 $mA.cm^{-2}$ showed a high overpotential, whereas Pt addition resulted in overpotential values of -0.103, -0.206, -0.239, and -0.169 mV. In summary, electrochemical characterizations confirm that platinum has a significant effect on improving the electrocatalytic activity of the electrode in HER.

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Optimizing Stability in Perovskite Solar Cells Through Encapsulation

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Perovskite solar cells (PSCs) have emerged as a potential leading photovoltaic technology owing to their high efficiency, low production cost and ease of processing. However, the challenge hindering the widespread adoption is long-term stability. Therefore, developing effective encapsulation methods is crucial for advancing PSC technology [1]. In this study, we assess two different encapsulation processes for PSCs in a regular architecture. Using a $Cs_{0.17}FA_{0.83}Pb(I_{0.83}Br_{0.17})_3$ composition, Nb_2O_5/TiO_2 (mesoporous) as the electron transport layer and spiro-OMeTAD as the hole transporting layers, we achieved an average photovoltaic performance of PCE of 14.5%, Jsc of 23.6 mA cm^{-2}, Voc of 0.98 V, and FF of 62.4%. Firstly, we encapsulated our PSCs by sealing a glass cover on the top of the device using UV-curable epoxy applied across the entire surface. For the second one, we applied the same adhesive only to the edges, ensuring no contact with the absorber layer. In both approaches, the curing process involved exposing the devices to a UV light (395 nm) for 20 seconds in ambient air. The sealing quality was evaluated by water submersion tests (25 °C and 50 °C). While the first method provided better protection against external agents, it tended to react with perovskite after extended periods. We evaluated the stability of the photovoltaic parameters for the unencapsulated and encapsulated PSCs by exposing both to a continuous light source (1 sun, AM 1.5G) at room conditions (25 °C and <30% RH). The efficiency of the encapsulated devices was reduced to lower than 80% of their initial values before 24 hours. On the other hand, we observed an improved capability of PSCs to retain their efficiency when encapsulated. In conclusion, this study contributes to extending the lifetime of the PSCs.

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Organic Semiconductors Applied to Organic Dye-Sensitized Solar Cells

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The increasing use of fossil fuels worldwide and the associated impacts, such as pollution and climate change, have motivated the scientific community to seek sustainable solutions. Energy generation is one of the main causes of this increase, making photovoltaic energy a crucial alternative to reduce pollution resulting from non-renewable sources. The main objective of this study was the analysis and characterization of semiconductor polymers for application in solar cells. FTO (Fluorine-doped Tin Oxide) and ITO (Indium Tin Oxide) substrates were used, on which grooves were made by sliding a polytetrafluoroethylene (PTFE) bar, followed by the deposition of the polymer Poly(9,9-N-Di-Octyfluorenyl-2,7-Diyl) (PFO). PFO films were prepared using the self-assembly technique, dissolving PFO in chloroform at a concentration of 2.5 g/L, with subsequent thermal treatment at 250 °C. PFO films on identical substrates, but without thermal treatment, were also prepared. Solar cells were assembled by depositing titanium dioxide (TiO2) paste on FTO or ITO substrates, with and without the PFO layer. The deposited thin film was then impregnated with organic dye. The cell was finalized with an FTO counter electrode. The substrates and the device were characterized by absorption spectroscopy and current-voltage (I-V) curves. The results showed that the device exhibited photovoltaic behavior, making it possible to determine its electrical parameters, demonstrating that the solar cell was capable of transferring power to the load.

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Pechini-Ink: Redefining 3D Printing of Electrodes with Novel Resin Technology for Advanced Energy Storage

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Lithium-ion batteries play an important role in efficient energy storage due to their high energy density and long lifespan and advancements in this technology require constant development of new materials and processing methods. Niobium and titanium oxide-based electrodes (NTO) like $TiNb_2O_7$ are increasingly studied for their good stability and high charging rate. However, conventional electrode preparation methods often face challenges related to uniformity, porosity, and chemical composition control. In this context, it is essential to develop new processing methodologies for these components. 3D printing of ceramic elements from resins containing oxide particles is gaining popularity due to its high resolution, printing speed, and efficient solid-phase dispersion [1]. The resin acts as a dispersing vehicle for the particulate material, eliminating the need for complex processing of filaments. However, this method may encounter challenges such as nozzle clogging due to solid accumulation. Therefore, this study aimed to 3D print NTO electrodes for batteries using resins derived from Pechini precursor synthesis. The ceramic material is formed only after printing, during a calcination thermal treatment process. A standard Pechini synthesis was carried out using Nb-oxalate and Ti-isopropoxide. The printer was fed with the resin, and an electrode was printed onto a ceramic substrate, followed by thermal treatment in two stages (organic elimination at 350°C and calcination at 900°C). As a result, a ceramic electrode with adequate porosity and excellent microstructural uniformity and monophasic composition ($TiNb_2O_7$) was obtained.

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Pechini synthesis of $NaNbO_3$ for use in obtaining hydrogen from sodium borohydride

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With the gradual increase in the use of fossil fuels worldwide over the years, there is notable global concern regarding the harmful effects that the use of such fuels brings to the environment and human health, resulting from the release of polluting gases. This issue is one of the tasks to be addressed by the UN's Agenda 2030. Thus, the search for clean energy sources has been gaining prominence year after year in research and investments to find alternatives to conventional energy sources that end up generating polluting gases. Among the clean energy sources that have been attracting considerable attention is hydrogen gas (H_2), which presents excellent properties as a good alternative, mainly because it can be generated with low pollution and because this gas has a higher calorific value than gasoline, for example [1]. Therefore, this work aims at the synthesis of sodium niobate ($NaNbO_3$) and its application as a catalyst for hydrogen production, using borohydride as a hydrogen storage source. The synthed materials were characterized by XRD and SEM and then subjected to H_2 production tests. At the end of this work, it was possible to conclude that the Pechini method synthesis of $NaNbO_3$ proved to be effective and that their application for H_2 production through the hydrolysis of $NaBH_4$ yielded satisfactory results.

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Photophysical Study of The Interfaces of Perovskite/P3HT and Perovskite/P3OT

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Organic-inorganic hybrid perovskite films are widely targeted for application in solar cells and other photovoltaic devices due to their optoelectronic properties [1]. Briefly, the photophysics of perovskites is relevant, but they face instability due to photophysical phenomena such as photoinduced phase segregation due to halide segregation. This phase segregation is observed in the evolution of the photoluminescence spectra of perovskite films, and although it has been extensively studied and documented for free-standing perovskite films, the influence of the interface on this phenomenon has not been adequately considered [2]. To address this gap, this work studied the influence of interfaces on the optical properties of organic-inorganic multication lead halide perovskite films. Interfaces of $Cs_yFA_{1-y}Pb(Br_xI_{1-x})_3$ perovskite films with regioregular Poly(3-octyl-thiophene) (P3OT) and regioregular Poly(3-hexylthiophene) (P3HT) were prepared for the study. Perovskite films were synthed by a one-step method, involving the dissolution of reactants in defined stoichiometric amounts, followed by deposition on fluorine-doped tin oxide (FTO) by spin-coating. The regioregular P3OT and regioregular P3HT were diluted in chlorobenzene in a ratio of 1/0.1 by mass and deposited on perovskite films by spin-coating. The study used traditional spectroscopy techniques, such as UV-Vis absorption and Photoluminescence (PL), and the X-ray Diffraction (XRD) technique was used to characterize the films.

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Phyto-assisted Synthesis of NiO Nanoparticles for OER Electrocatalysis

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Green hydrogen (H_2) is a promising energy source, mainly obtained through the water electrolysis. This process consists of two half-reactions, Hydrogen Evolution Reaction (HER) and Oxygen Evolution Reaction (OER), however, demanding high energy and high overpotentials, and electrocatalysts are requested. Thus, this work reports a green synthetic route using aqueous extract from the wild sage plant (Ipomoea asarifolia) as a stabilizing agent to obtain nickel oxide (NiO) nanoparticles. The materials were obtained using three different calcination temperatures (300°C, 500°C and 700°C) under in air. The three samples (NiO300H, NiO500H and NiO700H) were characterized by X-ray diffraction (XRD) and vibrational spectroscopy (FTIR and Raman) and scanning electron microscopy (SEM-EDS). The electrocatalytic performances in alkaline solution (KOH, 1.0 mol/L) were investigated by linear sweep voltammetry (LSV), cyclic voltammetry, electrochemical impedance spectroscopy (EIS), and chronopotentiometry. Experimental overpotential at J = 10 mA cm^{-2} were 307 mV, 321 mV and 312 mV, and Tafel slope were 60.35 mV dec^{-1}, 50.29 mV dec-^{1} and 53.36 mV dec^{-1} for the NiO300H, NiO500H and NiO700H samples, respectively. The synthetic route proves to be economically viable and does not produce secondary products that are harmful to the environment, in addition to producing electrocatalysts with excellent performance compared to other materials.

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Pluronic to Cooling: a barocaloric investigation

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Solid-state refrigeration, based on caloric effects, has been considered as an economically viable and environmentally friendly alternative to replace conventional vapor compression refrigeration. Among caloric effects, the barocaloric effect (σ b -CE) in polymers, plastic crystals, and composites with a polymeric matrix has shown some of the necessary characteristics for the success of its application as solid-state refrigerants, including: giant (or even colossal) values of adiabatic temperature change (ΔT S) and isothermal entropy change (ΔS T) over a wide range of reference temperatures under low to moderate pressures, good reversibility, and good availability at low cost [1]. Regarding the σ b -CE, the excellent values of ΔT S and ΔS T manifested have been associated with the conformational entropy variation of the system. However, this theoretical association lacks experimental confirmation. Therefore, this project proposes the use of non-ionic triblock copolymers (Pluronics) to investigate the influence of molecular weight on the σ b -CE, respectively. The Pluronics (Sigma Aldrich) evaluated were F-68 (8400 g mol -1) and F-127 (12600 g mol -1), which were inserted into the pressure chamber in the necessary quantity to form a cylindricalbody with a diameter of 12 mm and a height of 22 mm. The results obtained show a maximum adiabatic temperature change of 15 and 17 K for Pluronics F127 and F68, respectively, due to a sol-gel transition. These impressive values of temperature changes qualify Pluronics as a promising material for barocaloric refrigeration.

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POLYDIMETHYLSILOXANE COMPOSITES (PDMS) WITH GRAPHENE OXIDE AS PHOTOVOLTAIC MODULES ENCAPSULANT

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Due to aging process or delamination of the ethylene vinyl acetate (EVA) layers that protect (encapsulate) the solar cells the performance and useful life of photovoltaic modules is compromised, reducing the efficiency of photovoltaic cells. Here, we propose to replace the EVA layers by a composite of polydimethylsiloxane (PDMS) with the incorporation of graphene oxide. PDMS (silicone) can be deposited directly on the surface of the solar cells by casting, presenting fast curing, transparence in the region of interest and chemical inert. PDMS (Sylgard® 184) in a 1:10 curing agent ratio (3 g: 0.3g) can be used to disperse the nanostructures throughout the polymer volume prior to the drying process. Different samples with quantities of graphene oxide were tested, 25, 50, 100 and 150 microliters by sample, cured at 100°C during 30 min. Comparing the current generated in solar simulator, before and after the deposition of composite films over the photovoltaic cell, the better composition of graphene oxide in the composite increase 2,68% (25 microliters). In the next step the degradation under UV radiation will be tested to prove the use as encapsulant of cells.

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Polymeric Synthesis and Characterization of the High Entropy Oxide (Mg,Co,Ni,Cu,Zn)O

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The rising demand for electronic devices and the shift towards clean energy systems have increased the need for advanced energy storage solutions. High entropy oxides are showing great promise for these applications, particularly as electrodes in lithium-ion batteries. Notably, (Mg,Co,Ni,Cu,Zn)O ceramics exhibit great potential due to their excellent electrochemical properties [1]. High entropy materials are a new class of materials composed of multiple principal elements in equimolar proportions, resulting in high configurational entropy [2]. This high configurational entropy may stabilize single crystalline phases that improve material performance. In this study, we synthed the high entropy oxide (Mg,Co,Ni,Cu,Zn)O using a polymeric route based on the Pechini method to evaluate its electrical properties. We use X-ray diffraction and scanning electron microscopy to investigate the ceramics (micro)structural characteristics, including phase composition, grain and morphology. Additionally, we employ impedance spectroscopy to examine their electrical behavior.

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Powder-Based New Route for Processing Bulk Ti-Supported $TiNb_2O_7$ Electrodes for PEM Cells

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The advancement of new technologies aimed at hydrogen production unfolds in the emergence of new demands, such as new ways of manufacturing electrodes for polymer electrolyte membrane (PEM) electrolyzers. The anodes of these devices may consist of nanoparticulate oxide catalysts deposited on a metallic titanium substrate [1]. However, the oxide/metal adhesion via wet routes may not be satisfactory [2], impacting the performance and durability and physical anchoring could represent a promising alternative. This study aimed to produce $Ti/TiNb_2O_7$ electrodes through uniaxial compaction/sintering and evaluate their morphological/structural characteristics. XRD patterns indicate that the phases present before sintering were preserved after the heat treatment, while SEM micrographs indicated successful sintering of Ti, good dispersion of nanoparticles on the Ti surface, and satisfactory physical anchoring, resulting in a robust and durable structure.

Preparation and electrochemical activation of Co-Ni-Mn catalyst for efficient oxygen evolution reaction

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Aside from the high energy consumption of the modern society, the burning of fossil fuels has led to an environmental crisis that demands sustainable and carbon-free energy sources. Green hydrogen production, especially via water electrolysis, is a promising technology for the energetic transition. First-row transition metal-based electrocatalysts are promising due to their cost-effectiveness and abundance. Many approaches are described to improve the OER activity and stability of the electrocatalysts, one that has recently gained great attention is the combination of different elements. Trimetallic oxides based on Mn-Co-Ni have emerged as promising electrocatalysts for OER and has shown superior efficiency over the bimetallic and monometallic analogs. Herein, films of Mn-Co-Ni oxides were prepared by electrodeposition, via chronoamperometry, and subsequently activated by electrochemical activation by cyclic voltammetry (CV). The Mn-Ni-Co films were characterized by X-ray diffraction, Raman spectroscopy, scanning and transmission electron microscopy, and atomic force microscopy. Electrochemical characterization involved CV and electrochemical impedance spectroscopy. The electrodeposited Mn-Ni-Co hybrid films exhibited lower overpotential compared to benchmark catalysts and all individual oxide films. The Mn-Ni-Co film shows low overpotential of 430 mV at 25 mA cm−2 and a Tafel slope 104 mV dec−1, respectively. The high activity of the trimetallic film was attributed to the lower electron transfer resistance, high electrochemical active surface area, high intrinsic activity, in comparison to the monometallic films. Furthermore, the film was stable up to 2 h at a density current of 100 mA cm-2 and provided a high Faradaic efficiency. In conclusion, the Mn-Ni-Co electrocatalysts prepared by electrodeposition and activated electrochemically are promising materials to promote the water splitting for green hydrogen production.

Preparation and electrochemical evaluation of eco-friendly eutectic electrolyte-water for application in aqueous lithium-ion batteries

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Aqueous lithium-ion batteries have attracted much attention in academia due to the fact that they are safer because they do not contain organic and volatile solvents [1]. However, their electrochemical stability window (ESW) is limited due to the presence of water in the electrolyte [2]. It is because of that a new type of aqueous electrolyte called aqueous eutectic electrolytes has emerged; these electrolytes have a wide ESW, greater than 3.0 V [3]. Here we report a series of eutectic-water electrolytes based on LiCl or $LiClO_4$, urea and two of its derivatives. They were prepared and characterized by near-infrared spectroscopy to observe the interaction of water clusters in the electrolyte. Linear scanning voltammetry showed the ESW of the eutectic-water electrolytes, showed a range higher than 3.0 V. The ionic conductivity of the series of eutectic-water electrolytes, using 0.1 M KCl solution as standard, was carried out by electrochemical impedance spectroscopy tests, they showed that most of the eutectic-water electrolytes had a conductivity >1 mS cm^{-1}. Therefore, the new formulated eutectic electrolytes can be used in aqueous lithium ion batteries, due to the high ESW and excellent ionic conductivity.

Key words: Eutectic electrolyte, urea, aqueous lithium-ion batteries.

