Porous materials

https://doi.org/10.1038/s41563-022-01419-7

Materials for a changing planet

About 700 scientists from 45 countries gathered in Dresden for the first time since the start of the COVID-19 pandemic to share their latest findings on metal–organic frameworks and open frameworks compounds.

In September 2022, the 8th International Conference on Metal–Organic Frameworks and Open Framework Compounds (MOF2022) was held in Dresden. This was the first physical meeting after the COVID-19 crisis, bringing back the community and assembling a broad panel of intertwined disciplines from materials discovery and fundamental science to chemical engineering and manufacturing for industrial needs.

Since their inception in the late 1990s, metal–organic frameworks (MOFs) have evolved from laboratory curiosities to an extremely versatile class of materials offering the potential to contribute to technological solutions in many fields, from climate change and sustainable energy production to health[1]. The uniqueness of MOFs is rooted in their specific building pattern according to the reticular chemistry concept, where one starts from organic and inorganic molecular building units that are assembled together to make diverse frameworks[2]. In principle, the whole periodic table of elements becomes a playground to construct materials. In the past two decades, concepts have been presented to make hybrid porous frameworks, soft crystals showing crystal-to-crystal transformations and, lately, liquid and glassy states[3]. Although MOFs have attracted academic attention for a long time, their potential for applications was clearly demonstrated during MOF2022. Eye-catching applications include MOFs such as MOF-303 to collect water from the air[4] or CALF-20 showing exceptional CO_2 capture performance from flue gases[5]. For each application, molecular insights into performance were gained owing to advanced characterization and modelling efforts.

CALF-20 is a nice illustration of the path from the laboratory to industrial scale. This required a so-called de-risking procedure, where in addition to standard characterization tests done within the lab, a series of tests giving typical process metrics are necessary, providing information on how to overcome hurdles in the technology-readiness chain. The CALF-20 case also illustrates how material scientists should focus not only on the best material but also on the most reliable solid for a given process.

The control of crystal morphology, size and shape has become much more mature. This enables the manufacturing and integration of MOFs into real devices, especially for micro-electronics and molecular sensors. Considerable effort has been deployed over the past few years to fabricate highly oriented and polycrystalline MOF films to address a wide range of challenges. Special attention has been paid to gain an in-depth understanding by combining advanced experiments and modelling of the MOF/MOF and MOF/polymer interfaces. This fundamental knowledge is indispensable for the design of MOF@MOF core–shell systems and MOF mixed matrix membranes, respectively[6,7]. One example is the growth of KAUST-8 into flat nanosheets orientated with all their CO_2-selective channels lying in the same direction and sandwiched between layers of a polyimide polymer, leading to an exceptional purification of natural gas[8].

To further exploit MOFs, academics have learnt to integrate process requirements for the selection of the most appropriate MOF for applications, especially in terms of synthesis conditions such as temperature, cost and green solvent usage. This is particularly true for biological applications, such as with the use of biocompatible MOFs to deliver therapeutics or protect fragile molecules like enzymes from degradation[9].

Although thousands of MOFs have been screened and discovered so far, there is still a need to design novel architectures integrating much less explored metal centres. This is typically the case for titanium owing to its complex chemistry in solution making the design of ordered structures challenging[10]. To leap forwards from serendipitous discovery to rational design, fundamental insights are necessary. The importance of in-depth physical understanding was nicely illustrated for the development of a photo(thermal)catalyst for visible-light-driven transformations of C1 molecules (CO_2, CH_4 and CO) or cracking of ammonia towards valuable chemicals and fuels[11].

Most of these achievements are not possible without advancement in experimental and theoretical techniques to understand and predict MOF structures. The search for novel architectures should be enabled by a better understanding of crystal growth, which has been facilitated by advanced in situ techniques such as electron diffraction and microscopy imaging coupled with automated data processing[12]. Advanced electron diffraction techniques have now become a complementary technique to X-ray diffraction or electron microscopy for structural determination, also accessing information on the dynamics of linkers or positioning of guest species[12]. A remaining challenge is to follow MOF dynamics and obtain kinetic information on local or global dynamics. For the field of flexible MOFs, it has thus far not been possible to follow the transition from one phase to the other on-the-fly. Currently, experimentalists undertake the building of dedicated in situ cells to unravel the spatiotemporal response of MOFs under operating conditions[13]. From the modelling point of view, the challenge is how to model realistic crystal particles exposed to external stimuli and how to bridge the theoretical and experimental scales, as well has how to simulate materials that are disordered from the short to long range[14].

Modelling has been instrumental in understanding behaviour and is moving more and more from a tool to understand experimental behaviour towards rational prediction. This transition has been catalysed by integrating data science and machine learning, making high-throughput screenings much more efficient and conclusive. However, with the explosion of structures and associated data, the availability of reliable databases, unique identifiers of MOF structures and their properties becomes important[15]. Further incentives are necessary to stimulate researchers to deposit their data via publicly available databases. Noteworthy is the recently launched initiative of the universal standard archive file for adsorption data[16].

During MOF2022, it became clear that MOF chemists can synthesize complex and fancy structures. However, it was emphasized that crystallinity might not always be a prerequisite for applications; instead, MOFs may be extended by including amorphous or glassy structures. Although such highly disordered phases have been enforced by subjecting MOFs to extreme conditions, for example, pressure, we are now entering the era where rational design of hybrid architectures with porous MOF liquids or glasses is within reach[17].

The concept of reticular chemistry offers many more material design options. Covalent organic frameworks (COFs) constructed from purely organic building blocks are an attractive class of porous materials owing to their high-order porosity, facile surface modification, and high chemical and thermal stabilities. A platform of applications was widely covered. It was emphasized that COF processability is mature with several examples of three-dimensional printing and aerogel COFs; the next challenge is scalability.

The maturation of MOFs has found further ground with the establishment of an elected board of the International Zeolite Association to promote the scientific advancement and industrialization of MOFs, COFs and other advanced porous materials. Finally, MOF2022 was preceded by a young investigators symposium, giving a forum to future generations to showcase their research, and followed by a workshop to promote MOFs in industry. MOF2022 showed great challenges are ahead; however, with the participation of young scientists, the future looks bright.

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Published online: 28 November 2022

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Competing interests

The authors declare no competing interests.