

The Road Ahead for Metal–Organic Frameworks: Current Landscape, Challenges and Future Prospects

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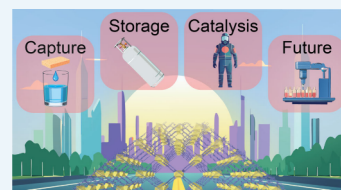
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ABSTRACT: This perspective highlights the transformative potential of Metal–Organic Frameworks (MOFs) in environmental and healthcare sectors. It discusses work that has advanced beyond technology readiness levels of >4 including applications in capture, storage, and conversion of gases to value added products. This work showcases efforts in the most salient applications of MOFs which have been performed at a great cadence, enabled by the federal government, large companies, and startups to commercialize these technologies despite facing significant challenges. This article also forecasts the role of nanoscale MOFs in healthcare, including strides toward personalized medicine, advocating for their use in custom-tailored drug delivery systems. Finally we underscore the potential acceleration in MOF research and development through the integration of machine learning and AI, positioning MOFs as versatile tools poised to address global sustainability and health challenges.



KEYWORDS: metal–organic framework, direct air capture, atmospheric water harvesting, large language models

INTRODUCTION

The Industrial Revolution, combined with historical practices of resource extraction without significant consideration for environmental impact, have contributed to the many challenges that our planet faces today. Climate change presents a growing concern, with rising temperatures and expanding populations leading to reduced water availability, increased air pollution, higher risks of pandemics, and a greater need for more individualized healthcare solutions. Metal–Organic Frameworks (MOFs), a class of crystalline, nanoporous, organic–inorganic hybrid materials, offer a wide range of structural and functional possibilities. As a result, they have been proposed for various applications, including energy efficiency, gas capture and storage, water purification, and emerging medical technologies.^{1,2}

However, due to the publication fervor, it can be challenging to identify the most practical and salient of these applications. In this perspective, we highlight a brief history of the benchmark MOFs for applications in gas capture, catalysis (conversion), and gas storage and identify some design rules, targets, and unique challenges to the deployment and the efforts of start-ups that have begun to commercialize MOFs. In addition, we discuss the prospects for how research in the field will likely be conducted with implementation of machine

learning and AI tools and how we can more effectively tailor MOFs for individually tailored medicine.

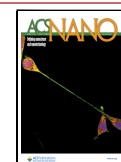
We emphasize the potential impact MOFs can provide considering current commercialization efforts, which are vast and varied in their readiness for commercial markets. In the U.S. and abroad large and small companies have begun to implement and push past the R&D phases. Governmental agencies have shown keen interest in the MOF market push. Additionally, numerous patents have been filed by private and academically affiliated individuals. These funding pushes are exemplified by private investments from Baden Aniline and Soda Factory (BASF) from 2005 to 2010, with later support from the Office of Clean Energy Demonstrations of Svante, a start-up for commercialization of MOFs for climate control, for a total of ~100 million U.S. dollars.

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CAPTURE

MOFs are excellent for gas capture and have been evaluated for a litany of gases. However, two of the most promising and pertinent areas where we see the most potential are the sequestration of CO₂ from ambient conditions, direct air capture (DAC), and the harvesting of water from ambient air, atmospheric water harvesting (AWE).

WATER

MOF's extensive structural diversity and precise functionalization offer many opportunities to tailor their design for capture of water from air.^{3–9} In addition, other conventional sorbents such as zeolites have high uptake at low relative humidity (RH) but require very high energies to regenerate. Other large pore materials perform well at high RH, such as commercial products like Drierite (Calcium sulfate) and household dehumidifiers, but are not suitable under arid conditions. Omar Yaghi was the first to demonstrate the potential of MOF sorbents for water harvesting while exploring the stability of a number of zirconium based frameworks.¹⁰ MOFs have been proposed for the capture and purification of water from several contaminants. In this perspective, we focus on the harvesting of water from air, which offers numerous advantages over contaminant purification, including the ability to capture anywhere (not limited to proximity to water sources) and providing an ultrapure source of water free of additional contaminants. Since then, Yaghi, Gagliardi, Farha and others have shown that this technology is scalable and implementable in devices simply using sunlight to regenerate water.^{11,12}

