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Reticular Chemistry: Past, Present, and Future*

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Reticular chemistry—stitching molecular building blocks with strong bonds to produce extended, crystalline, porous frameworks—has enabled a new paradigm in materials design. This article traces the field's evolution from early molecular hosts to the discovery of metal-organic framework (MOF)-5 and an expansive family of MOFs and covalent organic frameworks (COFs) characterized by ultrahigh surface areas and tunable pore chemistry. Selected examples (MOF-808, MOF-303, MOF-LA2-1, COF-999) demonstrate excellent performance in CO_2 capture and atmospheric water harvesting and show great potential for addressing environmental challenges. The article highlights scale-up and commercialization efforts and outlines the "Digital Discovery Cycle," where AI, robotics, and data-driven synthesis accelerate crystallization and screening. The piece concludes by situating reticular materials as promising, scalable solutions for climate challenges and by mapping directions for future research and deployment.

Keywords: Reticular Chemistry; Atmospheric Water Harvesting; CO_2 Capture; AI-assisted Materials Discovery.

I want to share with you my story about chemistry and how it can serve humanity. I went into science because I saw things like this when I was 10 years old, and I was captivated (Figure 1a). I had no idea what they were—I had never seen anything like them before. I opened a book, and there they were, and I just fell in love. My story is about how you can potentially make remarkable things from very unremarkable beginnings. I think that's something you should keep in mind when choosing a field of study: recognize what is pulling you in. As an undergraduate, I took a course in organic chemistry where we crystallized organic compounds—benzoic acid, for example. I crystallized it by adding ether to its solution, and the crystals that form look like snowflakes. When I saw the crystals, I knew I wanted to be a chemist.

When choosing a graduate school, I again followed beauty and my love of molecules. In those days, before the internet, we relied on booklets and leafed through them to learn what different professors were researching. We applied to the universities where we wanted to work with those professors, and this is something I saw (Figure 1b)[1]. I thought, "This is amazing; I would love to learn more and work on this," so I went to meet the professor. If the professor seemed like someone I would enjoy working with, I pursued joining the group. He interviewed well, and I joined his team. He proved to be a demanding mentor—which was exactly what I needed to learn rigorous science—and the experience was invaluable. My first project as a graduate student was to remove a proton from this

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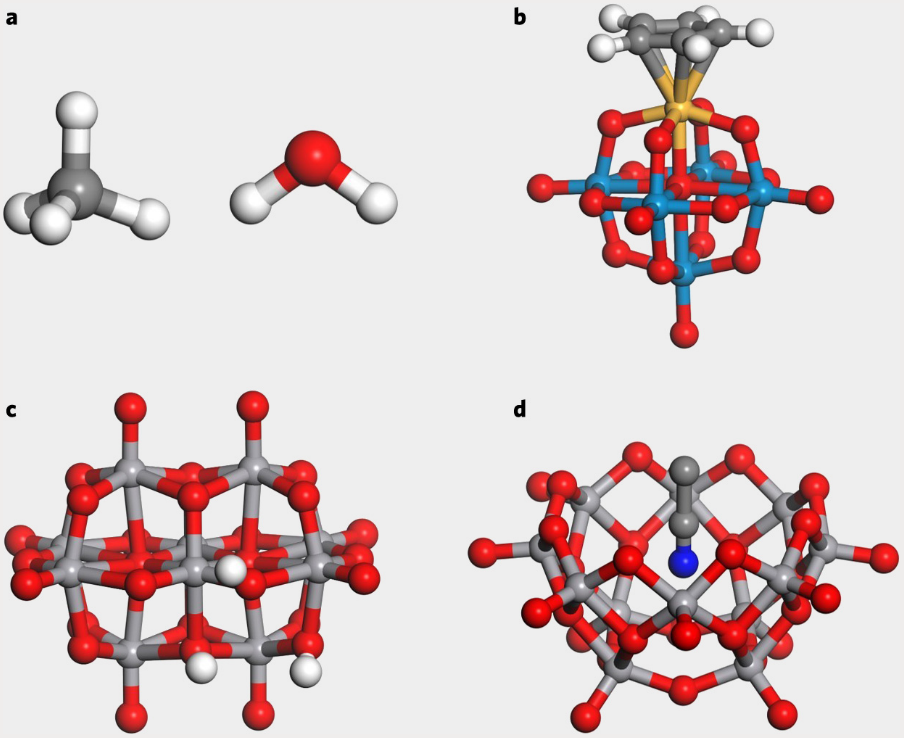