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Preparation of a catalyst based on Niobium Metal-Organic Framework ([Nb(BDC)]n) and bimetallic Pt/Co composition for hydrogen evolution via sodium borohydride hydrolysis

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The excessive consumption of fossil fuels and the severe climate consequences caused by their use have made evident the need to seek more sustainable energy sources [1]. Among these options, the use of hydrogen fuel (H2) stands out as an alternative to overcome the use of fossil fuels, due to its high calorific value and its combustion that releases only water as a by-product [2]. One of the safest ways to store the H2 produced is in solid form in hydrides, such as sodium borohydride (NaBH4) which has high storage capacity of H2 (~10.8% m/m) [3]. However, the dehydrogenation process of NaBH4 is extremely slow and requires a catalyst to be more efficient. The purpose of this study was to develop a metal-organic network (MOF) based on Niobium (Nb) and 1,4-benzenedicarboxylic acid (BDC), named as [Nb(BDC)]n, to act as a catalyst in the production of H2 fuel from NaBH4. The MOF was synthed by the solvothermal method, using ethylene glycol at 200 °C for 12 hours. After synthesis, the MOF was characterized by FT-IR, TGA, SEM-EDS, and DRX indicating that material was successfully obtained. The catalytic activity of the produced material was tested from various metals and bimetallic compositions, varying temperatures, NaOH concentration and amount of NaBH4 injected. As a result, the most promising catalyst is composed of [Nb(BDC)]/Pt-Co (4:6) and possessed a H2 generation rate of 1473 mL.min-1.g-1 with efficiency greater than 75%. The activation energy of the system is 19.2 kJ mol-1. The catalyst can be reused and can generate up to 20 cycles without loss of efficiency, thus becoming a promising catalyst for hydrogen evolution.

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Production of conductive polyetherimide nanocomposites for 3D printing and fuel cell applications

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This study aimed to develop multifunctional nanocomposites of polyetherimide (PEI) matrix reinforced with graphene nanoplatelets (GNP), carbon black (NF), and single-walled (SWCNT) and multi-walled carbon nanotubes (MWCNT). The nanocomposites were processed in the form of conductive filaments for 3D printing to manufacture bipolar plates, which could be used in ethanol fuel cells. The nanocomposites were prepared in the molten state using a mini-conical twin-screw extruder. Five test specimens were obtained for each composition with percentages of 1% of (SWCNT) and (MWCNT), 10% (GNP), and 20% carbon black (NF). The test specimens obtained were characterized by four-point electrical testing. The study indicated an increase in the conductivity of the polymer matrix with the introduction of nanoparticles, from a value of 10-15 S/cm for the pure polymer to values of the order of 10-3 S/cm. References:

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Production of Nb-doped SrTiO3 films by radiofrequency right angle magnetron sputtering at room temperature

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Niobium-doped strontium titanate is an n-type semiconductor that features high thermal stability, high oxidation resistance, non-toxicity and low cost. This oxide material has shown excellent thermoelectric efficiency (zT) results in bulk structure at temperatures close to ambient [1]. In addition to these perovskites (ABO3), they have applications in photocatalysis and photovoltaic cells. However, the production of crystalline films of this thermoelectric oxide is rarely found in international literature. In this work, we synthe Nb-doped SrTiO3 thin films by right-angle magnetron sputtering (RAMS) for the first time. The RAMS system has been widely studied for production at room temperature thin films of complex crystalline structures such as hydroxyapatite, ion substituted hydroxyapatites [2] and cubic tungsten carbide phase (β-WC) [3]. Our results show a production of crystalline cubic SrTixNbyO3 prepared at room temperature. These results are confirmed by grazing incidence X-ray diffraction (GIXRD), X-ray Energy Dispersive Spectroscopy (EDS), X-ray photoelectron (XPS), RAMAN spectroscopy and atomic force microscopy (AFM).

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"Exploring the Optical Properties of NbyOx for Technological Innovation"

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Brazil stands out for having the largest niobium reserves on the planet, in addition to having advanced technology for its exploration and purification. Although niobium has a wide range of applications in various areas of science and technology, such as computer hard drives, integrated circuits, thin film transistors, polymerization and dehydration processes, capacitors and optical systems, it is crucial to highlight its uniqueness and consequently , its value for certain applications, making it indispensable and boosting its consumption. In this interaction between supply and demand, niobium can emerge as an important agent of technological sovereignty, through the development of national devices, or as a significant commodity for export on the international scene. With the aim of investigating new technological applications for niobium, this study aims to analyze the optical properties of NbyOx thin films produced by the RF magnetron sputtering technique, following a 23 type factorial experimental design. Films deposited using a multiphase niobium oxide target revealed a significant result, the band gap energy is significantly influenced by the selected deposition variables. This discovery offers a valuable opportunity to modulate the band gap energy and consequently the technological application of these films.

Rationally designed interfaces to mitigate the electron losses in the hematite photoanode

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The rationally designed nanostructured interfaces of photoelectrodes have become a key factor to enhancing their photoelectrochemical performance for water splitting, by reducing the charge recombination rate, thus ensuring efficient photogenerated charge separation and transport. In this work, thin hematite photoanodes were prepared from a simple and scalable methodology recently submitted for an innovation patent [1], capable of mitigate the charge loss and recombination at all interfaces (i.e. FTO/hematite/, hematite-hematite, and hematite/electrolyte). Combining the Al_2O_3 interfacial layer to improve the electron injection from hematite to the FTO substrate, with the benefits of Nb^{5+} segregation at grain interfaces, enhancing the film accommodation and electron transport, the overall efficiency of almost 50% for water oxidation reaction was achieved compared to pristine photoelectrodes [2]. Electrochemical impedance (EIS) and intensity-modulated photocurrent spectroscopies (IMPS) were applied to probe and monitor the photogenerated charge carrier dynamics in every step revealing substantial improvement in charge separation and collection at the back-contact interface as well as partial mitigation of the surface states at the hematite-electrolyte interface. New possibilities to produce efficient, versatile and scalable materials for green hydrogen area have been opened. **Acknowledgments:** CAPES, CNPq, FAPESP (grants: 13/07296-2, 17/02317-2, 17/11986-5, 21/07459-5), Shell and ANP. **References:** [1] Souza, F.L.; Bedin, BR 1020230053726, Invention Patent (pending), deposited by the Brazilian Center for Research in Energy and Materials (CNPEM), 2023. [2] Bedin, K.C.; Roriguez-Gutierrez, I.; Peregrino, L.R.P.; Vayssieres, L.; Souza, F.L.; J. American Ceramic Society, 2023, 106, 79-92

Reductive pyrolysis of the NMC532 cathode of discarded LIBs with and without the addition of the anode material

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Spent lithium-ion batteries (LIBs) contain several valuable metals such as Li, Co, Ni, Mn, and Al and are hazardous industrial residues. Carbon-based reductive pyrolysis has proven to be a prospective method for recycling and recovering compounds from spent LIBs.[1] Despite notable advances, the technique still lacks further study. In this study, the reductive pyrolysis of the cathode of a typical spent LIB (NMC532) was investigated at different reaction temperatures with and without the addition of carbon from the anode material. The results showed that the pyrolysis of the cathode material without the addition of anode material started to collapse the material structure at 550 °C, resulting in Li2CO3, (NiO)0.75(MnO)0.25, and Li0.185Co0.815O compounds. However, by adding 5% of the anode material to the cathode material, Li2CO3 is the only product containing lithium for pyrolysis at 700 and 800 °C. Other reaction products were MnO, Ni, and Co, resulting from the decomposition and reduction of the metals in the (NiO)0.75(MnO)0.25 and Li0.185Co0.815O. These results offer valuable insights into the industrial-scale recycling of spent LIBs.

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Scaling-up Planar Perovskite Solar Cells and Modules Fabrication by Roll-to-Roll (R2R) Slot-die Coating

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Perovskites (PVSK) are an attractive third-generation photovoltaic technology that has developed rapidly and received widespread attention in recent years. Its unique physical and chemical properties allow the processing of solutions using high-yield, low-cost production techniques. However, despite its unique characteristics, there are still key factors to overcome for its commercial application, such as reliability and large-scale production. A high-quality solution for large areas processed with PVSK and interlayers is one of the main challenges due to the polycrystalline nature of the PVSK film. Here we report the scale-up of planar PVSK devices, from small area cells (0.55 cm2 active area) to large area coated modules (21.6 and 26.8 cm2). All devices were prepared in ambient atmosphere on flexible PET-based substrates using a DMF-free solvent system. Perovskite solar cells (PSC) manufactured by Doctor-blade sheet-to-sheet (S2S) coating and slot-die roll-to-roll (R2R) coating had their performances evaluated. Perovskite solar modules (PSM) prepared by both coating techniques had their interconnection design investigated, varying the number of serially interconnected subcells from 6 to 12. External Quantum Efficiency, Optical Absorbance and 1-sol Photovoltaic Performance were measured. The devices were successfully scaled up from a S2S process to an R2R process and high-quality PVSK films and interlayers were obtained in both methods. PSC and PSM fabricated by both techniques showed very similar power conversion efficiency (PCE). PSM showed a clear benefit in its performance by increasing the number of subcells due to a better fill factor. This trend can be explained by the reduction of film defects and the shortening of the electron path to the electrodes. The best PSC manufactured with S2S Doctor-blade coating achieved 14% PCE, while the most efficient module was 13% in a reverse scan. The R2R champion slot-die coated PSC was 13% and the PSM was 10%.

Self-Structured Graphene Oxide as a Supercapacitor Electrode

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The demand for compact energy storage devices is growing rapidly, driven by the increasing popularity of electric vehicles, smartphones, and other portable electronics. Supercapacitors offer a promising solution due to their high power density and long cycle life [1]. However, further improvements in supercapacitor performance are required to meet the demands of these applications [2,3]. In this work, we present the synthesis and characterization of self-structured graphene oxide (aerographene) for use as supercapacitor electrodes. Aerographene was prepared via chemical reduction of graphene oxide using ascorbic acid as a mild reducing agent, followed by hydrothermal treatment for 3 hours. The effects of temperature, reaction time, and reducing agent concentration on the synthesis were investigated. The resulting structure was stabilized by lyophilization for 24 hours. After synthesis, the aerographene was divided into two groups: with and without thermal treatment at 200°C. The morphology of the samples was characterized by scanning electron microscopy (SEM), and their electrochemical performance was evaluated by cyclic voltammetry using a three-electrode cell in 1M sulfuric acid. The results showed a specific capacitance of 260 F/g for untreated samples and 445 F/g for thermally treated samples.

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Silicate glass with recycled content and reduced melting point

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This study aims to address an innovative approach for producing silicate glass with recycled content from decommissioned photovoltaic cell cover glass, incorporating CaF_2 and Na_2CO_3 to lower the melting point. By using pieces of recycled glass along with CaF_2 and Na_2CO_3, we reduced the glass melting point to 1200 °C. These reagents are used based on previous studies where the melting point was reduced, but only in virgin material[1]. We empha that CaF_2 and Na_2CO_3 are readily available and easy-to-use reagents, making this process an economical and practical choice for the glass industry. Additionally, using recycled glass from solar panels addresses a growing waste issue, offering a sustainable solution. Lowering the melting point not only simplifies the production process but also has the potential to significantly reduce CO_2 emissions associated with glass production, thereby contributing to mitigating the environmental impact of the glass industry[2].

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Single atoms synthesis over g-C3N4 via Magnetron Sputtering Deposition for photocatalytic hydrogen production

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In recent years, the enhancement of photocatalytic performance with single atoms (SAs) has gained attention, particularly with graphitic carbon nitride (g-C3N4) [1] and modified poly-heptazine imides structures (PHI) [2], as a promising photocatalyst support for water splitting due to its suitable light absorption and electronic properties. However, the synthesis methods available for obtaining single atoms are limited due to the stability required to maintain a highly dispersed state over the support material, which is less than a nanometer in scale, and the techniques of characterization required to confirm the sole existence of single atoms. In this work, it was successfully synthed single atoms of Cu and Pt over g-C3N4 structure to assess their photocatalytic performance for hydrogen production under visible light. The support graphitic carbon-based material was prepared by pyrolysis using urea as precursor. Pt and Cu atoms are stabilized in the nitrogen-interstices of a graphitic carbon nitride (g-C3N4) framework using scalable, solvent-free, one-pot magnetron sputtering deposition. The photocatalytic activity of the Cu and Pt-loaded g-C3N4 was boosted to 93 and 173 µmol as compared to the pristine g-C3N4 (0.3 µmol). XAS characterization was done to elucidate the electronic structure, bonding environment, and oxidation state of the single atoms and. Scanning Transmission Electron Microscopy (HAADF-STEM) was also useful for the analysis of SAs. Our findings contribute to the field of hydrogen photocatalytic production and demonstrate how highly dispersed single atoms anchored to a suitable catalyst enhance its performance.

Sodium ion microbatteries

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In the field of energy storage, conventional batteries, such as lithium-ion ones, raise sustainability concerns due to resource depletion and environmental damage both during extraction and disposal. Alternative technologies, like sodium-ion batteries, offer an economical and environmentally friendly solution. Sodium-ion batteries exhibit performance comparable to lithium-ion batteries, with their components made from abundant elements like sodium, iron, and carbon, making them much cheaper and eco-friendlier. Sodium iron oxide electrodes are potential candidates for use in rechargeable sodium-ion batteries, and in this study, the electrochemical properties of charge capacity for thin films of NaFeO2 deposited by RF magnetron sputtering were investigated using a factorial experimental design. The results showed that the charge capacity depends on the deposition conditions, and the maximum capacity is higher than that obtained for the same electrode in bulk form. Thin films of NaFeO2 have potential applications as electrodes in rechargeable sodium-ion batteries, contributing to the sustainability of energy storage technology.

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[1] Electrochemical and Thermal Properties of α-NaFeO2 Cathode for Na-Ion Batteries. Jie Zhao, Liwei Zhao, Nikolay Dimov, Shigeto Okada and Tetsuaki Nishida

[2] New Insights into the Performance Degradation of Fe-Based Layered Oxides in Sodium-Ion Batteries: Instability of Fe3+/Fe4+ Redox in α-NaFeO2. Eungje Lee, Dennis E. Brown, Esen E. Alp, Yang Ren, Jun Lu, Jung-Je Woo, and Christopher S. Johnson

Sol-Gel Synthesis of α$NaFeO_2$: Performance in Sodium Battery

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In recent decades, the increasing production of electronics has driven the demand for energy storage technologies, with batteries being a key focus. Currently, lithium-ion batteries are widely used due to their high energy density and long lifespan. However, they face challenges such as element scarcity, flammable electrolytes, and high extraction and production costs. In light of this growing demand, the search for alternatives, such as sodium-ion batteries, becomes imperative [1]. These batteries have properties analogous to lithium-ion batteries and their elements are abundant in the Earth's crust, with lower extraction costs. An alternative approach proposes the use of sodium iron oxide electrodes (α-NaFeO2), synthed via the sol-gel route, known for their economic accessibility and environmentally friendly. The study aimed to characterize these electrodes and evaluate their electrochemical charge capacity, with the goal of replacing lithium-ion batteries. Results indicated a capacity of approximately 50 mAh/g, signaling promising potential for future sodium-ion battery applications. These findings suggest positive prospects, with future research aimed at optimizing their ecological efficiency. The transition to sodium-ion batteries may represent an economically viable and environmentally friendly alternative for energy storage technologies.

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Spinodal decomposition-mediated β-BCC Li nucleation within Li-Mg anodes for lithium metal batteries

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Mg-based interlayers or anodes promote homogeneous Li plating, and represent a possible cost-effective option for improving the cyclability of lithium metal batteries [1-2]. However, in addition to Li plating, simultaneous Li alloying in Mg-Li alloys can cause microstructural transformations during battery operation. Here, we use atom probe tomography in galvanostatically lithiated Li-Mg alloys to unveil a metastability cascade leading to the formation of compositional fluctuations in the range 30–80 at.% Li during the lithiation of Mg-25.7 at.% Li anodes. Such fluctuations appear to be consistent with a spinodal decomposition in the β-BCC phase, despite the absence of a reported miscibility gap in this system. These Li-rich regions reduce the energy barrier for Li plating within the bulk anode. Such reaction sequence is accelerated at grain boundaries due to equilibrium Li segregation to these interfaces. Our study reveals a new Li plating mechanism that could be used to optimize spinodal decomposition-forming anodes and interlayers based on microstructure engineering.

