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“Metal-Organic Frameworks and Hybrid Materials: From Fundamentals to Applications”

Porous metal-organic frameworks (MOFs) and dense hybrid frameworks are emergent multifunctional materials that have garnered major developments in the last decade. Indeed the incredibly rich structural diversity of this new class of materials in combination with its “designable” physical and chemical properties has caught the imagination of scientists, engineers and technologists from multiple cognate disciplines. By virtue of their immense versatility and functionalities, a number of promising applications have already been proposed many of which aimed at challenging industrial sectors, e.g. energy harvesting and storage, biomedicine, sensing and microelectronics, carbon capture and environmental sustainability.

In light of the rapid advances witnessed in the field, it is most timely for a themed issue which features cutting-edge research positioned right at the interface where crystalline engineering meets materials science, chemistry, solid-state physics and biology. Herein we are delighted to present a collection of thirty-one papers, including five review articles (Highlights). Together, this collection offers a unique coverage encompassing both the experimental and the computational domains illustrating the fruitful synergy between them, which will be appealing to a broad cross-section of readers.

Of all the Highlight articles, Allendorf and Stavila (DOI: 10.1039/C4CE01693A) provide the reader with an excellent overview of where the field stands after roughly 15 years of research by summarising the remarkable progress to date, and addressing the structure–function relationships from the perspective of crystal engineering. Notably, they further pinpointed the most pressing challenges that must be tackled for MOFs to reach their full commercial potential. The Highlight by Rösler and Fischer (DOI: 10.1039/C4CE01251H) addresses the innovative concept, termed “NP@MOF”, in which porous MOFs serve as novel hosts to generate metal nanoparticles potentially useful for hydrogen storage and heterogeneous catalysis. The review by Rossin and Giambastiani (DOI: 10.1039/C4CE00896K) presents a comprehensive survey illustrating the vast network topologies and crystal structures associated with the thiazole- and thiazyolidine-based MOFs, alongside potential exploitations in magnetism and luminescence. The Highlight by Chabal et al. (DOI: 10.1039/C4CE01406E) focuses on the critical issue concerning water interactions in MOFs, this information is key for devising new strategies to yield robust water-stable framework materials. The review on molecular simulations and modelling for hydrogen storage presented by Keskin and Basdogan (DOI: 10.1039/C4CE01711K) concerns state-of-the-art computational techniques and the accompanying deficiencies, thereby addressing possible factors surrounding observed discrepancies between experiment and simulation.

In addition to the aforementioned reviews, importantly this issue features twenty-six original papers comprising Articles and Communications, reporting the latest experimental and theoretical discoveries on MOFs and hybrid materials. New framework materials design and synthesis alongside crystal structure–property characterisation are reported by Lortsch et al. (DOI: 10.1039/C4CE01512F), Forgan, Fairen-Jimenez et al. (DOI: 10.1039/C4CE01379D), Kaskel, Glorius et al. (DOI: 10.1039/C4CE01400F), Volkmer et al. (DOI: 10.1039/C4CE01583E), Fröba et al. (DOI: 10.1039/C4CE00408F), Furukawa, Kitagawa et al. (DOI: 10.1039/C4CE01501K), De Vas et al. (DOI: 10.1039/C4CE01457J), Calleja et al. (DOI: 10.1039/C4CE01401D), Kosa and Major (DOI: 10.1039/C4CE01387E), Bureekaew, Schmid et al. (DOI: 10.1039/C4CE01574F), Eddaoudi et al. (DOI: 10.1039/C4CE01402B) demonstrated innovative fabrication of zeolite-like MOF thin films while Horcajada, Blanco-Prieto et al. (DOI: 10.1039/C4CE00885E) reported the potential applications of bio-oriented MOFs with antibacterial effects. Fundamental elastic properties and anomalous mechanical behaviour of MOFs and hybrid materials have been established in both experimental and theoretical works by Goodwin et al. (DOI: 10.1039/C4CE01572J), Zhang, Li et al. (DOI: 10.1039/C4CE01386G), Serra-Crespo, Gascon et al. (DOI: 10.1039/C4CE00436A), Bennett et al. (DOI: 10.1039/C4CE02145B), and Tan, Civalleri et al. (DOI: 10.1039/C4CE01564A). Additionally this themed issue features excellent contributions ranging from advanced reactivity characterisation (Walsh et al. DOI: 10.1039/C4CE01411A, Vandichel, Van Speybroeck et al. DOI: 10.1039/C4CE01672F) to understanding detailed host–guest sorption and separation capacities (Vittadini et al. DOI: 10.1039/C4CE01373E, de Lange, Gascon et al. DOI: 10.1039/C4CE01073F, Gómez-Álvarez and Calero DOI: 10.1039/C4CE01335B,}

We thank our colleagues who kindly contributed to this special collection and all the referees who have generously gave their time and expertise. While all the papers were solicited, we would like to emphasise that the majority of the contributions originated from authors who were also delegates at the EUROMAT2013 Congress held in Seville (9th-13th September 2013), specifically Symposium B41 on “Hybrid & Metal-Organic Framework Materials”. We sincerely hope that this unique collection of papers would not only inspire exciting future work, but also trigger new innovative directions in this vibrant research topic.

The guest editors wish to thank the CrystEngComm editorial staff, especially Dr. Debora Giovanelli and Dr. Anisha Ratan, who were instrumental for coordinating the reviewing and editing process, ensuring the entire operation was accomplished in accordance to schedule.

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