Figure 1. Ball and stick models of (a) CH_4 and H_2O. Color code: O, red; C, grey; H, white; (b) $(\eta^5\text{-}C_5H_5)Ti(Mo_5O_{18})^{3-}$, Color code: Ti, yellow; Mo, blue; O, red; C, grey; H, white; (c) $H_3V_{10}O_{28}^{3-}$, Color code: V, grey; O, red; H, white; (d) $V_{12}O_{32}^{4-}$, with an acetonitrile stick in the middle. Color code: V, light grey; O, red; N, blue; C, dark grey.

$H_3V_{10}O_{28}^{3-}$, which was kind of esoteric (Figure 1c)[2]. The only appealing thing about it was that it made for a nice research project with lots of beautiful colors. I was supposed to deprotonate it—one of the simplest reactions you can do—but it took me a whole year to get it to work. During that time, I walked between buildings to analyze my samples by vanadium NMR. At first the solution was a bright orange, but by the time I reached the NMR, it had turned brown. I turned to a senior postdoc in the group and asked, "What should I do with this?" He said it looked awful and told me to throw it away. I wasn't about to throw away a whole year's work. Instead, I set up a crystallization, and it turned out that the structure was unique: a bowl-shaped compound, reminiscent of a rice bowl, that trapped molecules containing a nitrile group, such as benzonitrile or acetonitrile (Figure 1d)[3]. The nitrile group stuck to the center of the pore, and the structure was selective for nitriles. This bowl-shaped complex was the very first inorganic host–guest complex and was the first soluble molecule that was able to trap other molecules inside it as well. There had been nothing like it before, and that unique complex started a whole new area of vanadate chemistry.

So, I was raised as a molecular chemist, learning about molecules. Chemists have been, over the last 100 years, honing their skills on designing these molecules with great precision. You can make pharmaceuticals and other things out of molecules that are very useful. What I was really interested in is what happens when I shove small molecules closer together and then connect them with strong bonds. I was interested in finding out what kind of things I could make and hoped that they would be beautiful first and foremost. But really, at the fundamental level, I wanted to understand how do I build large structures or extended structures by stitching molecules together in a designed or rational way. That is the question I set up to answer when I became an assistant professor with an independent group. So, my journey up to this point had nothing to do with being highly intellectual in my choice of a problem. It was just the love of doing research and the love of how beautiful molecules are, and I think very often your interest arises from things like this. You do not have to have a necessarily "well-planned" interest.

At this point in my career, I had to become serious because I was on a tenure track, and I needed to do something that would be useful. People used to make extended structures by what was called the "shake and bake" approach. They mixed stuff together, heated them up to a high temperature, and materials were produced. That wasn't satisfactory to me because I wanted to use organic structures that wouldn't survive at high temperatures. So, my question was, how do I take building units that involve organic molecules, which we can functionalize potentially in the future, and make designable materials. The problem was that as you stitch molecules by strong bonds to make these extended structures, the materials you get are usually not crystalline. In my mind, I needed crystals not only because I could wake up every day and enjoy my research but also because we could characterize crystals on the atomic and molecular level. That way, I could certify that I had made that material and then modify it and still be able to characterize it.

What ultimately worked was linking a transition-metal ion to a charged organic linker (Figure 2)[4]. This produced an infinite, layered structure with pyridine—present as part of the reaction conditions—occupying the space between the layers. We were able to remove the pyridine and reinsert it. This was the first time anyone had crystallized a metal–organic complex linked by such strong bonds. We then sought to develop this further and to understand the conditions under which these compounds crystallize.