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Structural and Electrical Properties of Water in Salt Electrolytes Confined in MXenes and Graphite by Molecular Dynamics

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Aqueous electrolytes are an efficient, safe, and environmentally friendly alternative solution to replace organic solvents electrolytes in energy storage devices but have a narrow electrochemical potential window (< 1.2 V) limited by water splitting reactions. However, increasing the concentrating of salt in an aqueous electrolyte expands the potential window [1]. In this way, supersaturated aqueous electrolytes (Water-in-Salt Electrolyte-WiSE) are considered good candidates for supercapacitor electrolytes and can be combined with different types of electrodes, for example, two-dimensional (2D) transition metal carbides, known as MXenes, which have excellent performance in terms of capacitance, when used as electrodes [2]. Here we present a detailed computational study of WiSEs in $Ti_3C_2F_2$ and graphite, employing molecular dynamics simulations with an extension of the constant potential model (CPM_X) [3] and using some unsupervised learning techniques for data analysis (clustering and kernel density estimation). The data analysis showed that independently of the WiSE and electrode, cations carry their hydrated spheres when they are either attracted to the negative electrode or repelled from the positive one and the behavior of water molecules inside the closest layers to the electrodes seems to be more sensible to the chemical nature of the electrode. The capacitances on negative electrodes are always higher than on positive ones, independently of the chemical nature of the electrodes, also the differential capacitances are smaller in cells containing MXenes, which is related to higher values of the potential drop in these cells.

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Study of magnetite hybrids with ionic liquid and their effect on electromagnetic properties

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The magnetite has been used in various applications due to its magnetic properties. In electromagnetic shielding, magnetite can play an important role due to its ability to absorb magnetic and electric fields. Carbon nanotubes have excellent properties, including high aspect ratio, electronic/electrical properties and high mechanical resistance [1]. CB has also been used to manufacture conductive composites, acting as filler and conductor [2]. Therefore, the use of hybrid materials with the aim of enhancing the material's electromagnetic properties has been investigated. Furthermore, to promote synergism between these materials, ionic liquids have been used to improve the dispersion and electrical/dielectric properties of the materials [3]. The objective of the work was to study magnetite hybrids containing carbon nanotubes and carbon black with ionic liquid for electromagnetic shielding. Characterizations containing mono- and multi-layer materials were carried out in order to evaluate the electromagnetic wave attenuation capacity and verify the influence of the composition and thickness of the material under study. The presence of ionic liquids in hybrid materials resulted in a decrease in the percentage of reflection for monolayer materials.

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Study of polymeric solid electrolytes based on semi-interpenetrating polymer networks with polystyrenes

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Improve the performance of fuel cells and electrolyzers; devices with polymeric solid electrolytes (ionic conductive membranes) have driven the development of new polymeric materials with ionic conduction, chemical, and electrochemical stabilities suitable for applications and with reduced make cost. This work aimed to compare different semi-interpenetrating polymer networks, SIPN, obtained with commercial linear polymers to control the SIPN's hydrophilicity necessary for use in direct ethanol fuel cells. Poly(styrene-co-anhydride maleic acid) (PSCAM), polystyrene-co-allyl-alcohol (PSAA), and polystyrene-co-acrylo-nitrile (PSCAN) were used as a linear polymer in the SIPN, which network was formed with diglycidyl ether of bisphenol A, DGEBA, using 4,4′-Diaminodiphenyl sulfone, DDS, as a crosslinking agent. It employed a molar ratio DGEBA/DDS 1:1, linear polymers from 30 to 50% m/m, and casting obtained membranes. The samples were characterized by FTIR, SEM, and electrochemical impedance spectroscopy (EIS). The EIS study (1mHz to 1 MHz) used membranes doped with H_3PO_4 from 20 to 90 °C temperatures. Membranes, SIPNPSCAM, and SIPNPSAA formed films with dimensional stability and slight roughness and were homogeneous second SEM images, and the SIPNPSCAN formed gel. FTIR confirmed the disappearance of the bands typical of the anhydride group at 957 and epoxy ring of DGEBA at 913 cm-1. The ionic conductivities (σ) of the SIPNPSSA and SIPNPSCAM samples reached (80 °C) values of 10^{-5} and 10^{-8} $\Omega^{-1}.cm^{-1}$, respectively, with the desired value being 10^{-1}-10^{-3} $\Omega^{-1}.cm^{-1}$. The SIPN membranes did not present the hydrophobic/hydrophilic phase segregation necessary in the nanostructure for high conductivity achievement, although the ethanol absorption has been controlled compared to other membranes previously obtained [1].

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STUDY OF THE STRUCTURAL STABILITY OF MAPI ON THE MAPI/P3HT INTERFACE DEPOSITED BY SPIN-COATING

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Poly(3-hexylthiophene) (P3HT) is commonly employed as a hole transport layer (HTL) in photovoltaic devices due to its high hole mobility and stability. Its absorption range aligns well with methylammonium lead iodide perovskite (MAPI), significantly enhancing the absorption spectrum without compromising light capture. However, the degradation of MAPI due to ambient humidity poses a concern for solar cell durability. Deposition of P3HT onto perovskite aims primarily to shield MAPI from moisture. X-ray diffraction (XRD) studies have shown that P3HT stabilizes and delays perovskite degradation. Furthermore, spectroscopic analyses did not reveal significant changes in the energy of photoluminescence (PL) spectra. The optical absorption spectrum confirmed the formation of the perovskite phase, evidenced by absorption at 760 nm, attributed to the transition between the valence band (VB) and the conduction band (CB) of perovskite. Interaction between organic and inorganic materials affects lattice properties, influencing the resulting material's band gap.

Sugar Cane Waste: A Renewable Resource for Energy Production and Storage

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The use of waste to create new materials is becoming a crucial tool to promote industrial sustainability and contribute to the production chain of processes that generate this waste. This significantly contributes to the circular economy, transforming waste from the production process into valuable resources. Sugarcane bagasse, in particular, has attracted interest due to its various applications, serving as a raw material for the production of materials that offer sustainable solutions for managing agro-industrial waste, reducing greenhouse gas emissions. Furthermore, when subjected to thermochemical treatments, there is the possibility of its use in the manufacture of electrodes for energy storage and in sensor production, thanks to its high carbon content and porosity. In this sense, the present study aims to characterize the residue from unburned sugarcane bagasse in the steam generation process, evaluating its energy and technological potential. The analysis of the High Heat Value allowed quantifying the energy potential of the residue, while techniques such as Scanning Electron Microscopy (SEM), Fourier Transform Infrared Spectroscopy (FTIR), X-ray Photoelectron Spectroscopy (XPS) were employed to characterize its structural and chemical composition. The results revealed the energy and technological potential of the material, highlighting its lower calorific value of around 24 MJ/kg and its composition, with approximately 70% carbon and 20% oxygen by mass. These characteristics enable the use of the residue as a precursor in routes for obtaining carbon-based materials, as well as its investigation as a base for energy storage materials.

Survey of piezomagnetic properties of Fe-35%Co alloys (% by mass) with addition of 0.5 and 0.7% of Nb

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The growing interest in smart devices demands further exploration of the potential of the piezomagnetism for application in force sensors, which are currently made with Fe alloys containing rare earth elements, Ga, and AlB. However, the narrow range of stress for which the rare earth and Ga options are applicable [1], as well as the high cost of the first, and the lower sensitivity of FeAlB alloys [2] open a gap in which magnetically soft FeCo alloys can fill up due to their high saturation induction and permeability. In this study, the potential of Fe-Co alloys with 35% Co is analyzed to mitigate costs and to improve the permeability of the binary alloy, by the additions of 0.5% and 0.7% of Nb in mass. Likewise, Nb can also reduce the brittleness of these alloys [3]. For both compositions, the microstructure and the magnetic, mechanical, and magnetomechanical behaviors were characterized. The latter was accessed by measuring the curves of magnetic induction as a function of the applied stress in the range from -100 MPa up to 100 MPa. Our findings revealed that the addition of 0.5% Nb provided higher sensitivities in the order of 10 mT/MPa for compressive stress measurements, while of 0.7% provided a wider margin for applicability. Therefore, both compositions demonstrate utility for larger compressive stress ranges than alloys with rare earths and Ga, while also outperforming FeAlB alloys in sensitivity.
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Synthesis and Characterization of Donor Polymers for Organic Photovoltaics (OPV)

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Organic photovoltaics (OPV) have been the subject of great interest in the last years because of its rapid development and advantages such as flexibility, lightness and semitransparency, in addition to a potencial low cost production via solution-process techniques. The recent materials developments in active layer (AL), interfacial layers and device architecture resulted in certified record efficiency values of 19.2% for cells and 14.5 % for modules (NREL, 2024). Nevertheless, these numbers come from research samples, fabricated on small s and under controlled conditions, hard to reproduce in a large-scale production line.

This study aimed at synthetizing conjugated polymers to be used as p-type material in the AL of OPV. A series of commercially known polymers and new molecular structures were fabricated, following the criteria for a large-scale production: solubility in green solvents, high yield, high molecular mass, low dispersity and high thermal stability. The synthed materials were alternated copolymers with Donor-Acceptor (D-A) monomeric units, based on thiophene, benzodithiophene and thienothiophene (donors) and benzothiadiazole, benzodithienedione, quinoxaline, pyrrolodione and carboxylated thienothiophene (acceptors). 33 conjugated polymers were synthed, purified and characterized.

PV cells with the best polymers synthed were produced following the PET/IMI/ZnO/Donor:Acceptor/HTL/Ag structure. All layers were deposited the blade coating method, except for the silver top electrode, which was evaporated. Good results were obtained reproducing the commercial polymers D18, PM6 and PTQ-10 and novel polymers also showed promising results, requiring continued research for further optimization.

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Synthesis and characterization of FeSe semiconductor nanoparticles in organometallic colloidal solution

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We studied the results of the synthesis to obtain semiconductor nanoparticles of FeSe using organometallic compounds and the hot-injection technique. Initially, we diluted 30mg of metallic selenium in 5mL of octadecene. To this solution, 0.4 mL of Trioctylphosphine (TOP) was added, and it was subjected to heating until the formation of the trioctylphosphine selenide complex (TOPSe). In the second stage, in a three-neck reactor, 12,8mg of $FeCl_3.6H_2O$ was dissolved in oleic acid and octadecene. Then, a solution containing 2.29g of chlorodihydrate hydrazine in 2mL of ultra-pure water was added. Finally, the reactor was heated to a temperature of 200°C, and at this temperature, 1mL of the TOPSe solution was injected. The rapid color change, from light yellow to brown, is indicative of the formation of FeSe semiconductor nanoparticles. The nanoparticles were characterized by Raman spectroscopy, this indicates the formation of peaks related to the Se e Fe, between 180 cm^{-1} and 215 cm^{-1}, also an intense peak around 230 cm^{-1} related with amorphous selenium; optical absorption measurements in the Uv-Vis region were made between 190 nm – 550 nm, a peak absorption band close to 360 nm is observed indicating an energy of 3.44 eV; when excited by a 405 nm laser, the photoluminescence measurement indicates an elongated band with a peak of 500 nm of 2.48 eV energy; The of the nanocrystal is estimated from optical absorption measurements and corresponds to around 10 nm, According to scanning electron microscopy analyses, the nanoparticles are polycrystalline with spherical shapes and highly agglomerated, possibly there are 3 crystalline phases, type FeSe, $FeSe_2$ and amorphous as in Raman measurements. The correlation of these measurements with the FeSe synthesis method is studied.

Synthesis and characterization of $LaNiO_3$ catalytic precursors for H_2 production from dry methane reforming: a design of experiments

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Hydrogen (H_2) is a potential fuel due to its clean burning capacity, as it does not produce direct emissions of pollutants or greenhouse gases. Among the processes for H_2 production, dry reforming of methane (DRM) stands out for using two gases responsible for the greenhouse effect (CH_4 and CO_2) to produce synthesis gas (H_2 and CO). $LaNiO_3$ perovskites have been used as a catalytic precursor due to their ability to exsolve Ni particles to the surface after activation, resulting in a catalyst with strong interaction between the active phase (Ni) and support (La_2O_3) [1]. Therefore, this work aimed to synthesize $LaNiO_3$ perovskites and apply them in DRM using a design of experiments (DOE). The parameters were defined through a 2^n complete factorial DOE, with n = 4 being the independent variables (synthesis temperature, time and pH, and DRM temperature). The lower levels of the variables were 160 °C (synthesis temperature), 6 h (time), 9 (pH), and 600 °C (DRM temperature). The upper levels of the variables were 200 °C (synthesis temperature), 24 h (time), 13 (pH), and 800 °C (DRM temperature). Finally, the central points were 180 °C (synthesis temperature), 15 h (time), 11 (pH), and 700 °C (DRM temperature). The XRD patterns showed that the samples synthesized at pH 9 and 11 presented the phases $LaNiO_3$, La_2NiO_4, NiO, La_2O_3, and $La(OH)_3$. While the samples synthesized at pH 13 presented only the $LaNiO_3$ and NiO phases. The SEM micrographs showed that all samples presented rod-shaped morphology. Regarding the DRM catalytic tests, the catalysts tested at 600, 700, and 800 °C temperatures showed a maximum H_2 yield of 38.86%, 58.53%, and 82.56%, respectively. Finally, the TGA analysis results of catalysts after DRM showed that the maximum percentage of carbon deposition at 600, 700, and 800 °C temperatures were 88.27%, 68.86%, and 87.75%, respectively.

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Synthesis and Characterization of Phosphate Glasses with Alkaline and Alkaline-Earth Ions

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Vitreous materials with good Li ionic conduction are potential candidates to replace liquid electrolytes on lithium batteries [1]. One of the most severe limitations to the ionic conductivity is the mixed-ion effect, which depends on structural properties of glass networks with two modifier species. To improve the understanding of the structure of these materials, two series of mixed glasses of Li as mono (Na^{+1}) and divalent (Ca^{+2}) cations , Li-Na and Li-Ca, respectively, were analyzed: $(1-x-y)Li_2O$ - xR - yP_2O_5, with R = CaO or R= Na_2O with $0{,}4 \leq y \leq 0{,}5$ (molar fraction), $0 \leq x \leq 0{,}6$ and substitution fractions $0 \leq [Li]/[Li+Ca] \leq 1$ and $0 \leq [Li]/[Li+Na] \leq 1$. Molar volumes and glass transition temperatures were studied as function of the alkaline and alkaline-earth cation ratio and the P_2O_5 concentration. High resolution ^{31}P Nuclear Magnetic Resonance (NMR) techniques were applied in order to analyze the short and medium range structures around the phosphate groups [2]. As a function of Ca and Na, the evolution of the average isotropic chemical shift, T_g and density were explained by the effect of the stronger ionic potential of Ca and weaker ionic potential of Na when compared to Li. Also, it was verified that bigger P_2O_5 concentrations produce less compact (packing fraction is reduced) and more rigid (increase of T_g) vitreous matrices. Finally, the ^{31}P-INADEQUATE [3] experiments to analyze the medium range order of the Li, Li-Ca and Li-Na series showed the existing connections between Q^n phosphate species for different compositions, revealing that the number of connection Q^2-Q^2 decreased and Q^1-Q^1 increased as the ionic potential of the modifier increased. The result also showed that the addition of another ion to the chain, in this case Li, made the amount of dimers decrease, this being the first experimental evidence of different organization in the medium range scale of mixed phosphate glasses.

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Synthesis and Characterization of the high entropy oxide (Mg,Co,Ni,Zn,Cu,Li)O

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High entropy oxides are part of a new class of materials known as high entropy materials, in which a solid solution not predicted by the phase diagram of the constituent elements can be obtained. A high entropy oxide was first synthed in 2015 [1]. As research on these materials progresses, intriguing electrical properties such as giant dielectric constant [2] and high ionic conductivity [3] have been reported for the (Mg,Co,Ni,Zn,Cu,Li)O system; however, the underlying mechanisms are still under debate. Therefore, there is a need to investigate the physical mechanisms that give rise to these electrical properties. In this study, we explored the synthesis of the high entropy oxide (Mg,Co,Ni,Zn,Cu,Li)O via a polymeric route to assess its electrical properties. The (micro)structural characteristics of the ceramics are evaluated using X-ray diffraction and scanning electron microscopy, while impedance spectroscopy is used to investigate their electrical properties.

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Synthesis and Scaling-Up of ZIF-8 Nanoparticles: Process Optimization and Parameter Influence

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The objective of this work was to develop an effective method for synthesising ZIF-8 nanoparticles, with a focus on scaling up to increase the mass yield of the particles. The process began with the production of a solution totalling 400 mL, and then scaling up was carried out by modifying the synthesis parameters (centrifugation time, speed, and temperature during drying) and doubling the volume of the solution to obtain more particles. Following synthesis, the particles were characterised using two main techniques: XRD and SEM. SEM allowed direct observation of particle formation, while XRD provided information on the crystallinity of the samples. It was observed that washing the samples resulted in an improvement in crystallinity. Despite variations in the experimental parameters, no significant influence on the final synthesis yield was observed. The yield was calculated through mass balance, and comparing synthesis with and without washing showed a decrease in yield from 51% to 31%. This decrease was attributed to impurity removal, confirmed by XRD between samples with and without washing, highlighting the increased crystallinity of ZIF-8. Regarding the scaling-up process, the importance of the solution mixing order was emphasised. Two distinct solutions were prepared and mechanically mixed: one composed of zinc nitrate and methanol, and the other containing methylimidazole and methanol. With the production of 400 mL, the zinc nitrate solution was added to the methylimidazole solution; for 800 mL, this order was reversed as proposed by Cravillon [1] for obtaining ZIF-8 particles. This study not only achieved successful synthesis of the desired nanoparticles but also provided valuable perceptions into the scaling-up process and the influence of the solution mixing order on the synthesis of these materials.

