


 Cite this: *CrystEngComm*, 2015, 17, 197

Metal–Organic Frameworks and Hybrid Materials: From Fundamentals to Applications

 Jin-Chong Tan^{*a} and Bartolomeo Civalleri^{*b}

DOI: 10.1039/c4ce90162b

www.rsc.org/crystengcomm

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 their “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 thiazolidine-based MOFs, alongside potential exploitation 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 Basdogan and Keskin (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 Lotsch *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 Vos *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 anti-bacterial 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:

^a Department of Engineering Science, University of Oxford, Parks Road, Oxford OX1 3PJ, United Kingdom. E-mail: jin-chong.tan@eng.ox.ac.uk

^b Department of Chemistry, NIS and INSTM Reference Centre, University of Turin, via Pietro Giuria 7, 10125 Torino, Italy. E-mail: bartolomeo.civalleri@unito.it

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, Walton, Millange *et al.*

DOI: 10.1039/C4CE01393J, Turnes Palomino *et al.* DOI: 10.1039/C4CE01265H, Münch and Mertens DOI: 10.1039/C4CE01327A, Baima, Casassa *et al.* DOI: 10.1039/C4CE01989J).

We thank our colleagues who kindly contributed to this special collection and all the referees who 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 (9–13th September 2013), specifically

Symposium B41 on “Hybrid and 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 area.

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