Gaining insights into what our instrumentation can reveal about real-world water capture performance is essential for advancing industrial applications. In Figure 1a–c we highlight some of the key regimes and important measurements for potential sorbent candidates. Potential sorbents have different relevant pressure regimes when it comes to capture (Figure 1a); the onset of the rapid uptake of water (labeled as iv) is material dependent but crucially important to the working range and capacity of the material. By shifting to lower pressures, we can create sorbents that are efficient in the more arid environments. The upper end of the pressure regime (iii) is also important, as this is where we release our captured water for use. The area in green is a rough metric for the working capacity of the sorbent and is important to determine the volume (L) of water per day per kg of MOF. However, material performance in single component isotherms is not a fair comparison to real world conditions; multicomponent breakthroughs are important to ascertain the guest–host interaction time to determine the relative selectivity to differentiate gases which are present in much higher concentrations than the desired target gas (e.g., competing analytes such as N₂ in arid environments) as seen in Figure 1b. One of the last key features of sorbent candidates is the ability to withstand many cycles and exposure to elevated temperatures and pressure cycles, as these conditions are crucial for material regeneration. This evaluation is conducted by studying the uptake after accelerated exposures, exploring the effect on crystallinity or cyclability through Thermal Gravimetric Analysis (TGA) and several other means, as seen in Figure 1c. All three of these metrics are important for developing and commercializing sorbents for the capture of H₂O.

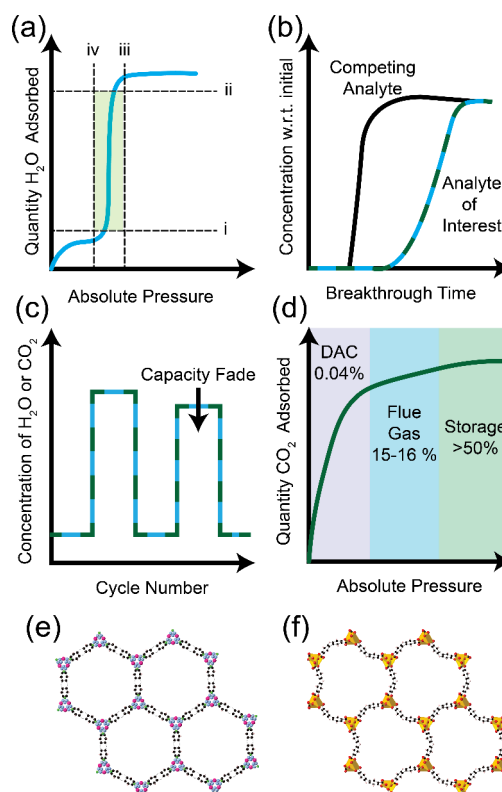


Figure 1. Overview of capture metrics and top performing illustrative MOFs for capture applications. (a) shows the relevant regions in the water sorption isotherm: (i) the Quantity adsorbed at (iv) the lowest RH (or pressure of H₂O) and (ii) the Quantity adsorbed at (iii) the highest pressure. The area highlighted in green is a proxy for the working capacity of the sorbent with thermal cycling, and (b) shows the respective ideal breakthrough curves in mixed gas streams of CO₂, H₂O, N₂, etc. respectively with the analyte of interest being CO₂ or H₂O and the competing analyte is N₂ or the other respective gas (e.g., when H₂O is the analyte of interest the black trace of the competing analyte represents N₂ or CO₂). (c) shows the cycling performance as evaluated through capture and regeneration cycles. (d) shows the most relevant regimes in the CO₂ isotherm for direct air capture (DAC), flue gas, and CO₂ storage (it should be noted that an isotherm alone does not equate to overall material performance in application), percentages on graph represent percent of gas by volume in feedstock. (e) shows the structure down the *c*-axis of M₂Cl₂(BTDD) where M can be several transition metals (M = Mn, Co, Ni). Finally, (f) shows the structure of mmen-dobpdc down the *c*-axis. For atomic structures disordering has been removed for clarity and yellow = Mg, black = carbon, green = Mn, pink = Cl, blue = N.