Acknowledgments:
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SYNTHESIS AND STUDY OF PARAMETERS FOR OBTAINING PM6 NANOFIBERS BY COAXIAL ELECTROSPINNING

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The objective of this work was to study the parameters for obtaining PM6 nanofibers as the nucleus of the core-shell structure synthed by Stille coupling. In this structure, the shell layer was PMMA. These structures will be used as the active layer of a BHJ-type solar cell. The synthed PM6 polymer was characterized by NMR, GPC, UV-vis, VC and TGA. The first parameter studied was the concentration of the solution used as the shell layer (PMMA in acetone), and concentrations of 5% and 10% by weight in relation to the solvent was tested. However, the electrospinning parameters studied were the distance between the needle and collector, the application of the electric field and the pump flow rate for the core and shell layers. The distance value was varied between 12.5 cm and 15 cm. The applied electric field values were 17 KV and 20 KV. The pump flow rate was changed to values of 0.5 ml/h and 1.0 ml/h for the shell layer, while for the core layer, the pump flow was 0.10 ml/h and 0.25 ml/h. The morphology of the core-shell structure was analyzed using SEM with EDS, TEM, and fluorescence microscopy. To remove the shell layer, the PMMA was washed in acetone. Furthermore, XRD, Raman and FTIR analyses of the nanofibers were carried out to verify the complete absence of the shell layer.

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Synthesis, characterization and photocatalytic application of bismuth vanadate in the photodegradation of norfloxacin

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Norfloxacin (NOR) is an antibiotic belonging to the group of fluoroquinolones, commonly used to combat bacterial infections. Studies have highlighted the presence of this medicine in bodies of water, raising concerns due to its resistance to conventional treatment methods. In this work, the efficiency of bismuth vanadate ($BiVO_4$) as a photocatalyst in the degradation of NOR under UV-visible irradiation was investigated. $BiVO_4$ was produced by hydrothermal synthesis [1]. Photolysis and photocatalysis tests were carried out with NOR solution (20 ppm), analyzing the influence of the photocatalyst concentration (500 and 1000 ppm). NOR degradation was evaluated through the formation of short-chain organic acids, identified by ion chromatography, UV-Vis absorption and pH. The synthesis of $BiVO_4$ resulted in the monoclinic scheelite phase material with a band gap of 2.35 eV, confirmed by diffuse reflectance analyzes and a high degree of crystallinity, evidenced by XRD analyses, compared with the crystallographic chart (JCPDS no. 14-0688) [2]. FTIR results showed the characteristic vibrations of the bonds between Bi, V and O, highlighting the purity of the material. For the photocatalysis tests, $BiVO_4$ concentrations of 500 and 1000 ppm resulted in a degradation rate of 61.0% and 54.9%, respectively. Ion chromatography studies allowed the identification of organic acids such as acetate and formate, confirming the degradation of NOR through the formation of short-chain organic acids. Thus, the results obtained indicate that $BiVO_4$ presents good performance in removing NOR when irradiated by UV-visible light.

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Synthesis of $BiVO_4/Bi_2S_3$ Heterostructures for Photocatalysis

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With an environmental crisis caused by the use of fossil fuels, the development of viable energy alternatives is a crucial strategy, and photocatalysis for energy production stands out as a promising clean process. In this context, bismuth vanadate ($BiVO_4$) has emerged as a suitable candidate for this application because of its band gap energy, non-toxicity and chemical stability [1, 2]. In particular, regarding Bi_2S_3, its heterostructure are reported as relatively easy to synthe and with increased photocatalytic performance [1]. The present work aims to synthe $BiVO_4/Bi_2S_3$ heterostructures via a hydrothermal route for photocatalytic applications and to characterize those. The obtained pristine $BiVO_4$ has a monoclinic structure, as observed by XRD, which is known for having a greater photocatalytic activity [3]. Furthermore, it has an excellent bandgap of 2.55 eV as observed by UV-Vis spectroscopy. The $BiVO_4$ and Bi_2S_3 (orthorhombic structure) phases in the heterostructure were confirmed by XRD, along with a bismuth oxide phase, and its bandgap was estimated to be 2.45 eV. Alternatively, the heterostructure will be synthed via magnetron sputtering deposition of metallic bismuth followed by sulfurization. Structural modifications will be investigated through XRD, XPS and UV-Vis analysis, and samples will be tested for O_2 evolution.

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Synthesis of nanocatalyst from battery waste for enhanced hydrogen evolution from borohydride

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Hydrogen is a highly dense energy source and an interesting strategic energy reserve. Its evolution and storage from sodium borohydride (NaBH4) offer considerable advantages, such as chemical stability and non-flammability at room temperature [1]. However, the hydrogen evolution reaction from NaBH4 is known for its slow kinetics. To overcome this challenge, metals such as Pt, Co, and Ni are commonly employed as catalysts to accelerate the reaction hydrolysis of NaBH4. Therefore, this study aimed to synthe a new nanocatalyst from battery waste and evaluate its effectiveness in producing hydrogen via hydrolysis of NaBH4. Graphene oxide (GO) was obtained from graphite rods of spent Zn-C batteries and then used to support Co and Ni bimetallic nanoparticles (Co/Ni NPs), with Co and Ni obtained from spent ion-Li batteries. The developed nanocatalyst was subjected to detailed characterization using specific techniques, FTIR, SEM, BET, and DLS. The GO-Co/Ni NPs have an average particle of 125 nm, a leaf-like morphology, a surface area of 1.37 m^2/g, and pores measuring around 30 nm. The catalytic material was evaluated for hydrogen evolution, presenting a hydrogen generation rate (HGR) of 1447.8 mL min-1 g-1 and activation energy of 17.32 kJ mol-1. The nanocatalyst maintained its effectiveness over eight hydrogen production cycles. This new material, derived from electronic waste, presents promising performance in the evolution of hydrogen through the hydrolysis of NaBH4, standing out as a sustainable and efficient approach to energy generation.

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Synthesis of V_2O_5/Nb_2O_5 heterostructures applied in the photodegradation of organic compounds and in the photoreduction of CO_2

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Water pollution and excessive CO_2 release into the atmosphere pose significant environmental threats, prompting the exploration of various methodologies to address these issues. Heterogeneous photocatalysis emerges as a promising solution, enabling the degradation of organic compounds in water and the reduction of CO_2 into valuable materials [1]. However, these processes' rapid recombination of photo-generated charges is a challenge. Heterostructure formation addresses this challenge by physically separating these charges, prolonging their lifespan, and accelerating reactions. This study focused on synthesizing V_2O_5/Nb_2O_5 heterostructures through an oxidative peroxide method followed by hydrothermal treatment. Both oxides can be obtained individually through this method [2,3]. Characterization techniques included XRD, FTIR, Raman spectroscopy, DRS, and SEM-EDS, with surface analysis conducted via the BET mathematical model. Photocatalytic properties were assessed through UV tests using rhodamine B dye and amiloride pharmaceutical compound, revealing superior performance of the heterostructure compared to isolated Nb_2O_5. Additionally, CO_2 photoreduction experiments demonstrated that the heterostructure produced 21% more CO and 309% more CH_4 than Nb_2O_5, generating 18% less H_2. This result indicates a preference for CO and hydrocarbon formation over H_2, suggesting enhanced selectivity towards CO_2 photoreduction over water hydrolysis. Overall, the employed methodology proved effective in synthesizing heterostructures between these oxides, thereby improving the photocatalytic properties for organic compound degradation and CO_2 photoreduction.

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Tailoring properties of platinum catalysts supported on reduced graphene oxide for ammonia electro-oxidation

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Ammonia electro-oxidation reaction (AOR) is essential for developing new strategies to replace fossil-based energy sources with renewable technologies for producing green hydrogen and clean energy. Designing and developing new materials and understanding reaction mechanisms are crucial to achieving this goal. This work aims to synthe platinum-based catalysts supported on graphene oxide (GO)-based materials with selectively controlled properties for AOR. The metallic phases were incorporated on the supports of GO using the solid-state method of synthesis called "shake and bake," which eliminates solvent and residue generation. Samples were synthed in different temperatures (220, 250, and 300°C) and characterized by XRD, TG/DTA, DSC, FTIR-ATR, Raman spectroscopy, XPS, and SEM. The general electrochemical characterization of the materials was evaluated using cyclic voltammetry (CV), chronoamperometry (CA), and rotating disc electrode (RDE) in acidic and alkaline media. Spectroscopic and thermal analysis data revealed that GO supports were simultaneously reduced with the platinum precursor to form a Pt/rGO hybrid material in a one-step synthesis. Particle and crystallite s ranged from 16.3 to 4.1 nm and systematically decreased with increasing baking temperature, which allows for systematic control of essential properties. The measured AOR catalytic activity in alkaline media depended on the different catalyst parameters. The study allowed a better understanding of the relationships between material properties, catalytic activity, and reaction mechanisms and contributed to improving the technology for critical electroconverting processes involving a future ammonia-based energy matrix.

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The evaluation of the impact of the CuS counter electrode synthesis conditions on the efficacy and stability of the CIS quantum dot sensitized solar cell.

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The collapse of the energy production system, an environmental crisis and developing sustainable means of production are some of humanity's concerns. To solve this problem, the Quantum Dot Sensitized Solar Cells (QDSSDs) is a good choice because it uses renewable energy, doesn't produce harmful gases, is cheap to make, and has a theoretical efficiency of about 44%[1]. However, although the development of this technology has brought efficiency close to 20%, low stability is still a problem[1,2]. One way to reduce energy losses and increase the useful life of the QDSSCs is to reduce the charge transfer resistance at the counter electrode (CE)/electrolyte interface and improve its mechanical and chemical stability[2]. We studied how the temperature and reagents concentration affects the deposition of CuS on fluorine doped tin oxide substrates. This had an impact on the power efficiency and stability of CdS QDSSCs. Based on the results obtained, it is concluded that CE CuS produced at 80 °C using a concentration of 0.2 $\mathrm{molL^{-1}}$ showed better performance and stability in QDSSC due to the morphology. This increased the number of active sites and due to the adhesion of the CuS.Furthermore, it was observed that CuS particles were released into the electrolyte and could contaminate or passivate the photoanode, depending on the amount that was adsorbed on the surface.Using the Impedance Spectroscopy technique, it was feasible to monitor the charge transfer processes throughout the day, thereby enabling the determination of the moment at which the CE degraded.

Acknowledgments

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The relation between the power factor and doping level of PEDOT:PSS

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Thermoelectric materials present a promising ability to convert heat into electrical energy through the Seebeck effect, making them applicable in generators and sensors. Moreover, conductive polymers applied in thermoelectric power generation present significant advantages such as low-cost production, non-toxicity, and good flexibility, opening possibilities for their use in wearable devices [1]. Among these polymers, PEDOT:PSS, a p-type material, stands out as the most studied in thermoelectric applications, exhibiting interesting values of Figure of Merit [1]. Typically, secondary doping is applied in commercial PEDOT:PSS inks to enhance the thermoelectric properties, electrical conductivity, and Seebeck coefficient. In this context, we investigated the influence of the doping level on the power factor of PEDOT:PSS. PEDOT:PSS inks were synthed through oxidative polymerization, varying the ratio of the oxidizing agent Na2S2O8 and the monomer EDOT, resulting in PEDOT:PSS inks with adjustable doping levels. The doping level were verified via the presence of polaronic and bipolaronic band in the UV-Vis-Nir spectra. The Seebeck coefficient of PEDOT:PSS thin films were determined using a homemade system. Using the same system, electrical conductivities were measured through IV curves, from which the Power Factor (PF= S^2.σ) of PEDOT:PSS was calculated. Our results highlight that the sample with the highest doped level presents the highest Seebeck coefficient.

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THERMAL STABILITY OF THE POSITIVE ELECTRODE LiCr(MoO4)2 FOR LITHIUM ION BATTERIES

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The popularization of electric vehicles (EVs) depends on pending improvements in the safety, cost, and energy density of lithium-ion batteries (LIBs). A crucial component to this is the positive electrode since its active material decomposes if heated 'charged', releasing oxygen – which can trigger electrolyte combustion and cause fires – and it also contains cobalt, costly metal. Given this scenario, this work investigated the high-temperature thermal stability of LiCr(MoO4)2, an active cobalt-free material with a high specific capacity. The material was synthed by solid-state reaction preceded by wet milling and characterized by x-ray diffraction (XRD), Raman spectroscopy and scanning electron microscopy, where the effect of heating the material (which is synthed already in the 'charged' state) in two different environments was compared: one in air, with the material alone; and another in argon atmosphere, with the material as a component of the slurry (active material + PVdF + conductive carbon) that is used in the electrode, simulating the environment to which the active material is exposed inside the battery. XRD and Raman results showed that it remains stable in the air throughout the investigated temperature range (300 K - 973 K), i.e., it neither undergoes structural phase transition nor decomposition. In this range, it showed negative thermal expansion (NTE) along the b-axis due to MoO4 tetrahedra rotation. As a slurry component, when heated in an argon atmosphere, it undergoes chemical attack from pyrolysis products of PVdF and starts to decompose at ~450 °C, more than 100 °C above the decomposition temperature of commercial positive electrodes NCA, LCO and NMC. Thus, LiCr(MoO4)2 has higher safety than 3 of the 4 major commercial positive electrodes (with only LFP as an exception) and is, therefore, a promising candidate for application as a positive electrode in LIBs.

The Role of Formamidinium Ions on The Perovskite Layers' Durability

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Perovskite Solar Cells (PSCs) have advanced in energy conversion, achieving efficiencies of over 26%. Ensuring long-term stability is a challenge, mainly for PSCs fabricated in uncontrolled environments [1]. The presence of formamidinium ions (FA+) enhances the durability of PSCs prepared under uncontrolled conditions [2]. Formamidinium perovskites (FAPI) may exhibit two phases, a photoactive (α) and a non-active (δ). To stabilize the α-phase, methylammonium chloride (MACl) facilitates grain growth through more efficient ion exchange [3].
In this study, perovskite layers were prepared using MA+ and FA+ in different proportions, varying from MAPI (MAPbI3), FAPI (FAPbI3), FA0.5MA0.5PbI3, FA0.25MA0.75PbI3 and FA0.125MA0.875PbI3, to identify the impact of FA+ in perovskite layers durability. Perovskites and measurements were made in uncontrolled environments, with relative air humidity ranging from 40-60%.
X-ray diffraction (XRD) patterns of all perovskites show a small residual PbI2 peak at 2θ = 12.65º, which enhances the photostability of perovskites. XRD of FAPI layer shows a peak at 13.93º attributed to α-phase. The intensity of this peak is predominant over the peak at 11.75º, attributed to the δ-phase. Decreasing the concentration of FA+ ions, the peaks shift towards slightly higher angles near 14º, indicating a reduction in the tolerance factor due to the increase of MA+ ions, which have a lower radius than FA+.
Further experiments, including absorption spectra, electron microscopy, and XRD are underway to assess the durability of perovskite layers over time. The photovoltaic parameters of PSCs prepared with these perovskites will be monitored to identify any trends in device durability.
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The search for sustainable solutions: The use of scrap tires in the production of nanocomposites for electrochemical hydrogen storage

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With the growing demand for alternative energy sources and the need to reduce dependence on fossil fuels, the urgency of developing new production and storage systems for renewable energy is becoming increasingly evident. To face this challenge, this project presents a solution focused on the electrochemical storage of hydrogen, using carbon black from discarded tires (NFP) as a precursor material to produce nanocomposites. Functionalized multi-walled carbon nanotubes (FMWCNT) and bismuth (III) sulfide (Bi2S3) were incorporated into NFP. Bi2S3 was incorporated into FMWCNT (Bi2S3-FMWCNT) using a hydrothermal method. The formation of FMWCNT/NFP and Bi2S3-FMWCNT/NFP nanocomposites was carried out by wet impregnation. The morphological study was carried out using scanning electron microscopy (SEM-FEG) and presented characteristic images of the nanocomposites. Analysis by energy dispersive X-ray spectroscopy (EDS) showed the presence of atoms characteristic of the FMWCNT/NFP and Bi2S3-FMWCNT/NFP precursor materials. Furthermore, the nanocomposites were evaluated for their performance in electrochemical hydrogen storage using cyclic voltammetry and charge/discharge techniques. The copper electrodes were modified by drop-casting with nanocomposite suspensions and the studies were carried out in 3.0 mol/L KOH solutions. The results showed the synergy of the nanocomposites, since there was an increase of almost 20% in the specific hydrogen discharge capacity (mAh g-1) in the electrode containing the Bi2S3-FMWCNT/NFP.

