Editorial: focus on waste-heat harvesting via thermoelectric conversion: materials, devices and systems for sustainable energy technologies

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Editorial: Focus on Waste-Heat Harvesting via Thermoelectric Conversion: Materials, Devices and Systems for Sustainable Energy Technologies

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Abstract

The Focus collection on Waste-Heat Harvesting via Thermoelectric Conversion: Materials, Devices and Systems for Sustainable Energy Technologies collates several research articles and a Roadmap highlighting the most recent advances in the field of thermoelectricity from the viewpoint of both basic and applied research, with a special eye on the work of the Italian community.

To face the worldwide continuously growing energy request, and mitigate the health and environmental consequences of the consumption of fossil fuels, a two-fold path seems to be the best route to follow: on the one hand, sustainable sources need to be exploited, such as wind, solar, geothermal and chemical energy of renewable fuels; on the other hand, energy saving has to be implemented. In the framework of energy saving, harvesting plays an important role since, in average, about 66% of the yearly world energy consumption is currently discharged in the environment and lost as waste heat. A possible response to this issue is represented by thermoelectricity by means of the Seebeck effect, that allows the generation of a difference of electrical potential as a response to a temperature difference settled between the two sides of a conductor. The current flows between the two sides when the circuit is closed by another conductor characterized by a different Seebeck coefficient. The effect is exploited in thermoelectric generators (TEGs), thus allowing to harvest at least a portion of waste heat by direct conversion into electricity.

The research on thermoelectricity experienced variable fortunes during the past century since the discovery of the Seebeck effect, mainly due to the limited output power provided by generators and the cost and toxicity of many elements contained in the most efficient thermoelectric materials. Nevertheless, the efforts of the scientific community never stopped, and nowadays they are especially focused toward the substitution of toxic elements and critical raw materials (CRMs), as well as the design of new materials with reduced thermal conductivity, also resorting to computational methods.

The present Focus Collection, facing the vast topic of energy harvesting in terms of thermoelectricity, consists in several research articles, as well as in a „Roadmap to Thermoelectricity". The whole collection aims at providing a bird-eye view on the state-of-the-art of thermoelectric research with a special focus on the challenges taken by the Italian community, from the viewpoint of both basic and applied research.

Sustainable materials containing earth-abundant and low-cost elements are the most represented in the collection: among them, binary [1] and multinary [2] chalcogenides, skutterudites [3,4], half-Heusler phases [2,5] and silicides [6]. Filled skutterudites for instance, are Zintl phases with a crystal structure characterized by a large cavity which can be easily filled with foreign atoms. A proper filling modifies not only the electronic, but also the thermal properties of the material, possibly making it a good candidate for thermoelectric applications [4]. Noticeable is the attempt to fabricate skutterudites thin films, with the aim to obtain flexible and robust modules [3].

Experimental investigations are often supported by computational tools. On the one hand, high throughput DFT calculations and machine learning can be used to predict the stability of new thermoelectric compounds. On the other hand, atomic-level modelling allows to establish correlations between properties and structure, as well as to predict the electrical and thermal transport behaviour of new materials [1].

In the case of half-Heusler compounds, the synergy of experimental and computational investigations [5] evidenced the crucial role of point defects and residual secondary phases on the transport properties of the TiNiSn model system. The concentration and type of defects and secondary phases in the material depends on the processing routes, affecting the thermoelectric properties. In view of the development of thermoelectric modules based on half-Heusler alloys with reproducible properties, reliable and cost-effective methods for the synthesis of these compounds are needed.

The size of the grains or crystallites is a further fundamental factor in view of thermoelectric properties. In particular, nanostructuring represents an effective approach to reduce thermal conductivity. A new sintering technique, named Ultrafast High-temperature Sintering (UHS), which consists in heating and cooling of samples within seconds, is a viable candidate for processing nanostructured thermoelectric materials. The advantage of the ultrafast high-temperature technique is also the low energy involved, resulting in a low production cost. In the case of silicides, such as Mg_2Si, a non-toxic and low-cost material, the UHS technique proved to process dense samples while limiting grain growth and Mg evaporation, with low energy demand [6].

A materials class of rising interest is the one of chalcogenides. In these, a multinary nature has been shown to be a promising strategy to suppress phonon transport [2]. Additionally, ab initio investigations on monolayer SnX_2 (X=S, Se) and Janus SnSSe, revealed that the symmetry breaking in the latter compound can lead to a strongly suppressed thermal conductivity, while maintaining good electronic properties. Calculations predict a zT value ranging from 0.5 to 3 from 300 K to 700 K upon optimization of the *p*-type carrier density, pointing to an interesting candidate for experimental validation [1].

Moreover, the focus collection addresses two different aspects related to TEGs. In the first case, the performance of a commercial TEG was characterized under mimicked operating conditions by means of a thermostatic chamber [7]. In the second case, the latest advancements in the development of novel thermoelectric device architectures and functionalities based on nanostructured semiconductor materials, including silicon and III-V semiconductor compounds (*e.g.* InAs), were considered. In this frame, nanowires are given particular attention, due to their large aspect ratio allowing for reduced thermal conductivity with respect to the bulk counterpart, and thanks to the reliability of device fabrication protocols and control methods. Leveraging on unique combinations of newly engineered nanowire heterostructures, advanced nanofabrication techniques and innovative control strategies , such as electrolyte gating, seminal results were recently achieved including the giant reduction of thermal conductivity in twinning superlattice InAsSb nanowires [8], and the demonstration of heat-driven transistors at the nanoscale [9].

We hope that readers will enjoy this focus collection, dealing with a well-established but continuously evolving research field facing one of the hardest challenges of our time.

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