From the laboratory to the market, Dinca and Yaghi have shown success in the early stages of applying three different MOF systems. Dinca set record performances in 2017 with M₂Cl₂(BTDD) (M = Mn, Co, Ni); BTDD = bis(1*H*-1,2,3-triazolo[4,5-*b*],[4',5'-*i*])dibenzo[1,4]dioxin for water capture (as seen in Figure 1e).¹³ Since then, Dinca has worked with Transaera, a startup focused on developing new air conditioning technologies, to commercialize these materials and others, such as MIL-100 (used by Air Joule and Montana technologies) for cooling and water capture applications. Dinca was one of eight finalists challenged to redesign air conditioning units to reduce emissions on a warming planet. Similarly, Yaghi has pushed the limits of water adsorption with

MOF-LA2-1(furan) and MOF-LA2-2(furan).¹⁴ Yaghi founded water startups Atoco and Water Harvesting Inc. and is exploring MOF-303 and other high performing materials to implement commercialized water capture units for arid environments. They even demonstrated capture of 210 mL H₂O/kg of MOF of water in one of the driest, hottest, climates in the world, Death Valley National Park.¹⁵

CO₂

MOFs for the capture of CO₂ have been extensively studied for catalysis, conversion, and capture in both CO₂ laden streams (such as flue gas or exhaust) and ambient conditions where concentrations are as low as ~400 ppm, which is referred to a direct air capture (DAC). It should be noted that the material requirements for adsorption are quite different in both applications. At point sources, traditional capture materials such as liquid amines and cryogenics are commonly used. In DAC conditions, metal hydroxides and amine impregnated materials are typically selected.¹⁶ MOFs have an advantage over traditional mesoporous materials (alumina, silica) that capture CO₂ through capillary condensation of CO₂; this condensation makes regeneration more energy intensive, where MOFs, by contrast, can have rigidly defined pores optimized for the size of CO₂ molecules and can be more reasonably regenerated from an energy perspective.¹⁷ MOFs for CO₂ capture can be roughly broken into 5 categories: (1) Open metal site; (2) Amine decorated (node/linker); (3) Fluoride based; (4) Metal OH modified; (5) Flexible MOFs.¹⁸ Top performers among them include: KAUST-7,¹⁹ Mg-MOF-74,²⁰ and CALF-20.²¹

Understanding what our instrumentation can tell us about the real-world CO₂ capture performance is important for development in industrial applications. In Figure 1b–d we highlight some of the key regimes and important measurements for potential sorbent candidates. Potential sorbents have different relevant pressure regimes when it comes to capture. As shown in Figure 1d, high uptake in the ultralow pressure regime can indicate an effective capture material, and the isotherm can dictate if the MOF is a good candidate for DAC vs point source capture. However, as discussed in the previous section, material performance in single component isotherms is not a fair comparison to real world conditions; multi-component breakthroughs are key to understanding performance in practical conditions with competing analytes. One of the last key features of sorbent candidates is the ability to withstand many cycles and exposure to high humidity conditions, which are common in the solid adsorbent regeneration cycle.²² This evaluation can be done by studying the uptake after accelerated exposures, as discussed in the previous section. All three of these metrics are important for developing and commercializing sorbents for capture of CO₂.