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Thin films of BiVO4:Ti deposited by RF Magnetron Sputtering

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The research on new materials for clean and renewable energy production has gained prominence due to the need to expand the availability of sustainable energy. Semiconductors stand out for their ability to efficiently and cleanly convert light energy into electrical energy, and $BiVO_4$ has emerged for its favorable optoelectronic properties for the production of photovoltaic devices. One strategy to improve the photoelectric properties of this material is to dope it with another transition metal, aiming to stabilize the separation of photogenerated charges. With the aim of investigating the effects of titanium incorporation into $BiVO_4$ ($BiVO_4$:Ti), thin films were deposited by RF magnetron sputtering from a target composed of 50% $BiVO_4$ and 50% TiO_{2-x}. To optimize the photovoltaic conversion properties, the films were produced following a 2^3 factorial experimental design, considering power, pressure, and heat treatment as variables. The film that exhibited the best photo-generation characteristics was deposited under the configuration of 100W, $1.5x10^{-2}$ mbar, and 500°C, indicating that optimization depends on the plasma characteristics. This film demonstrated a band-gap of 2.6 eV and a current density of $1.4\mu Acm^{-2}$, emerging as a promising candidate for further investigations in its applications for photovoltaic devices[1],[2].

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Transition Metal Decorated Graphenylene as Single Atom Catalyst for Hydrogen Evolution Reactions

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The increasing energy demand and aggravation of CO2 emissions due to fossil fuel exploitation urge the need for an energetic transition. Green hydrogen (GH) is a promising eco-friendly energy carrier with high energy density with applications in energy storage and production. Electrochemical water splitting is among the most promising routes to produce GH without harmful emissions in the cathodic hydrogen evolution reactions. However, its large-scale implementation remains challenging due to the high demand for efficient and abundant catalysts to compete with benchmark materials (e.g. Pt). 2D carbon-based materials have attracted large research interest in catalysis due to their large surface area, low cost, high stability in harsh environments and tunability[1]. In this work, we employ first-principles calculations based on DFT and the Computational Hydrogen Electrode Model (CHE)[2] to explore the catalytic properties of transition metal decorated Graphenylene (GPY). Our results show that the decoration of Sc, Ti, Mo, Zr, Pt, Ni and Co promotes the catalytic properties of GPY reaching $|\Delta G_H| < 0.1$ eV. Crystal Orbital Hamilton Population (COHP)[3] analysis shows that bonding states below the Fermi energy modulate the binding strength of the adsorbate (H), tailoring the free energy of adsorption.

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Unraveling Organic Photovoltaics (OPV) Modules High Reproducibility: A 5 Year Case Study

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Organic photovoltaics (OPV) represent an attractive class of photovoltaic materials with unique characteristics such as low temperature processability, high production throughput, semitransparency, lightweight and flexibility, which make OPV well-suitable for several applications. They are based on solution-processed photoactive polymers that can be deposited over flexible substrates applying coating and printing techniques such as roll-to-roll (R2R) processing. For this technology to remain competitive in the market, a few challenges must be overcome, such as power conversion efficiency (PCE) and lifetime reproducibility at a large-scale fabrication. In this study inverted OPV modules were prepared by slot-die coating and screen-printing with layers deposited over a pre-patterned PET-based substrate. Electron transport layer, active layer, and hole transport layer were coated in a single station 110mm-wide R2R lab machine in air under environmental laboratory conditions and using non-halogenated solvents. The 21.6 cm2 active area modules, consisting of 6 individuals serially connected sub-cells, were finalized by the screen printing of a silver paste. Modules composed of two different AL systems, a blend of a low band-gap copolymer (1.67 eV) and a PC60BM fullerene-derivative acceptor and P3HT:PC[60]BM, fabricated in the last 5 years were investigated. External Quantum Efficiency, Optical absorbance and Photovoltaic performance at 1-sun were measured. Lifetime and stability were assessed by accelerated aging tests according to international standard protocols and outdoor measurements at ONINN, in Belo Horizonte. The results indicated the high reproducibility of the modules fabricated with an average PCE maintained within 5 years investigation. Devices presented similar lifetime with stable performances over years, suggesting that the materials and processing conditions applied are well-suitable for the fabrication of reproducible OPV modules at large-scale.

Use of metal-organic framework (MOF) based on niobium as a catalyst for the green hydrogen evolution

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Growing environmental concerns have intensified the search for clean and renewable energy sources. In this context, there is a need to explore technologies capable of contributing to this energy transition [1]. Among the viable alternatives, there is the possibility for hydrogen (H2) evolution from metal hydrides, such as sodium borohydride (NaBH4). However, this reaction has slow kinetics, requiring the use of catalysts. Due to the high porosity and large surface area of the MOFs, they significantly increase the contact area with the catalyst, enhancing catalytic performance in green H2 evolution [2]. Thus, this work aims to develop a metal-organic framework (MOF) based on niobium (Nb), named as Nb-MOF, to serve as a catalyst for H2 evolution from NaBH4, adding value to this metal that has large reserves in Brazil, but little explored. The material was synthed via the solvothermal method, using 1,5-pyridinedicarboxylic acid and benzene-1,3,5-tricarboxylic acid as organic ligands, and a Nb salt as the metal source. The synthed MOF was characterized using FT-IR, SEM, XRD, TGA and BET, revealing that the MOF was successfully synthed. As a result, Nb-MOF presented high thermal stability and significant surface area (183.96 m^2/g) with pore of 2.5 nm. For H2 evolution experiments employing Nb-MOF, some parameters are being evaluated, such as the most efficient bimetallic composition (Pt, Ni, Pd, Co), temperature variation (283-323K), and concentration of sodium hydroxide. These experiments are in progress, and the results will be presented during the event.

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Visible light-induced photocatalytic reactions with Ag3PO4/TiO2 nanocomposite catalysts– An EPR spin trapping analysis

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Ag_3PO_4/TiO_2 nanocomposites are potential candidates for effective visible light photocatalysis in advanced oxidation processes (AOPs) [1, 2]. For that it is essential to consider their photostability concerning photo-corrosion and the role of oxygen vacancies. Due to the bandgap scheme of the hybrid structure of Ag_3PO_4/TiO_2 [1], visible light is primarily absorbed in Ag_3PO_4, generating electron-hole pairs that separate at the interface. The holes are transferred to TiO_2, while the electrons remain in the conduction band of Ag_3PO_4. The primary photocatalytic processes involve direct oxidation by holes or indirectly through the formation of hydroxyl radicals (•OH). However, electrons in the conduction band of Ag_3PO_4 do not have enough energy to produce superoxide radicals ($\bullet O_2^-$) from molecular oxygen dissolved in water. In this work, we studied Ag_3PO_4/TiO_2 synthed by a slightly modified process from the literature [3]. EPR in the solid-state and EPR coupled with the spin trapping methodology were employed to understand the catalytic reaction mechanisms involved. We used the spin traps DMPO and PBN, in addition to the redox probe hydroxy-TMP. Compared to the pure catalysts, the composite nanomaterial showed enhanced visible light photocatalytic production of hydroxyl radicals in water and water/ethanol mixed solvent. To our surprise, in acetonitrile solvent, an aprotic solvent, the nanocomposite catalyst also showed the formation of superoxide radical adducts, although the conduction band of Ag_3PO_4 is below that of the $\bullet O_2^-/O_2$ electron transfer reaction. EPR analysis of the solid nanocomposite allowed us to attribute the visible light-induced •O2-radical formation to oxygen vacancy defects in the TiO_2 structure.

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Voltage control in the synthesis of TiO2 nanotubes

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Metal oxides, especially TiO2, have attracted significant attention in nanoscience due to their diverse applications. TiO2 is known for its cost-effectiveness, durability, mechanical strength, low density and corrosion resistance. Its remarkable magnetic, optical and catalytic properties are crucial not only in medicine, but also in green fuel production, particularly in the generation of H2 through photoelectrochemical oxidation of water [1]. Although pure titanium naturally forms a passive oxide layer, the anodization process allows the growth of controlled artificial TiO2, such as nanotubular structures, improving the surface area and the main physicochemical properties for H2 production reactions [2]. This study investigates the influence of voltage control during the synthesis of TiO2 nanotubes, producing three distinct samples anodized at a)30V, a)60V and a)90V for one hour using an electrolyte solution of C2H6O2, NH4F and H2O. Characterization via FEG-SEM reveals that the increase in voltage directly impacts the diameter and height of the tube, resulting in an increase in pore diameter from a)78nm to a)150nm and a)215nm, and in height from a)0.9µm to a)2µm and a)3.5µm. The evaluation of the photoelectrochemical properties of the samples will be carried out using electrochemical impedance spectroscopy (EIS), Mott-Schottky measurements and linear voltammetry, followed by the demonstration of photocatalytic efficiency through the photodegradation of the methylene blue dye.

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Water Splitting Process promoted by $NaNbo_3$

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In the last years, due to concerns about the problematic use of fossil fuels as an energy source, the use of clean and renewable energies has been a growing area of research. Among the existing alternatives, the use of hydrogen gas obtained by the water splitting reaction has stood out as a promising strategy for generating hydrogen (H_2) as a clean and highly efficient energy source [1-2]. However, there are still gaps to be filled regarding the synthesis route used, morphologies and crystal structures of $NaNbO_3$ in order to assess its efficiency in generating H_2 by water splitting. In this work, $NaNbO_3$ was synthed using the hydrothermal and polymer precursor (Pechini) methods. The material was subjected to photocatalytic tests to generate H_2 by water splitting with the aim of evaluating the influence of the morphology and particle of this material on the generation of H_2.The results suggest that this material may be promising for generating H_2 through the water splitting process. However, special attention must be paid to the particle and morphology of the material.

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Xanthan flexible photovoltaic substrates with PEDOT:PSS and graphene oxide

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The main challenges in photovoltaic technology are related to solar cell efficiency, durability and cost production. Nanomaterials, especially graphene oxide (GO), enhance device properties such as electrical conductivity and light absorption, potentially reducing manufacturing costs [1]. Combining poly(3,4-ethylenedioxythiophene):poly(sulfonated styrene) (PEDOT:PSS) with GO is a way to improve electrical conductivity, stability over time, and mechanical properties of biopolymeric substrates. Biopolymers like xanthan offer versatility, cost-effectiveness, and environmental friendliness, forming transparent, flexible membranes with plasticizers and crosslinkers. [2] This study aimed to optimize electrical properties for organic photovoltaic devices by preparing xanthan substrates with PEDOT:PSS and GO. Different concentrations of GO were added to xanthan dissolved in deionized water, with glutaraldehyde as a crosslinker and ethylene glycol as a plasticizer. Two methods were tested for adding PEDOT:PSS: in-situ, during xanthan substrate synthesis, or via spin-coating deposition. Raman spectra of GO were obtained and computationally simulated using Density Functional Theory (DFT) within Quantum Espresso (QE) free software, fitting with experimental data. [3] Simulated GO configurations were adjusted to match the oxygen/carbon concentrations observed in experimental data, favoring the identification of characteristic peaks in the samples through comparison with theoretical results. Preparation methods were correlated with morphological, electrical, and optical properties, revealing a significant enhancement in electrical conductivity and stability, also after solar spectrum light exposure, in samples combining GO and PEDOT:PSS.Acknowledgements:CAPES, FAPERJ.References:[1]J.E.D Vieira et al. Revista Eletrônica de Materiais e Processos 11, 54 (2016)[2]F.C. Tavares et al. J. Appl. Polym. Sci. 5976 (2018) [3]P. Giannozzi, et al. J.Phys.: Condens.Matter 21, 395502 (2009).

ZIF-8, MoS2 and FMWCNT-based nanocomposites applied for electrochemical hydrogen storage

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The hydrogen energy to replace fossil fuels can significantly contribute to the reduction of polluting gas emissions and the transition to a more sustainable energy matrix. However, hydrogen gas has physical characteristics that make it difficult to store and transport, such as a low boiling point and low density in the gaseous state. Solid hydrogen storage has aroused interest due to its safety characteristics and overcoming difficulties. Electrochemical hydrogen storage is considered one of the most promising systems due to its operation at low temperatures and pressures, and high reversibility. This work aimed to develop hybrid nanocomposites based on the formation of the composite of ZIF-67 and carbon nanotubes modified with molybdenum sulfide for the electrochemical storage of hydrogen. SEM and Electron Dispersion Spectroscopy (EDS) analyses were carried out to investigate the morphology and composition of the nanocomposites. SEM analyses showed that the characteristic morphologies of ZIF-67 and FMWCNT did not change after the formation of MoS2/FMWCNT and incorporation of ZIF-67. EDS analyses confirmed the presence of reagent elements in the composites after the synthesis processes. Cyclic voltammetry curves showed hydrogen adsorption-desorption peaks/shoulders and charge-discharge measurements indicated gravimetric specific capacitance of approximately 96.48 F g^{-1} and specific hydrogen discharge capacity of 34.4 mAh g^{-1} at an applied current density of 1 A g^{-1}.

ZnO nanorods electrosynthed and applied as a photoanode in CdS-sensitized solar cells

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This study presents the use of ZnO nanorods as a semiconducting oxide in quantum dot sensitized solar cells. The NRs-ZnO film was electrosynthed by chronoamperometry at -1.3 V for 1 min and -1.0 V for 29 min on a fluorine-doped glass/tin oxide substrate, followed by sintering at 300 °C for 30 min. The sintered films were sensitized with cadmium sulfide (CdS) quantum dots (QDs) using the SILAR method with solutions of CdCl2.5H2O 1.0 mol.L-1 and Na2S 1.0 mol.L-1. The photovoltaic cell was assembled using the prepared photoanode, polysulfide electrolyte (S2-/Sn2-) 1.0 mol.L-1 and brass counter electrode. The NBs-ZnO films were characterized by X-Ray Diffraction (XRD), Scanning Electron Microscopy (SEM), Electron Scattering Spectroscopy (ESS), Ultraviolet and Visible absorption spectroscopy (UV-Vis). The photovoltaic device was evaluated by Cyclic Voltammetry (CV) and Electrochemical Impedance Spectroscopy (EIE). XRD analysis showed the hexagonal pattern of wurtzite, which is characteristic of ZnO. SEM analysis showed the formation of NRs-ZnO with good homogeneity and deposition density, but poor organization and alignment. After sensitization, the EDS spectrum showed a predominance of Zn (63,5%) and O (22,6%) and Cd (0,65%), indicating sensitization by CdS. The absorption spectrum showed a peak at 365 nm (transition) characteristic of ZnO with a band gap of about 2.93 eV. Photoelectric tests showed a current of 0.19 mA and a long lifetime, indicating a low recombination rate and consequently good stability of the cell using the ZnO-CdS photoanode. While the achieved photoconversion efficiency of 0.075% is modest, this work demonstrates the successful sensitization of ZnO NRs with CdS quantum dots.

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SS04-Advances in Microscopy/Spectroscopy of Materials for Sustainable Processes and Environmental Protection

Conversion Lithium Batteries: Polymers as cathode materials

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On March 8th, International Women's Day, we achieved a significant milestone at the Federal Fluminense University (UFF) by constructing the university's first prototype of lithium batteries. While the timing coincided with this notable day was an announcement of high achievements, the preliminary results reveal a groundbreaking advancement. Our battery introduces an innovative type of conversion cathode, surpassing traditional oxygen and sulfur batteries, and demonstrates an impressive specific capacity exceeding 1600 mAh/g. In our presentation, we will delve into the fundamental principles of lithium batteries and discuss the journey that led to the creation of PANflon. Where PANflon, protected under patent BR 10 2024 007382 7, stands for polyacrylonitrile (PAN) and Teflon (PTFE), both of which are integral components of the cathode and crucial to the battery's conversion process. In the presentation, we will outline the synthesis of PANflon, present our experimental findings, and utilize molecular dynamics to address fundamental aspects of the process.