It is widely known that copper or zinc acetates have a paddlewheel structure, where the core of these molecules is a dimer of metal ions, either copper or zinc that is bridged by carboxylates, referred to as chelation[5]. Our idea was that if the carboxylates are substituted by dicarboxylates, then it would be possible to extend this structure infinitely. Now the key to crystallizing the structure is to make sure that the building units can attach themselves and then break away while they're being crystallized so that any mistakes can be fixed. For example, if molecules approach in the wrong geometry, they can detach and come back and fix correctly. It's like asking a number of people to go out in the field and make a big circle. That doesn't happen instantly, since there will be a lot of holding hands and corrections in positioning. To make such a circle takes time. The kinetics of the reaction must be controlled. If the kinetics is too fast, then too many mistakes are made and there's no time to correct, while if it's too slow, then the material cannot grow to the size that you want. The kinetics mentioned above can be controlled by changing the experimental conditions, and what we did was to take the dicarboxylate, a very common material called terephthalic acid, and a solution of zinc nitrate to conduct a very simple reaction. Under these conditions you can crystallize an extended structure.

Well, how does it work? Who made it work is a student that I met when I was also a student on an internship in China. Later, when I became an assistant professor, he wrote me a handwritten letter that said, I see that you have become a professor at Arizona State University (ASU), and I see that you are making these extended structures. I think I can do a better job than you. I responded, fine, if you can do better than I can, then please come. Later, he came to join our team at ASU. What he did was brilliant, as he was able to slow

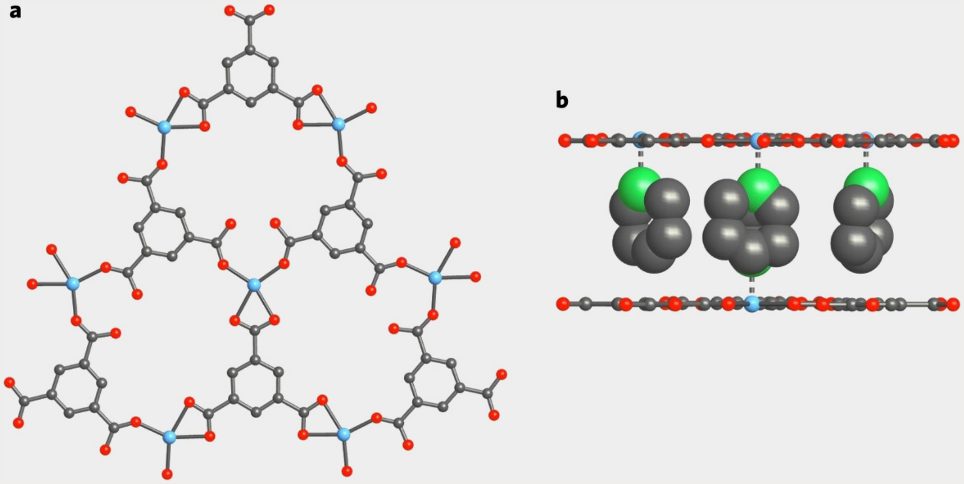


Figure 2. (a) Ball and stick models of a layer of $CoC_6H_3(COOH)_{1/3}(NC_5H_5)_2 \cdot 2/3NC_5H_5$. Co, blue; O, red; C, gray. (b) A perspective drawing of the structure of $CoC_6H_3(COOH)_{1/3}(NC_5H_5)_2 \cdot 2/3NC_5H_5$ perpendicular to the z-axis. Pyridine guest molecules are represented by their space-filling van der Waals radii to show their occupation of the channels within the structure.