These MOFs no longer exist exclusively in the laboratory—startups such as Svante, Captivate Technologies, Promethean Particles, and Mosaic Materials (in venture with Baker Hughes) have begun to commercialize these systems and explore their potential in both flue gas and direct air capture.^{23–25} While the exact framework systems are still proprietary, it is likely that they are utilizing some form of CALF-20 (Svante) and N,N'-dimethylethylenediamine (mmen) dobpdc appended (Baker Hughes/Mosaic Materials) frameworks from PR releases from both companies and patent licensing.^{23,25–27}

CALF-20 is notable for its efficient and selective carbon dioxide (CO₂) capture capabilities, particularly under conditions with up to 40% relative humidity, and shows robustness to acidic and basic environments. CALF-20 distinguishes itself by its low regeneration energy requirement, robustness to steam and acid gases, and the ability to suppress water sorption in the presence of CO₂, as confirmed by computational modeling and dynamic breakthrough experiments and is largely being proposed for flue gas capture.²¹ The N,N'-dimethylethylenediamine (mmen) dobpdc appended frameworks first reported in JACS by Long et al. exhibit remarkable CO₂ adsorption capabilities, particularly under conditions simulating both air and flue gas environments due to its channel pore architecture and strong binding sites (as seen in Figure 1f). This MOF demonstrates an exceptional ability to capture CO₂ at low pressures, crucial for applications in DAC. It can be efficiently regenerated and maintains high selectivity and capacity for CO₂ over multiple cycles.²⁸

CATALYSIS

MOFs have been extensively investigated for the catalytic conversion and detoxification of chemicals.²⁹ Owing to their permanent porosity and possibility for open metal sites upon removal of labile solvent, MOFs are amenable to both installation of catalytic species and possession of an inherent catalytic ability. Taking inspiration from the groundwork laid by zeolite catalysts, the chemical versatility of MOFs has been exploited for use in important conversions, such as hydrogenation, oxidation, and coupling reactions. More recently, increasing structural and chemical complexity programmed into these materials has led to the development of MOFs for electrochemistry, biomimetic CO₂ conversion, and detoxification of chemical warfare agents (CWAs). Following fundamental catalytic studies, efforts to engineer practical media for real-world applications have led to the development of composite MOF materials.³⁰ For example, Numat has designed suits featuring MOF composites for the detoxification of CWAs in the field.

With the growing threat of rising greenhouse gas levels, MOFs have been extensively researched for the capture of CO₂ as discussed earlier in the text. We envision that this will be taken a step further, with the development of MOFs that may not only capture but upcycle CO₂ into commodity chemicals that benefit society. To this end, efforts toward the CO₂ reduction and sustainable production of commodity chemicals may be combined. This combined capture and utilization would advantageously allow for efficient recyclability of the MOF, as the upcycled chemical may be removed to allow for capture and conversion of more CO₂. Such MOFs must be highly selective toward CO₂ capture, stable in humid and high temperature conditions, and electronically tuned for C–C bond formation.

Currently, a number of start-ups are leveraging the MOF technology for CO₂ conversion. For example, Metafuels, an Oslo-based company, is producing jet fuels using MOF-catalyzed CO₂ upconversion.³¹ This is a promising route, given that the infrastructure exists for liquid fuels in vehicles and aircraft, opening avenues for a more circular carbon economy.

In nature, carboxylases and CO₂ fixing enzymes can rapidly and efficiently convert CO₂ into C₂ and higher products. Since these enzymes rarely maintain their conformations in practical, ambient conditions, methods to enhance their stability outside of buffered conditions have been employed. MOFs in