MagnetoElectroCatalysis of ammonia and urea on platinum and nickel-magnetic iron oxide nanoparticles

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Urea and ammonia are compounds that can cause harm to the aquatic ecosystem. Ni-based materials and Pt-based presents high electrocatalytic activity towards urea electro-oxidation reaction (UER) and ammonia electro-oxidation reaction (AmER), respectively [1,2]. Magnetic iron oxide nanoparticles (MNP) have attracted considerable attention due to their ability to generate heat under an alternating magnetic field (AMF) [2]. The objective of this work was to study the effect AMF on Ni-MNP and Pt-MNP nanoparticles towards UER and AmER, respectively. The main idea consists of using AMF to generated heat in MNP that is transferred to Ni and Pt nanoparticles, improving the catalytic activity towards UER and AmER. The Ni-MNP material was prepared in a mass ratio of Ni:MNP 3:2 and Pt-MNP of Pt:MNP 1:4. The X-ray diffraction analysis showed the presence of Ni, NiO, Pt, $Fe3O4$ and/or γ-$Fe2O3$. The images obtained by transmission electron microscopy showed Ni, Pt and MNP nanoparticles with average diameters of 3, 5 and 100 nm, respectively. The materials were supported on carbon cloth, which was used as working electrode. The chronoamperometric (CA) measurements carried out in 0.33 mol L-1 urea in 1 mol L-1 NaOH for 1800 s at 0.55 V vs Hg|HgO, under AMF of 14.9, 29.8, 44.8, 56.6, 74.0, and 88.9 mT were conducted. It was observed an increase of 6% in the current density from UER for the lowest amplitude of AMF and 52.5% for the highest one. The CA experiments in 1 mol L-1 NaOH with 0.5 mol L-1 $NH4OH$ at - 0.2 V for 1800 s under AMF of 29.8, 44.8, 56.6, 74.0, 88.9, 103.9, 118.4, and 133.5 mT showed that the current density from AmER increased from 2 to 51% with lowest to highest AMF.

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Seeing Atomic-Level Surface Dynamics on Metal and Oxide Nanoparticles through *In Situ* TEM and Artificial Intelligence

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Nanoparticle systems often show high degrees of instability which are strongly influenced by and ambient environment. These dynamic structural changes modify material properties such as reactivity, phase changes and catalysis. Atomic-level surface dynamics may play a significant role in defining particle structures and functionalities but characterizing nanoparticle surface structures with high spatial and temporal resolution simultaneously has proven challenging. Ultrafast transmission electron microscopy (TEM) can now achieve picosecond temporal resolution but is limited to a spatial resolution of about 2 nm. Fortunately, modern detectors now provide readout rates in excess of 1000 frames per second, offering the potential to investigate atomic-level structural evolutions with time resolutions down to a millisecond. However, in most situations, the need to limit electron dose rates results in high temporal resolution movies that are dominated by shot noise, which often obscures surface structural dynamics. In order to address this challenge, we propose a fully-unsupervised AI denoising framework, which enables recovery of atomic-resolution information from such data. The unsupervised deep video denoising framework improves the signal-to-noise ratio (SNR) by a factor of 30 at a spatial resolution of 1 Å and time resolution of 10 ms. For this investigation, we explore structural dynamics of metal and oxide nanoparticle particles under combinations of CO and O_2 at temperatures up to 300°C. The enhanced time resolution reveals that supposedly stable, low-energy surfaces can display highly active dynamics, triggering nanoparticle instabilities resulting in rapid structural fluctuations. The new spatiotemporal capability enabled by the proposed framework dramatically enhances our ability to explore surface dynamics and the evolution of metastable states in nanoparticles at the atomic level, offering new insights into their functionality.

Towards Quantitative Maps of Lithium in the Electron Microscope

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This work will present where we are to perform quantitative EDS and EELS maps of Lithium-based materials with the Hitachi SU-9000 dedicated STEM having electron beam energies between 0.1 to 30 keV. State-of-the-art results acquired will be shown. This microscope has EELS capabilities that allow Li detection. It is also equipped with the Extreme EDS system from Oxford Scientific that can detect the Kα line of Lithium. The SU-9000 has a resolution of 0.22 nm in bright field STEM without aberration correctors and this allows lattice imaging. Even if the X-ray Kα line was not seen for this material with the Extreme EDS detector, the ionization edges are visible for Fe, Li, and Si. A Li EELS jump ratio map of an Al 2099 alloy taken with the Hitachi SU-9000 at 30 keV shows δ precipitates (Al3Li) which are spheres between 5 to 20 nm and T1 plates (AlCuLi) that have thicknesses between 2 to 6 nm. The fact that the edges are always ionized is a strong advantage for EELS since it does not matter if there is not an electron transition leading to X-ray emission, where is often the case that there are no Li Kα line with oxides cathode-based materials. Also, the emission rate in EELS is greater than about 10,000 than that of EDS owing to the fluorescence factor. The downside of EELS is the need for a transparent specimen and beam damage can also be an issue. Results obtained with a cryo-holder to minimize beam damage will be presented for Spodumene and other materials.

In situ and ex-situ investigation of ROS-generating ZnO nanostructures applied as photocatalysts

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Some semiconductor materials have characteristics that can make them environmental remediators and can be used in photocatalytic processes for the degradation of organic and inorganic pollutants [1]. The photodegradation process occurs via redox reactions mediated by reactive oxygen species (ROS) formed by the activation of semiconductors [2]. Particularly, ZnO, an n-type semiconductor with a band gap energy (Eg) of 3.24 eV, is widely used in photocatalysis under UV irradiation. Variations in particle morphology and ionic defects in ZnO may impact the formation of ROS and modify its photocatalytic properties. Thus, paramagnetic resonance spectroscopy (EPR) and spectrofluorimetric analysis were used in combination to elucidate in situ and ex-situ the formation dynamics and reactivity of ROS of different ZnO nanostructures synthed by the microwave-assisted hydrothermal method. XRD results demonstrate the formation of single-phase ZnO with a P63mc hexagonal structure. Microstructural analysis by SEM and TEM/EDX demonstrated the formation of ZnO nanostructures with sphere, rod, and flower-like particle morphology. Furthermore, the presence of ionic defects was evidenced by EPR analysis, mainly interstitial oxygen, or zinc vacancies, and varies according to the particle morphology. In situ spin trapping measurements by EPR in combination with ex-situ spectrofluorimetric results of the photohydroxylation of terephthalic acid showed that the ZnO sample with flower-like morphology presented the highest ROS formation, confirming its greatest photocatalytic degradation of the dye pollutant.

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Study of the photocatalytic activity of protonated niobates HNb_3O_8 and $K_{4-x}H_xNb_6O_{17}$ using the RNL dye

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The photocatalytic activity of layered potassium niobates is directly linked to the degree of distortion of their octahedra. Naturally configuration, niobate tends to exhibit distortions due to its small atomic radius, resulting in Nb-O bonds with double bond length. However, when subjected to an ion exchange reaction with molecules that promote the relaxation of these distortions (such as H_3O^+), a reduction in photocatalytic activity is observed [1]. Protonated niobates were obtained from precursor potassium niobates using an ion exchange reaction with a 6 mol/L HNO_3 solution [2]. Structural analyses by XRD, UV, Raman, and PL confirm the structural alteration caused by protonation, including the substitution of K^+ ions by H_3O^+. This ion exchange is evidenced in the X-ray diffraction patterns, where shifts in peaks corresponding to the lamellar planes are observed. Broadening of UV spectra bands and reduction in intensities of Raman and PL spectra bands are also observed, indicating a possible reduction in octahedral distortion. Photocatalytic tests using the RNL dye confirm the reduction in activity when niobates are protonated (C/C_0 = 100% for both potassium niobates, 16% and 38% for HNb_3O_8 and $K_{4-x}H_xNb_6O_{17}$), attributed not only to the lesser distortion of octahedra but also to the trapping of photo-generated electrons, which hinders their photocatalytic performance.

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The effect of Sn^{3+} centres on SrSnO3's photocatalytic activity: An EPR study

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The increased growth in recent years of the use of photocatalysis has allowed its application in different areas including environmental remediation, hydrogen generation, sustainable fuels and chemicals. [1]. In this context, different materials have been used for such applications, including $SrSnO_3$, which has also been used as dielectric materials, capacitors and sensors [2]. One advantage of $SrSnO_3$ is the absence of expensive rare metals and the large abundance of its elements. In this work, $SrSnO_3$ was synthed by Pechini-modified method and after calcination, $SrSnO_3$ was characterized using X-ray diffraction (XRD), UV-Vis absorption spectroscopy, Field emission scanning electron microscopy (FE-SEM), Scanning transmission electron microscopy (STEM) and Electron paramagnetic resonance (EPR) spectroscopy. The FE-SEM micrographs for all systems show spherical shaped particles grouped together forming large clusters and may be associated with the applied synthesis method. HAADF-STEM image shows of crystal oriented along <201> direction. Attempt was done to elucidate the species formed upon electron excitation and trapping, and provide an improved fundamental understanding of its photoactivity. EPR measurements associated to irradiation of the sample confirmed the presence of a defect sensitive to visible irradiation despite the broad band gap. X-band measurements associated to simulation confirmed the presence of Sn^{3+}, sensitive to visible light and probably responsible for the photocatalytic activity of $SrSnO_3$, similar to Ti^{3+} species in TiO_2. Despite being already detected in other materials, it is the first time that Sn^{3+} is identified in perovskites.

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The role of structure and ionic defects in SnO_2 photocatalysts: A diffraction and spectroscopy study

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Heterogeneous photocatalysis is an advanced oxidative process that could mitigate emerging and persistent pollutants in water by the reactive oxygen species (ROS) formed in the process[1]. SnO_2 is an n-type semiconductor with a large band gap value between 3.6 and 4.0 eV very active under UV irradiation [2]. Tin oxide SnO2 nanoparticles (SnO_2-NPs) were synthed by a modified Pechini method, followed by annealing at 700 ºC, and applied as catalysts for cationic and anionic organic dyes degradation. The SnO_2 samples were characterized by XRD, infrared (IR), Raman, UV-Vis spectroscopy, scanning electron microscopy (SEM), transmission electron microscopy with energy dispersive X-ray spectroscopy (TEM/EDX), zeta potential, and electron paramagnetic resonance (EPR) spectroscopy. The short and long-range structural characteristics and electronic properties of SnO_2-NPs strongly depend on the annealing time, which plays an important role in the photocatalytic properties. It was evidenced that the increase in the annealing time led to an increased short- and long-range order, which was strongly linked with the magnitude of structural and electronic defects, cumulatively affecting the formation of ROS and, therefore, changing the photocatalytic performance of SnO_2-NPs. As a result, to obtain high photocatalytic activity toward the organic dyes degradation, it is important to choose appropriate synthesis conditions to fine-tune the properties of a desired material.

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Zn(II)-modified SiO2 as photocatalyst for the degradation of glyphosate herbicide

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The demand for agricultural products makes Brazil one of the most polluting countries [1]. The scientific community has searched for different methods and strategies to remove agricultural pollutants from the environment; in this regard, heterogeneous photocatalysis has been a great ally in environmental remediation [2]. Thus, this study aimed to synthe Si1-xZnxO2 (x= 0.10; 0.20; and 0.30 Zn mol%) materials by the polymeric precursor method for applications in the photodegradation of glyphosate herbicide. Samples were characterized by X-ray diffraction (XRD), Infrared (IR) and UV-Vis spectroscopy, Scanning Electron Microscopy (SEM), and BET surface area analysis. XRD analysis confirmed the successful synthesis of the oxides after calcination at 800 °C for 4 h. IR spectra showed the presence of bands related to Zn-O and O-Si-O vibrations and, according to the UV-Vis spectra, Six-1ZnxO2 materials exhibited band gap values of 2.98-3.0 eV, consistent with the literature. SEM micrographs revealed the formation of particles with irregular spherical shapes in the samples with lower Zn2+ content, but rod-like morphology was observed in Zn2+-richer oxides. SEM results agree with BET analysis, which indicated a decreased surface area (SBET) with the increase of Zn2+. These characteristics may influence the photocatalytic performance of Six-1ZnxO2 toward the degradation of the herbicide. SiO2 and Si0.90Zn0.10O2 exhibited the highest photodegradation efficiencies, reaching a degradation of 86.2 and 93.6% of 10 ppm glyphosate aqueous solution, respectively. Additionally, the photocatalytic efficiency decreased when the tests were performed using 20 ppm of the herbicide solution.

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Antimicrobial activity of improved mortar grout by incorporation of zinc oxide nanoparticles (ZnO-NPs)

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Recently, there has been an increasing interest in the durability of construction materials, especially those with cementitious binders. This study investigated the effect of surfactant on the synthesis of zinc oxide nanoparticles (ZnO-NPs), used as additives in antimicrobial mortars. The antimicrobial efficacy of these nanoparticles was evaluated compared to samples without surfactants, analyzing the impact of surfactants on the morphology of ZnO-NPs. SEM analysis revealed filamentous structures in ZnO-NPs without surfactants, while samples with surfactant showed interrupted filaments. Surfactants interact with zinc ions, controlling the and shape of the particles. Minimum inhibitory concentrations (MIC) were used to assess the antimicrobial activity of ZnO-NPs against S. aureus, E. coli, and A. niger, with Ampicillin and Amphotericin as control substances. Despite the surfactant effect, the results of antimicrobial activity, determined by broth microdilution, indicated that MIC varied from 0.2 to 78.12, from 25 to 1250, and from 160 to 1250 in control versus samples (with and without surfactants). Mechanical damage resulting from contact with the cell membrane contributed to the antimicrobial activity of ZnO-NPs, facilitating their rupture. In conclusion, the incorporation of ZnO-NPs in mortar improved its antimicrobial properties, suggesting potential contributions to cleaner environments.

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Cement matrix composed of rock powder for photodegradation of methylene blue dye

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The construction sector consumes large amounts of natural resources, generating significant environmental impacts. To mitigate these impacts, the recycling of waste, reintegrating it into the construction cycle has become increasingly relevant and frequent. Rock dust, a by-product of basalt mining, presents characteristic compatible with cementitious composites [1]. However, a relevant feature of this by-product and little explored, is its potential to act as a semiconductor photocatalytic. Heterogeneous photocatalysis is one of the processes that can be used in effluent treatment. The interaction of a semiconductor with light leads to the formation of highly reactive radical species, which act in degradation of polluting compounds [2]. In this work we developed cement matrix composites with basalt rock powder replacing partially natural sand (25, 50 and 75%), aimed at application in effluent treatment. The photocatalytic potential of the material was tested with these mortar plates immersed in 500 mL of methylene blue dye (concentration 10 mg/L), kept under UV radiation (18 W lamp) for 2 hours. Mortars with 75% powder of basalt rock demonstrated greater photocatalytic efficiency than mortar control by up to 48%. Therefore, this composite material can contribute to minimization of extraction of resources such as natural sand, as it reuses a by-product of basalt mining activity and reduces the accumulation of waste generated. Therefore, the use of basalt rock powder is viable in replacing aggregates in cementitious composites and provides photocatalytic activity useful for the water effluent treatment.

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Characterization by Scanning Electron Microscopy (SEM) and Energy Dispersive Spectroscopy (EDS) of biochar from Taperebá waste (*Spondias mombin L.*)

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Taperebá (*Spondias mombin L.*) is a fruit from the north and northeast regions and widely used to obtain juice [1]. This work aims to characterize morphologically and chemically the biomass derived from taperebá, both in its naturals form and in charcoal. The taperebá biomass was obtained after collecting the fruits and separating them from their pulp, the seeds were dried in an oven at 100 °C. The seeds were then crushed and separated in particle using Tyler sieves with varying mesh syzes. 10 g of the mass was placed in a crucible, which remained on a 14 mesh sieve and taken to a muffle oven, carbonization was carried out at a maximum temperature of 800 °C. To characterize by SEM/EDS, the fresh and carbonized biomass were placed in the SEM sample holder (stub) and non-metallized and metallized samples with a thin layer of Au/ PD. The metallized samples were characterized by a SEM-FEG and the non-metallized samples by SEM/EDS. The obtained micrographs by SEM-FEG demonstrated the fresh samples are fibrous and smooth on their surface, while on the surface of the coal there is the appearance of pores, caused by the burning process. The coal porosity of the taperebá biomass indicates that it may have potential as an adsorbent product. The SEM/EDS results demonstrated the presence of the chemical elements, C, O, K, Ca, P, S, Fe, Cl, Mg, Al and Si, for both *in natura* and in coal. The presence of these elements can indicate the taperebá biomass could be used as fertilizer.

