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Introduction to molecular engineering in MOFs: beyond reticular chemistry

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Over the last twenty years, the field of metal–organic frameworks (MOFs) has experienced huge growth. At the core of this growth is the modular structure of MOFs, which allows us to design materials with atomic-level precision by judicious choice of the inorganic and organic building blocks. The term "reticular chemistry" was coined to describe the chemistry of MOFs, which relies on the linking of such molecular building blocks by strong bonds to make crystalline open frameworks. Testament to the success of reticular chemistry in tapping a virtually limitless chemical and structural space, is the ever-growing number of known crystal structures of MOFs, now exceeding 100 000 and counting, based on almost any metal of the periodic table and organic linkers bearing a wide range of coordinating groups.

Originally dominated by chemists, the field of MOFs has progressively attracted researchers with a diverse background – including materials scientists, chemical engineers, physicists and computational scientists – moving towards new, application-driven directions and opening itself to approaches inspired by the emerging multidisciplinary field of molecular engineering. The principles of reticular chemistry developed since the early days of MOFs have, therefore, become a key tool to either design new materials or purposely modify known ones, with the aim of fine-tuning the structural features and physicochemical properties to fulfil a specific function. However, nowadays there is much more than just reticular chemistry in the constantly evolving field of MOFs.

The central importance of understanding of the links existing between molecular structure, properties, and function in the context of molecular engineering requires to combine a wide array of advanced experimental and computational methods. The recent advent of sophisticated computational tools to design and evaluate the proficiency of MOFs for specific applications *in silico* has further accelerated the progress of the field by helping to better explore the immense landscape of hypothetical and existing MOFs in search of the best performers, providing precious insight to guide experimental efforts. The increasing focus on practical application is stimulating researchers to look beyond the atomic scale and to draw inspiration from materials science and engineering to master: the preparation of MOF-based composites with other classes of materials (*e.g.*, polymers and ceramics), the growth of MOFs on surfaces, the deposition of thin films, the shaping of powders, the control of their morphology and particle size, and so on.

This themed collection is an excellent representation of the diversity of molecular engineering approaches currently applied to MOFs targeting properties and functions relevant for both "classical" applications, such as gas separation, catalysis and sensing, and newer ones, such as heat reallocation, electronic and ionic conductivity, electrochemical energy storage and luminescence.

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