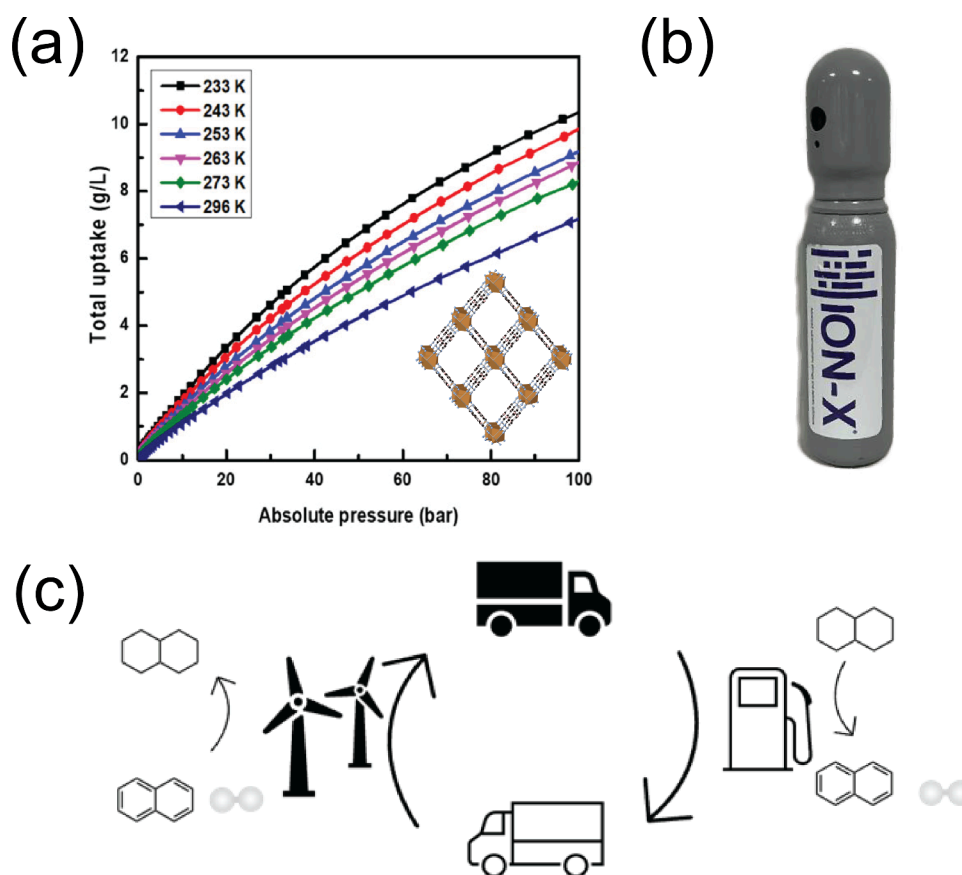


Figure 2. (a) High H₂ storage capacity of NU-2100 demonstrated at elevated pressures (inset shows the crystal structure). Reprinted (Reprinted in part) with permission from [Sengupta, D. et al., Air-Stable Cu(I) Metal–Organic Framework for Hydrogen Storage. *J. Am. Chem. Soc.* 2023, 145 (37), 20492–20502. [10.1021/jacs.3c06393](https://doi.org/10.1021/jacs.3c06393)]. Copyright [2023] [JACS] Copyright 2023 American Chemical Society). (b) Schematic of ION-X gas cylinders loaded with MOFs to store hazardous gases at low pressures. (c) Simplified schematic for distribution of LOHCs in the transportation sector.

particular have shown success in stabilizing certain proteins upon their encapsulation by preventing outside factors, such as solvent, pH, and heat, from impacting protein folding.^{32,33} In this vein, we envision that future MOF studies will aim to stabilize CO₂ fixing enzymes such that they may upconvert the environmental pollutant to useful chemicals while maintaining their secondary and tertiary conformations.

STORAGE

Due to their unprecedentedly low density and large void space, MOFs have demonstrated their capability for storing gases in high volumes utilizing lower pressure and higher capacity than state-of-the-art gas storage technology. Critical metrics for evaluating a sorbent's performance include volumetric capacity, or amount of adsorbate stored per unit volume of the material, and gravimetric capacity, which refers to the amount of gas stored per unit mass of the material. While a delicate balance of both metrics is needed for storage applications, a high volumetric efficiency is crucial to meet the energy density requirements for practical deployment. MOF nanomaterials that have achieved such benchmarks are being explored in the US and abroad by small start-ups and large companies (such as Samsung and BASF).

HYDROGEN

One limitation to the development of hydrogen-fueled technology is the challenge of safely storing and transporting

reserves of hydrogen that would uproot the current infrastructure landscape in place for refueling vehicles. The Farha group has demonstrated that Cu(I)-based MOF (NU-2100) has the ability to capture and store hydrogen approaching the department of energy (DOE) target of 4.5 wt % and 30 g/L at 700 bar as shown in Figure 2a.³⁴ In addition, NU-2100 has shown high performance at ambient temperatures and pressures, which would make loading less expensive and overall storage safer as cylinders can be stored at much lower pressures.