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Coagulant evaluation sodium aluminate alkalized at material removal organics from industrial effluent from the dairy industry

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The food production area is one of the most consume water and produce effluents liquids per unit of production. In the dairy sector , one of the main branches , there are one production significant amount of effluent liquids with a high matter load organic . You waste generated by this industry they are characterized by the great presence of matter organic, which makes essential to use an Effluent Treatment Station (ETE) for treatment of these effluents before disposal in bodies of water. So, this works he had as goal propose the implementation of a decantation system primary at the ETE of a dairy industry, aiming improve the efficiency of the treatment system. An approach adopted involved the execution of the jug test using 2,000 mL containers, with the aim of evaluating the pollutant removal capacity. The process included adjusting the pH to 8.5, through the incorporation of Sodium Aluminate Alkalized and the application of different dosages of coagulant - 0.4 ml, 0.6 ml and 0.8 ml of PAC - and flocculant - 6 ml, 8 ml and 10 ml. You results obtained indicated that the Sodium Aluminate Alkalized demonstrated efficiency to the collaborate at separation between the components solids and liquids of the liquid to be treated in the phases subsequent ones. That contributed to adapting the effluent to the requirements settled down by standards environmental in force, facilitating your destination to the receiving body in a way more effective.

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Construction of an Equipment for The Automation of The Photocatalysis Test of Nanoparticulated Semiconductors

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In this work, equipment was developed with the purpose of automating the laborious and repetitive process of analyzing substances subjected to photocatalytic processes, creating a new system intended to expedite current analytical techniques, one of which is Beer's Law. In addition to reducing the costs of implementing high-value equipment compared to those commercially available, the electronic system was developed with this form of application in mind, based on Deshmukh S. D. [1]. At the current project stage, a low-cost spectrophotometer was designed and constructed. It utilizes an ESP32-WROOM integrated circuit along with modules for a Stepper Motor and GY-2561 light sensors. These sensors measure the luminous flux in Lux units. The source of lights are eight monochromatic LEDs operating in visible light spectra and infrared frequency. The components were attached to a structure made of ABS (Acrylonitrile Butadiene Styrene) material using 3D printing techniques, with the receptacle modeled in Fusion 360 software. Absorbance tests conducted with various dyes in this created system and in a commercial spectrophotometer were carried out with the objective of validating the new system and evaluate its reproducibility and robustness.

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DESIGN OF NANOPARTICLE OF PRUSSIAN BLUE COORDINATION COMPOUND

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Prussian blue nanoparticles (PBNPs) have been the focus of intense research due to their applications in various areas such as biomedicine, (bio)sensors, diagnosis, and catalysis [1]. This work focuses on the preparation of Prussian blue nanoparticles (PBNPs) using the double precursor synthetic route [2] and applying them in the photocatalysis process with crystal violet dye at a concentration of 10 ppm using short ultraviolet (UV-C) light. The of the Prussian blue nanoparticles was controlled using Polyvinylpyrrolidone. The structural characteristic of the material was investigated using X-ray Diffraction (XRD), which showed the crystallographic planes related to the face-centered cubic phase of the Prussian blue nanoparticle complex, with the crystal [2]. Based on the Scherrer equation, the estimated crystal is 9.57 nm for the peak at $2\theta = 17°$, confirming that the inorganic core of PBNPs is coated with PVP [2]. UV-Vis spectroscopy analysis showed a maximum absorption band at 690 nm, attributed to the interband transition and a band gap of 5.5 eV. Regarding the application of nanoparticles in dye degradation, it exhibited an efficiency of 33.47% in 3 hours of monitoring.

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Detection of Metal Single-Atom Catalysts Supported on Carbon Nitrides by CO DRIFT-FTIR

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Carbon nitrides (C_3N_4) are highly promising semiconducting polymers widely used in energy conversion reactions through photocatalysis due to their stable two-dimensional structure and excellent electronic properties. These materials, especially the most crystalline ones, offer exceptional coordination sites for stabilizing isolated atoms, making them particularly well-suited for use as photocatalysts in single-atom catalysis. This study employed the DRIFT-FTIR technique to investigate the adsorption of CO molecules on supported metals. Specifically, Ni-PHI was prepared from sodium poly(heptazine imide) (Na-PHI), a highly crystalline carbon nitride support, to examine the impact of different metal loadings on the coordination mode of CO probe molecules. The experimental process involved heating the sample to 350°C using helium, followed by cooling and introducing CO, then purging with helium. The resulting spectra exhibited distinct bands, indicating chemisorbed CO with different coordination modes. Lower wavenumbers (below 2100 cm^{-1}) suggested CO coordination with multiple metals (bridging coordination), especially in samples with a high metal load, indicating cluster formation. Conversely, higher wavenumbers (above 2250 cm^{-1}) indicated monocoordinated CO, suggesting the presence of isolated metallic atoms. Additional studies with different metals and concentrations are planned to validate these findings, potentially revolutionizing the characterization of single-atom catalysts.

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Eco-friendly Metal-Organic Framework ([Ni(BDC)]n) is successfully synthed and applied to extract contaminants from fish samples

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Contaminants such as pesticides and dyes pose substantial challenges to environmental and human health, especially when found in aquatic ecosystems and ingested through the food chain [1]. In this scenario, this study presents the elaboration of a metal-organic framework (MOF), named as [Ni(BDC)]n, to serve as solid adsorbent for the determination of pesticides, including atrazine, bifenthrin, chlorpyrifos, endrin, heptachlor, flutriafol and permethrin, as well as dyes such as crystal violet (CV) and Congo red (CR) in fish samples. The material was synthed employing solvothermal method, and using nickel (Ni) salt and 1,4 benzenedicarboxilic acid (BDC). MOF characterization using SEM, FT-IR, TGA, XRD, and BET, indicated the success of the obtained MOF. BET analysis indicated MOF surface area and total pore volume of 2700 m2 g-1 and 0.0136 cm3 g-1, respectively. The adsorption study revealed high affinity of the MOF for the target analytes, with qmax ranging between 4.18-208.33 mg g-1. The kinetic study demonstrated that the adsorption mechanism follows a pseudo-second order model for all analytes. Furthermore, employing [Ni(BDC)]n, an efficient extraction method using Matrix-Solid Phase Dispersion (MSPD) combined with GC-MS and UV/Vis spectrophotometry for determination of pesticide and dyes, respectively was developed. The methods showed satisfactory linearity for both contaminants (pesticides and dyes), with recovery efficiency ranging from 81-103% and precision < 13% (n=3) for the analytes. Linear ranges covering 10-500 µg L-1 (R2 > 0.995) for pesticides and 100-1000 µg L-1 (R2 > 0.988) for dyes. The limits of detection (LOD) and quantification (LOQ) ranged from 0.5-1.6 µg L-1 and 1.7-5.6 µg L-1 for pesticides, respectively, while for dyes, LOD and LOQ ranged from 2.0-12.0 µg L-1 and 7.6-39.6 µg L-1, respectively.

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Effect of CTAB addition on Ni/CeO$_2$ vacancy aiming CO$_2$ catalytic methanation.

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The effects of cetyltrimethylammonium bromide (CTAB) addition in the sol-gel synthesis of Ni/CeO$_2$ catalysts, aiming to induce changes in the crystal structure by promoting oxygen vacancy formation, were evaluated to develop catalysts with favorable characteristics for the catalytic reaction of CO$_2$ conversion into CH$_4$. The specific surface area of the catalysts was assessed by nitrogen physisorption, along with pore , averaging 124 m^2/g, with slight variation. Each synthed catalyst showed distinct pore variations, ranging from 12 to 8 nm in diameter. To assess the structural parameters, such as crystallite , the Scherrer equation was applied using the full width at half maximum of the reflection peak from crystal planes, and the Bradley-Jay function was used to determine lattice parameters, obtaining a slight decrease in crystallite , reflecting the minimal change in specific area for this type of catalyst. Raman spectroscopy was employed to characterize the CeO2 cell structure in the catalyst bulk, revealing the distortion of the fluorite structure and the F$_2$g cubic phase field of ceria, distorted by the formation of shoulders at 466 cm^{-1}, possibly due to the active phase-support interaction and the formation of vacancies and structural defects related to vacancy with the addition of CTAB. X-ray photoelectron spectroscopy was used to determine the surface composition of the materials. An increase in oxygen vacancy formation with CTAB addition was observed through the increase in Ce^{3+} concentration and the decrease in Ni^{3+} concentration, potentially resulting in less resistance in catalysis. The morphology of the formed powder was evaluated by scanning electron microscopy, showing a decrease in average with the addition of CTAB.

EVALUATION OF THE DURABILITY OF COMPOUND MORTARS WITH BLAST FURNACE SLAG AND BAMBOO LEAF ASH

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Industrial waste with pozzolanic and hydraulic properties is commonly used in cement manufacturing globally. Among the various reasons for this practice, the improvement of durability properties stands out. Blast furnace slag (BFS) is utilized in numerous nations because of its unique ability and recently agro-industrial ashes have been globally evaluated and utilized. The purpose of this research is to examine how BFS and BLA affect the durability of compound mortars. Mortars were produced with partial cement replacement: 20%BFS, 20%BLA, and a ternary blend with 20%BFS+20%BLA. Prismatic molds (16×4×4 cm) were used in electrical resistivity measurements, starting with demolding and continuing up to 28 days of curing. Additionally, cylindrical specimens (Ø10 cm and a thickness of 5 cm) cured for 28 days, were used for chloride migration coefficient test. In the results, it is observed that the reference mortar exhibited an electrical resistivity of 44.2Ω.m after 28 days of curing. The compound mortars with 20% BFS and 20% BLA showed resistivities of 60.67Ω.m and 114.35Ω.m, respectively. The ternary binder showed a resistivity of 190Ω.m. Higher electrical resistivity means an evolution towards greater closure of porosity and reduction of interconnected porosity. In the migration test the depth of chloride penetration is used to calculate the chloride migration coefficients of mortars. Was observed a range of migration coefficients ranging between 3.2x10-12 m^2/s (20BFS20BLA) and 13.53x10-12 m^2/s (Control mortar). The intermediate values were observed for mortars with 20%BFS (10.33x10-12 m^2/s) and 20%BLA (5.34x10-12 m^2/s). As conclusion it is possible to observe that all composite mixes show an electrical resistivity much higher than reference mortar related to lower interconnected porosity. In addition, both, binary and ternary mixes improved durability against chlorides.

Evaluation of the photocatalytic properties of SnO_2 doped with Zn^{2+} and Ni^{2+} in the degradation of polychlorinated biphenyls

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The application of pesticides in the control of weeds, insect pests, and fungal diseases has been bringing significant impacts to the environment. Pesticides based on Biphenyls (PCBs) are compounds with high resistance to degradation, bioaccumulation capacity, and wide environmental distribution[1]. In this context, the present study aimed to prepare SnO_2 oxides doped with Zn^{2+} and Ni^{2+} by the polymeric precursors method for application in the photodegradation of the pesticide PCBs. The materials were characterized by X-ray Diffraction (XRD), Infrared Spectroscopy (IR), and UV-vis Absorption Spectroscopy. Regarding the photocatalytic tests, we used a reactor with a UVC lamp (4.9 eV) and a solution of 5 and 10 ppm of the pesticide PCBs with a reaction time ranging from 1 to 4 hours of monitoring. Through X-ray Diffraction (XRD) analyses, we confirmed the successful preparation of the modified oxides by the method. The infrared and Raman spectra showed characteristic bands of the modified oxides, and the band gap values of the materials calculated from the UV-visible spectra ranged from 3.0 to 3.1 eV. In relation to photocatalytic efficiency, the samples with 3% and 6% of Zn^{2+} showed better results with efficiencies of 77.6% and 87.2% for 4 hours of reaction, respectively, compared to samples doped with Ni^{2+}.

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Fabrication of eco-efficient glass from the recycling and utilization of agro-industrial wastes

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This work aims to present a sustainable, innovative and low-cost method for the production of eco-efficient glass materials, using wastes from the agro-industrial sector. Different residues were used: rice husk (RH), chicken eggshell (CES) and coconut husk (CH), as raw materials for the production of silicate glass. These residues, after physical-chemical beneficiation process, present chemical and mineralogical characteristics suitable for addition to glass formulations [1,2]. The wastes (RH, CES and CH) were subjected to beneficiation steps, such as washing, oven drying, grinding to reduce particle , and calcination to eliminate organic matter. They were subsequently characterized by FTIR, FRX, XRD, SEM and EDS and incorporated into glass samples, to evaluate the potential for replacing the raw materials SiO2, CaO and K2O in the composition of a soda-lime silicate glass. Samples were produced by melting of wastes proposed in this work (RH, CES and CH). The composition was melted for 1 h at 1600°C and heat treatment at 530°C for 3 h. The glass samples were analyzed by FTIR, FRX, DRX and UV-VIS transmittance. The glasses produced with the 3 residues presented a final composition analogous to the commercial reference composition, thus confirming the feasibility of incorporating agro-industrial wastes into glass materials with properties compatible with commercial glasses.

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Nanoparticles of Ni supported on Hierarchical ZSM-5 Zeolites: Synthesis and Characterization

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Metallic nanoparticles supported on zeolites are widely used as catalysts due to their unique properties, such as high thermal stability and uniform microporosity. The use of hierarchical ZSM-5 zeolites, obtained from desilication processes, promote the increase of mesopores, which increase the accessibility of pores and active sites and confine metallic nanoparticles, avoiding metal sintering [1]. Furthermore, a structure with voids, called "hollow" zeolites can be obtained. In this work, Ni supported on desilicated ZSM-5 zeolites were prepared. The ZSM-5 zeolites were synthed with a Si/Al molar ratio of 80 and 40. The catalysts were prepared by dry impregnation of the ZSM-5 zeolite with an aqueous solution of $Ni(NO_3)_2.6H_2O$. Then, desilication was performed using an aqueous solution of Na_2CO_3 at 80°C for 12h. The same desilication procedure was performed for a commercial ZSM-5 zeolite. The X-ray diffractograms of the catalysts are similar to that of the respective parent zeolite, showing that the treatments performed did not cause the structure collapse. For all catalysts, no significant changes were observed in the volume of micropores after the alkaline treatments. However, the results showed that the alkaline treatment caused an increase in mesoporosity The SEM images of the catalysts supported on synthed zeolites indicated an extraction of Si in the internal regions, forming hollow structures. For catalysts supported on commercial zeolites, it was not possible to observe significant changes. This result suggests that there is a higher concentration of Si in the inner regions of the synthed zeolites, while commercial zeolites exhibit a more homogeneous distribution of Si.

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OBTAINING ZINC OXIDE FROM STEEL WASTE VIA LEACHING FOR APPLICATION AS A COATING ON METALLIC PIPES

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The need to reuse steel mill waste rich in zinc is a difficulty faced by Brazilian steel industries for years [1]. On the other hand, the study of ceramic oxides aiming to inhibit the corrosion of metallic pipes is a well-known problem [2]. In the present work, the recovery of zinc oxide (ZnO) was obtained from steel residue dedusting powder, using leaching with sulfuric acid, pH adjustment with sodium hydroxide and heat treatment in a muffle furnace [3]. To confirm the formation, characterizations such as X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM) with Energy Dispersive Spectroscopy (EDS) and Fourier Transform Infrared Spectroscopy (FTIR) will be carried out. XRD analyses showed a high purity crystalline material. Using SEM, it was possible to observe clusters of nanoparticles [4], while FTIR and EDS analyses confirmed that zinc oxide was obtained without secondary phases. The results of the work show that the recovery process adopted for steel waste was effective in obtaining ZnO, in addition to allowing the oxide formed to be studied as a corrosion inhibitor.

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Photocatalytic Activity of Copper Oxide/Zinc Oxide for the Degradation of Organic Dyes

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Zinc oxide (ZnO) is a semiconductor material with direct bandgap energy of 3.37 eV and is a promising and favorable material in optoelectronic, biomedical, and photocatalytic applications. However, the effective use of solar energy in photocatalytic applications remains a challenge because sunlight contains only 4–5% UV light. Therefore, to improve the photocatalytic efficiency of ZnO induced by visible light, certain metals or oxides are often introduced to its surface. CuO has energy band gap of the range 1.21-2.1eV and as a mandatory p-type narrow band gap semiconductor can be used to extend the photocatalytic efficiency. In this study we developed ZnO/CuO nanocomposites by a hydrothermal method in aqueous solutions using eco-friendly low-temperature, short time, non-toxic and economical compounds. The crystal phase was investigated by X-ray diffractometry, bond vibration was determined using Fourier-transform infrared spectroscopy (FT-IR) and the Diffuse Reflectance Spectroscopy (DRS) was used to investigate the optical properties. Furthermore, photocatalytic performances were investigated for methylene blue (MB) degradation and the effect of pH on the degradation was conducted with a pH value without modification and 5, 7 and 9. The photodegradation obtained was 50.4 and 93% for CuO and ZnO, respectively, for solutions of the order of 10−5 mol/L using UVC light with 240 min of irradiation. In the experiments without pH modification 100 % of decolourisation was achieved with ZnO photocatalyst. However, according to the results, the best photocatalytic performance with short time is observed in ZnO with 20 wt % CuO, mainly at high pH value (9). The results indicated that the insertion of CuO in the ZnO contributes to the absorption of visible light and the reduction of the recombination rate because the band gap was 2.6 eV. Furthermore, ZnO/CuO compounds have large surface area that allow a strong photon absorption at the surface.