The future will see MOF catalysts leveraged for storage, particularly for hydrogen. Hydrogenation/dehydrogenation coupling reactions may provide a recyclable hydrogen source for more efficient storage with the use of hydrogen powered technology. Indeed, Liquid Organic Hydrogen Carriers (LOHCs) have been investigated as alternative means to transport and store hydrogen, as shown schematically in Figure 2c.

HAZARDOUS GASES

The success of certain MOFs as storage media for hazardous gases was shown by Numat who commercialized the first MOF product in 2016, ION-X (Figure 2b). ION-X is a subatmospheric storage solution used to store and transport the toxic gases used in ion-implantation processes in the semiconductor industry. Traditional gas cylinder storage relies on high pressure storage in cylinders. In the context of toxic gases,

arsine (AsH_3), phosphine (PH_3), and isotopically enriched boron trifluoride (BF_3) gases, used in the semiconductor industry, present significant hazards. By introducing an adsorbent, MOFs, within the gas cylinders, it is possible to store gas sub atmospherically (below 1 atm) while still having comparable cylinder delivery capacity to a high pressure cylinder.^{35–37}

CHALLENGES

Many MOF skeptics will make sweeping generalizations due to perceived challenges such as cost, stability, and synthesis limitations; but many of these concerns often lack context and are highly application dependent. For example, water stability is irrelevant for applications like gas phase catalysis or separation of hydrocarbons where water exposure is minimal. Similarly, higher cost may be justified for the production of very high-value-added products. It's also worth noting that the high cost of MOFs is often linked to the organic linker. However, if a linker demonstrates superior performance in a valuable applications, it is likely that the community will develop methods to produce the linker in high quantities at lower cost in the same way the semiconductor industry was able to with silicon due to economies of scale and innovation in semiconductor manufacturing.³⁸ Moreover, reducing the complexity of linker synthesis and increasing the overall yield can be achieved through reaction optimization, such as the use of efficient catalysts or by pivoting toward simpler linker designs.

Stability, as discussed briefly, of MOFs is also crucial and highly application dependent. It is important to define what is meant by "stable." Many groups when reporting stability provide an evaluation of thermal stability within the TGA, however this gives no indication of the material's crystallinity or porosity. But very general strategies to increase the stability of the framework to structural fluctuations in separations applications revolve around the introduction of 3D bulky linkers, which have more steric hindrance and prevent pore flexibility.³⁹ By contrast, in CO_2 capture applications, stability is generally defined as structure retention in the presence of water. However, making sweeping generalizations about improving material stability is challenging, as it is highly system dependent.⁴⁰

Scaling and commercialization of any new material technology comes with its challenges.⁴¹ In the past decade, several efforts to scale-up MOF production on an industrial level have been taken on by such chemical giants as BASF, Exxon, and GE, and smaller start-ups with the help of federal funding (i.e., Savante). Currently, the biggest hindrance to the rapid scale-up of these materials include the prohibitively expensive organic linkers, large volumes of required solvent, and downstream processing, such as filtration, activation, and extrusion.⁴²

Applied research and pilots will aid in the scale-up of MOF syntheses, which may differ in reaction conditions from lab-scale syntheses. In the future, we might look toward greener strategies for large-scale preparation, such as water-based or mechanochemical synthesis. With the use of batch reactors for MOF synthesis scale-up, there will be a significant push toward hydrothermal syntheses using water in place of toxic solvents and at lower temperatures and pressures. This has shown success for MOFs such as Al-fumarate and CALF-20 but may prove infeasible for challenging MOF syntheses that require more precise reaction conditions. For example, water may

impact the crystallization kinetics of certain MOFs whose linkers exhibit low solubility or possess incompatible functional groups. Conventional batch processing equipment such as filter presses, agitated stirring tanks, and centrifuges for washing and belt and spray dryers for activation currently exist at scale. However, similar to synthesis, washing techniques will require a shift toward water as opposed to organic solvents to limit the cost and environmental concerns. Finally, postprocessing, such as pelletization, granulation, and extrusion, will be highly application dependent. While equipment at scale also exists here, for example, in the pharmaceutical industry, to shape drug products, more fundamental and applied research into the impacts of these processes on MOF performance will be needed. For example, some MOFs cannot withstand the pressure required during postprocessing and will either undergo conformational changes or amorphize completely.⁴³