Photocatalytic activity of pillared clay containing Al and Ce applied in the treatment of textile effluents

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Photocatalytic activity of pillared clay containing Al and Ce applied in the treatment of textile effluents

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The constant use of contaminating materials, often improperly discarded into the environment, has concerned the research community, thus becoming a subject of investigation to mitigate such issues. This study focuses on the analysis of photocatalytic properties through advanced oxidative processes (AOPs) for the treatment of textile effluents[1]. A natural clay was pillared with aluminum and impregnated with cerium, being applied in the photodegradation of methylene blue dye (MB). The samples were characterized by XRD, FE-SEM, XRF, UV-Vis, and N2 adsorption-desorption isotherms. The materials were prepared using the traditional pillaring[2] and incipient wetness impregnation procedures. The results were positive and satisfactory, achieving around 55% dye photodegradation with a 25ppm dye concentration in a short period.

Acknowledgements: Pillarization, rare earth, dye.

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Photodegradation of different classes of dyes with the supported green nanocatalyst based on phosphorus doped Nb and Ti

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The environmental pollution of wastewater is mainly due to organic compounds, which are improperly disposed of and require advanced water treatments [1]. Heterogeneous photocatalysis consists of generating •OH and $•O_2^-$ through a semiconductor activated with energy-promoting oxidation-reduction reactions [2]. Titanium (Ti)-based oxides are for use in the photodegradation of organic pollutants highlighting the titanium niobate ($TiNb_2O_7$) involving the transfer of five electrons [3]. Nanocatalyst doped with phosphorus pentoxide ($TiNb_2O_7$@P) was synthesized by green/hydrothermal and impregnation, characterized, and tested in heterogeneous photodegradation containing dyes separated (106.5 mg L^{-1}) for 120 min. $TiNb_2O_7$@P demonstrated crystalline phases of titanium niobate and phosphorus pentoxide, rod-shaped particles with an average particle of 146 nm, and a negative surface charge of -17.3 mV. Ideal condition used was of [$TiNb_2O_7$@P]=1.20 g L^{-1}, pH=10, and T=298.15 ± 2 K with degradations separately of dyes: MB (38.8%/k=0.0044 min^{-1}), CV (16.4%/k=0.0020 min^{-1}), Rh B (17.2%/k=0.0014 min^{-1}), R 6G (15.5%/k=0.0014 min^{-1}), TT (25.7%/k=0.0025 min^{-1}), BB (16.5%/k=0.0017 min^{-1}), SY (14.8%/k=0.0015 min^{-1}), MO (22.1%/k=0.0022 min^{-1}), MR (23.6%/k=0.0024 min^{-1}), and EbT (20.1%/k=0.0017 min^{-1}) due to the (e_{CB}) of the $TiNb_2O_7$@P. It is worth noting that other photocatalysis tests at different temperatures will be carried out to demonstrate the catalyst's energy combined with a machine study. Therefore, it was possible to synthesize a nanocatalyst doped with P_2O_5 showing great potential for treating wastewater.

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Photodegradation of metylene blue dye mediated by Fe_3O_4-ZnO nanoparticles

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The Methylene Blue dye, commonly used in the textile industry, can be toxic to aquatic ecosystems if discarded without adequate treatment. Heterogeneous photocatalysis mediated by magnetic nanoparticles as catalysts appears as a viable alternative for the degradation of organic dyes in aqueous media. Studies demonstrate that ZnO, photocatalytic semiconductor, when associated with Fe_3O_4 forms an effective, recoverable and reusable magnetic nanocomposite [1]. The photocatalytic activity of Fe_3O_4-ZnO nanoparticles was evaluated through experiments with aqueous solutions of 0.02 g/L concentration of Methylene Blue dye and 2 g/L concentrations of magnetic nanoparticles, in the original form and recovered after 1 cycle photodegradation using a magnet and subsequent cleaning and drying in an oven. Three solutions were prepared for comparison: 1 aqueous solution of 250 mL of dye and 0.5 g of nanoparticles, 1 aqueous solution of 250 mL of dye and 0.5 g of nanoparticles recovered, and 1 aqueous solution of 250 mL of dye without the addition of magnetic nanoparticles. The solutions were exposed to sunlight for 4 hours, and in the first 30 minutes, 2 mL aliquots of each solution were removed every 10 minutes and the absorbance was measured at λ= 668 nm. After the first 30 minutes, 2 mL aliquots of each solution were removed every 30 minutes and the absorbance was measured. The results showed that the magnetic nanoparticles degraded the dye by 69% on first use and 48% after reuse. The solution without nanoparticles had a degradation rate of 23%. Therefore, the effectiveness of magnetic nanoparticles in dye photodegradation was confirmed, highlighting the high rate of degradation, even after reuse, compared to the solution containing only the dye. Acknowledgements: this study was financed in part by the CNPq grants (174402/2023-6). A.K. thanks the CNPq grants (306096/2023-4). References: [1] M. L. D. C. Silveira et al. Research, Society and Development 11(2), e3811225373 (2022).

Plasma-Activated Water Using an Affordable and Portable DBD Reactor: Enhancing Accessibility to Sustainable Technologies

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Plasma technology has revolutionized material adaptation over the past decades, facilitating the creation of microchips, touch-sensitive screens, and enhancing the durability of various industrial tools. In recent years, this innovative approach has extended its reach to a fundamental resource in industrial, commercial, and domestic settings: water [1].

By subjecting water to plasma, a process known as plasma-activated water (PAW) is generated. The versatility of PAW has been increasingly evident in recent years, with numerous studies showcasing its efficacy in surface sterilization, enhancing seed germination rates, and a myriad of other applications [2], [3].

This study aims to delve into the effects of water activation using plasma generated by a portable, cost-effective Dielectric Barrier Discharge (DBD) reactor developed at the Laboratory of Plasma and Applications (LPA) at UNESP Guaratinguetá.

For the activation of 25ml of water, a consistent power level of 3.15±0.04 W was maintained, with a fixed distance of approximately 10 mm from the samples, while varying treatment durations from 1 to 30 minutes.

Comprehensive analyses were conducted to assess changes in water properties, including pH, oxidation-reduction potential (ORP), electrical conductivity (EC), and total dissolved solids (TDS), both before and after treatment. Additionally, UV-Vis spectra were employed to identify reactive oxygen and nitrogen species (RONS) introduced into the water post-treatment.

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Production and characterization of sustainable composites from natural rubber and snake plant fibers

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Currently, the integration of resources from renewable sources into the production industry demands alternatives that meet requirements as durability, strength, and application of these products, which increasingly challenges researchers [1]. As a means to contribute to the implementation of such resources, this study aims to evaluate the potential application of fibers from the plant commonly known as "Snake Plant," scientifically named Dracaena trifasciata, in natural rubber elastomeric composites to enhance their mechanical properties and act as a filler. In total, four samples were prepared, varying the quantity of filaments in the composition, namely 0 (pure rubber), 10, 20, and 30 phr concerning the natural rubber matrix. From the investigated properties, it was observed that rheometry values, conducted according to ASTM D2084, revealed that the curing time of the composites did not undergo abrupt changes with the introduction of filaments. Tensile test results, according to ASTM D412, showed a significant increase in values compared to the reference sample. Hardness tests were conducted following ASTM D2240, demonstrating an increase in results with higher quantities of filament in the samples. Finally, the investigation of morphological properties by FTIR revealed that the interaction between fiber and rubber is of a physical nature, in other words, interfacial adhesion. With these results obtained from the conducted tests, it is concluded that fiber composites enhance their mechanical properties, enabling their application in products such as shoe soles, automotive mats, among others.

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Scanning Electron Microscopy Characterization of Umari (Poraqueiba sericea Tul) seeds

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Amazon is a region formed by great fauna and flora diversity. However, even with a vast list of research, there are still great biodiversity to be studied. Umari (*Poraqueiba sericea Tul*) is fruit and it is found and consumed in the Amazon region. The consumption part comes from the pulp and Most of the pits are discarded [1]. This work presents the characterization by Scanning Electron Microscopy (SEM) of pits umari. Umaris were collected in the UFPA, the pulp was extracted and reserved, the pits were broken and dried in an oven at 100 °C for 24 h, after which they were ground and separated by granulometry, for carbonization process in muffle furnace. They were heated at 800 °C and at 1000 °C. The obtained yield in the first stage was 27% and in the second stage was 24%. For SEM characterization, the carbonized samples were macerated for comparison with the *in natura* samples. Samples were metallized with an Au/Pd thin layer by sputtering process. In SEM results, the *in nature* samples presented porous with an average diameter of 1.5 mm and an average diameter of 5 mm for coals samples. Umari porosity indicates a great potential for application as bioadsorbent.

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Sustainable Cadmium Extraction in Sewage Sludge Samples by Hydrophobic Deep Eutectic Solvents (HDES) and Ultrasound-Assisted Extraction

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One of the aims of green Analytical Chemistry is to reduce or eliminate the use of products that are toxic to the environment and humans. In this context, the use of hydrophobic deep eutectic solvents (HDES) is an alternative in the extractions process. The HDES has been highlighted by its interesting characteristics, such as biodegradability and high extraction efficiency [1]. In this work, the objective was to synthe a solvent based on acetic acid, pyruvic acid and DL-menthol and use it to extract Cadmium (Cd) from sewage sludge samples. For this, initially the solvent was prepared by stirring for 15 min at 200 rpm, with heating at 60 °C and characterized by DSC, TG, ATR-FTIR, density and viscosity. A 3^3 Box-Behnken experimental design (15 experiments), evaluated the parameters that could influence the extraction, namely: sample mass (150; 225; 300 mg), HDES volume (2.0; 3.0; 4.0 mL), and ultrasonication time (15.0; 22.5; 30.0 min) from a sewage sludge certified reference material. The best condition was used in the extractions of three different sewage sludge samples from the state of São Paulo. The Cd analyzes were performed by ICP-MS using KED mode and calibration curves in the concentration range 0.500 –50.0 $\mu g\ L^{-1}$. The LOD and LOQ values were 0.280 and 0.933 $\mu g\ L^{-1}$ [1]. For sewage sludge samples A, B and C, the values obtained were, respectively, $2.10 \pm 0.11\ \mu g\ g^{-1}$, $2.07 \pm 0.23\ \mu g\ g^{-1}$ and $5.32 \pm 0.14\ \mu g\ g^{-1}$. The recovery of the method was 104% using a sewage sludge certified reference material, demonstrating that it is a sustainable alternative for use in the extraction of sewage sludge.

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Synthesis and characterization of a Gemfibrozil cocrystal

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Cholesterol is a lipid that performs important functions in the human body, for example, as a structural component of cell membranes, and synthesis of hormones and vitamin D. However, nowadays, high cholesterol is one of the biggest problems that public health is facing, as it is associated with metabolic and neurological diseases, such as Alzheimer's and diabetes [1]. Gemfibrozil (GEM) is an API (active pharmaceutical ingredient) from the fibrate class and is in class II of the Biopharmaceutical Classification System [2], which means it has low solubility and high permeability; this becomes an obstacle to the application of this compound in inhibiting myotoxins. An alternative to overcome this problem is the prospection of new multicomponent solid forms, such as salts. In this context, this project aimed to synthe a GEM salt using the mechanochemical method, to optimize its physicochemical properties. The synthesis used a no-grinding (NG) and liquid-assisted grinding (LAG) approach in the mechanochemical method in a vibrating ball mill, and, also, a mortar-pestle grinding approach. This system with L-lysine (LYS) was prepared in a 1:1 stoichiometric ratio, with a frequency of 15 Hz. The system was characterized using Thermogravimetry and Differential Thermal Analysis, Differential Scanning Calorimetry (TG-DTA and DSC), X-ray diffraction (XRD), and Infrared Spectroscopy (IR). Furthermore, based on the modification, disappearance, and appearance of other peaks at 2θ of the diffractograms (such as the 1704.58, originally present in the GEM´s one), the detachment of bands from the infrared spectrum, and the melting point of the intermediate system and the precursors, it is possible to confirm that the system is, in fact, a salt.

Acknowledgments: PIBIC

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Synthesis of graphene from disposed battery graphite.

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The extensive use of batteries in everyday life raises serious concerns about disposing of this material after usage, due to the toxic content present in the batteries. Xing et al. (2018) showed the recovery of zinc via the hydrometallurgical route through oxidative alkaline leaching, managing to obtain cathodic zinc with a purity of 99%. In this context, the great efforts of the scientific community to create a viable process for recycling cells and batteries are evident, aiming at the development of more sustainable and economically viable production processes. The main effort in the battery recycling process focuses on the recovery of metals due to economic and environmental interests. Graphite has become a by-product of battery recycling, currently with little reuse. The recycling process becomes more efficient by using a graphite rod to obtain graphene. According to Sabisch et al. (2018), about 3% of the total mass of batteries consumed is recovered, a small part is incinerated and a large percentage of waste with recycling potential is disposed in landfills. The use of a graphite rod for graphene synthesis is an economically viable recycling process due to the great market value of graphene, contributing as a new option for obtaining graphene by the Top-Down method, which is currently restricted to natural graphite and synthetic graphite. In the present work, it was verified that the methodology applied with graphite free of any chemical treatment proved to be less efficient, while the Hummers method with acid washing proved to be the most satisfactory. Therefore, recycling batteries is a sustainable alternative by recycling and adding value to a material that poses a risk to the environment and human health in case of incorrect disposal.

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Synthesis of Ni-doped ZrO2 and Evaluation on the Photocatalytic of MB in Varied pH Conditions

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Currently, environmental issues represent a significant global challenge, with environmental problems directly related to pollution production and energy consumption. Ongoing industrialization exacerbates pollution resulting from urbanization over time [1]. The synthesis of photocatalysts has attracted great interest within scientific community due to their potential in converting solar energy into chemical energy and in removing organic pollutants, using accessible, non-toxic and chemically stable materials [2]. ZrO2 is a robust semiconductor with a wide band gap energy, however, to make it an effective photocatalyst, it is necessary to modify its surface and reduce the band gap. Ni(II) doping emerges as a promising approach as it reduces the band gap and prevents electron-hole recombination, improving photocatalytic performance [3]. In this study, the synthed compounds Ni-ZrO2 were characterized using X-ray diffraction (XRD), UV-visible absorption and Fourier Transform Infrared (FTIR) spectroscopy. The photocatalysts was synthed through hydrothermal synthesis and photocatalytic tests were carried out on the orange organic dye G and methylene blue (MB) dyes, in different pH conditions (pH = 2, pH = 7 and pH = 10), in the presence of 2 UVC lamps with power of 18 w, with 5 hours of reaction. The degradation of orange G in the neutral pH obtained 20% as the best performance in 1 hour, the basic pH reached 28% in 1 hour and the acidic pH obtained 44% of degradation, with concentrations of 0.1 g.mL-1 of the photocatalyst. The variation of the degradation rate as a function of pH reveals that the maximum and minimum degradation rates are in acidic (pH = 2) and neutral (pH = 7) conditions.

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The effect of synthesis conditions on the photocatalytic behavior of $Na_2Ti_3O_7$

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Sodium trititanate ($Na_2Ti_3O_7$) has been investigated and used in different applications, especially in heterogeneous photocatalysis [1]. Thus, this work aimed to synthe $Na_2Ti_3O_7$ materials using a Pechini method, varying the calcination temperature (700, 800, and 900 °C) to be applied in the photodegradation of methylene blue (MB) dye. The samples were characterized by X-ray diffraction (XRD), Infrared (IR) and Raman spectroscopy, UV-Visible (UV-vis) spectroscopy and Scanning Electron Microscopy (SEM). XRD structural results confirmed the formation of a monoclinic structure with space group P21/m. Infrared and Raman showed active modes referring to the monoclinic structure of trititanate. Photohydroxylation was carried out with terephthalic acid, showing a distinct evolution in the formation of hydroxyl radicals (OH) according to the calcination temperature. In the photodegradation tests, it was observed that the sample calcined at 800 °C takes only 15 min to reach 98% of MB dye photodegradation, while the sample calcined at 700 °C only reached this percentage after 300 min and the one calcined at 900 °C does not achieve such photodegradation percentage even after 480 min. All the results indicate that changing the calcination temperature leads to structural changes in the materials, which impact directly in the photocatalytic efficiency of the materials.

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