With the expansion of applied research and exploration of alternate strategies to synthesize, process, and form MOFs, we will see a reduction in the currently high production costs,⁴⁴ which are likely to mirror those of zeolites and porous carbon materials.

FUTURE PROSPECTS

The future of MOFs is challenging to forecast yet appears promising. In this section, we outline potential advancements in automating the discovery and analysis of MOFs. The forefront of the field is pushing more toward crystal structure prediction (CSP) to determine structures before synthesis, machine learning (ML) approaches coupled with Bayesian optimization to accelerate materials discovery and design, and artificial intelligence to assist researchers to generate models, identify trends, and analyze large bodies of literature.

We also introduce exciting new applications for MOFs in personalized medicine. This approach shifts the paradigm of producing generalized medications for specific diseases to utilize the structural diversity of MOFs to create customized treatments for individual patients and their unique health conditions.

AUTOMATING THE FUTURE OF MOF DISCOVERY

Expediting materials discovery has never been more vital than in the 21st century. Because of the wide structural diversity of possible MOFs, modeling structural and performance-based parameters, machine learning, and artificial intelligence are the next forefront in MOF design and application optimization. Modeling the MOF performance can assist in screening and tailoring design rules for new framework topologies.

A large limiting factor in machine learning approaches for screening of MOFs is the absence of null data, as publications almost exclusively focus on positive results. Herein, we see an opportunity for high-throughput synthesis enabled by autonomous synthesis (Figure 3a) as demonstrated by Aspuru-Guzik and Cooper groups.^{45,46} High-throughput MOF synthesis and characterization allow for unparalleled access to determine phase boundaries and more crystallization parameters, and assist in linking structure property relationships. By integrating machine learning with large data sets of MOF parameters, we can suggest new metal/ligand combinations and predict the performance and structures for many of the applications discussed earlier.⁴⁷

Lastly, the way we do research is constantly evolving, but artificial intelligence can be a powerful tool to more rapidly

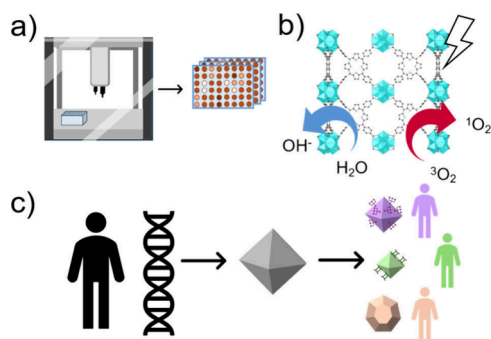


Figure 3. (a) Schematic of high-throughput techniques for automated MOF synthesis. (b) Structure of Hf-containing RiMO-301 (reprinted from Lu et al. with permission from *Nat. Biomed. Eng.* 2018). (c) Illustration of the concept of personalized medicine.

perform literature reviews, summarize broad fields and assist younger researchers to solve their problems faster.^{48,49} Yaghi and co-workers have shown preliminary successes in training specific large language models (LLMs) to assist in summarizing literature and even assisting graduate students in which experiments to pursue next based upon existing MOF literature. In addition, Smit et al. have utilized LLM (Chat GPT 3) as a replacement for ML models and found that the AI approach (Random forest, neural networks, and the Automatminer)⁵⁰ outperforms traditional ML models with far less training.

MEDICINE

In the past few decades, nanoscience and nanotechnology have been rapidly developing in the biomedical space. Nanomaterials, which have been employed for cancer treatments and diagnostics, are advantageous due to their tunable sizes, biocompatibility, and high drug loading. Modifying surface properties has led to the possibility of targeted therapies and personalized medicine.

MOFs have garnered attention for these biomedical applications due to their analogous tunability and availability of void space that may carry drug payloads. The first MOFs proposed for drug delivery were Cr(III)-MIL-100 and MIL-101 by Férey and co-workers,⁵¹ whereby the controlled release of Ibuprofen was monitored. Shortly after, Morris and co-workers identified CPO-27 (MOF-74) as a candidate for NO (nitrous oxide) delivery for vasodilation, capitalizing on high gas storage capacity and open metal sites to deliver payloads.⁵² More recent work from the Morris group developed this technology to make mixed-MOF thin films that allow for sustained delivery of NO using two different mechanisms.⁵³ Spinoff start-up companies, including Zeomedix and MOFgen, were founded with the intent to commercialize this technology.

In the immunotherapy realm, clinical trials for RiMO-301, a nanoscale Hf-based MOF, are ongoing for treatment of head and neck cancer (Figure 3b).⁵⁴ Another area of biomedicine where MOFs are making waves is wound healing. The modular physicochemical properties of MOFs allow for dual antimicrobial activity, with the controlled release of metals, and bioactive agent delivery to promote wound healing and skin regeneration.⁵⁵

The main challenges that MOFs face for biomedical applications involve a lack of understanding of their *in vitro* and *in vivo* toxicity as well as the biodistribution. This issue

becomes increasingly complicated when considering personalized medicine, whereby the unique physicochemical makeup of the individual must be considered when designing nanomaterial properties. Despite this, a seemingly infinite combination of properties is possible within MOFs, which is a convincing platform from which to explore personalized medicine (Figure 3c). By tuning the properties of a particular material, we can tune drug release kinetics, biodistribution, and biorecognition to fit the unique therapeutic needs of an individual. The use of high throughput and machine learning techniques to identify the best candidate MOFs will be of paramount importance and can help in surmounting some of these challenges. The biomedical start-up Vector Biosciences out of the University of Cambridge is one example of a commercial effort to use machine learning to drive the discovery of MOFs for personalized drug delivery.

Following extensive toxicity studies for these materials, we will likely see the ushering of an era in which MOFs are increasingly considered for biosensing, controlled drug release, and targeted immunotherapy for precision theranostics. The future will see MOFs whose properties are tuned for maximum efficacy toward the treatment or diagnosis of the individual.

CONCLUSIONS

Metal–organic frameworks hold promise to address many different challenges faced by society today. Despite their nanosize, the wide array of tunability and functionality allows for seemingly endless possible applications. In this Perspective, we summarize the most promising of these applications in the areas of capture and release, storage, and catalysis. We look to a future where MOFs are used in arid climates to pull the small amount of available humidity from air to provide fresh water sources for at-risk communities. Additionally, we envision future MOFs as capable of not only capturing and storing toxic chemicals or greenhouse gases, such as CO₂, but up-converting them to commodity chemicals. In terms of hydrogen storage for cleaner energy vehicles, we will see MOFs as both means of storage and catalysts for the cycle of LOHCs.

Next, we describe a more distant future in applications of personalized medicine, which heavily relies on the development of automated synthesis and discovery. This builds upon progress of personalized nanomedicine, which is already making waves, whereby the tunability of MOFs is highly advantageous in their exploration for diagnostics and medical treatment tailored to individual patients. Finally, we highlight some of the biggest challenges that the field faces in scale-up and commercialization. Ultimately, the advancement of applied research to bridge gaps between synthesis at the lab and industrial scales, including the reduction of waste, excess solvent, and cost, will be key. The integration of advanced manufacturing techniques, coupled with a deeper understanding of MOF behavior in relevant conditions for their real-world use, will prove critical for driving these materials from the lab to large-scale.

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Notes

The authors declare the following competing financial interest(s): W.M., B.H., and O.K.F. have a financial interest in Numat Technologies, a startup company that is seeking to commercialize MOFs.

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