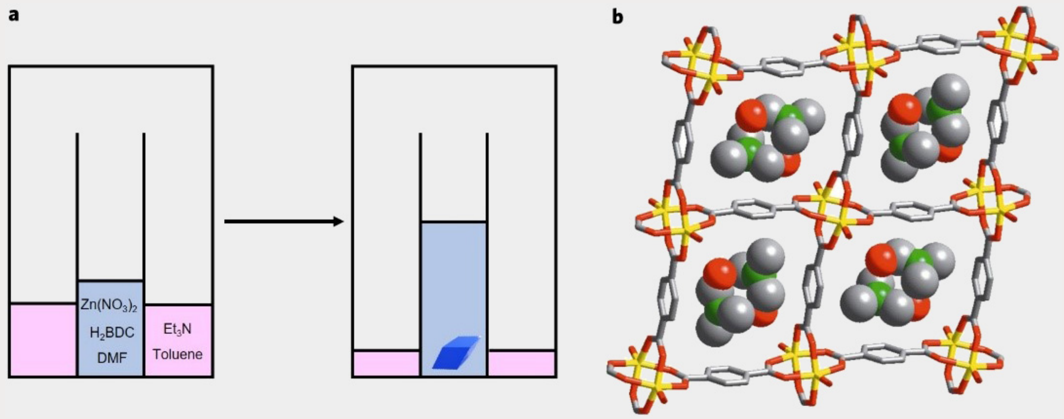


Figure 3. *(a) Schematic of the diffusion-based crystallization setup used to grow MOF-2. (b) A perspective drawing of the structure of MOF-2. Zn, yellow; O, red; C, gray. DMF molecules are represented by their space-filling model. Copyright © 1998 American Chemical Society.*

down the reaction. For the reaction between zinc nitrate and terephthalic acid, the two materials will not react unless the base deprotonates the acid. To slow down the reaction, he diluted the base in toluene and let it slowly diffuse into the reaction system. This image shows how the reaction works (Figure 3a). The inner vial contains a solution of zinc nitrate and terephthalic acid in dimethylformamide (DMF), while the base was diluted by toluene and put in the outer vial. In this way, the base in toluene can diffuse slowly into the inner vial to start the reaction. This was a classic crystallization, a very simple strategy, and it was successful. What we got is a crystal with extended structure, which is exactly what I described before, linked infinitely to make a two-dimensional grid (Figure 3b)[6]. Since terephthalate is a long linker and the cluster itself is large, the resulting framework has enough space to trap the solvent molecules (DMF) present during the reaction. Later we showed that these DMF molecules could be removed and the structure still stands.

If you can do one reaction, you can do the other. It turns out that diethylformamide (DEF), produces very small amounts of diethylamine when heated, which can deprotonate the acid slowly and can make good crystal. This crystal is a primitive cubic made from tetra zinc units. The molecular version of this tetra zinc cluster is called basic zinc acid, which has been known since Bragg's time in the 1920s, and the cluster structure was studied with X-ray crystallography[7,8]. They have been known for a long time in chemistry, but no one had either thought about linking them together or succeeded because of the crystallinity challenge. But here, we now have a three-dimensional structure; it's not layered, but it extends in three dimensions, and this is what it looks like (Figure 4a). The yellow ball indicates the space within which you could trap things, and this is the N_2 isotherm (Figure 4b)[9]. This isotherm shows that nitrogen enters and exits the pores along the same path, indicating that the framework remains open in the absence of any guest molecules. This was truly powerful because up until this point, all porous materials like zeolites were inorganic or porous carbon. Porous carbon is not crystalline, and it can't be functionalized because it's made of carbon and there are no C–H bonds. But here, there were plenty of C–H bonds in our structure, and terephthalate is not the only option. Longer dicarboxylates can be used to expand the pores, and different functionalities can be introduced to make functionalized pores. The surface area for this material was 2,900 m^2/g, which was derived from the nitrogen isotherm. This value was three times that of the most porous carbon at the time and six times that of the most porous zeolite.

For a young assistant professor, this was terrifying because you're actually breaking a thousand-year record of porosity. We verified this result by sending it to an independent company to measure it, and they were getting 2,900, sometimes 3,300. When the paper describing these results came out in 1999, I was invited to give a talk at the German Zeolite Conference. The renowned professors in the front of the auditorium did not believe any of this, but there was somebody in the audience, his name is Ulrich Mueller, who was especially interested in what I had said. Ulrich later revealed that he thought the number for the surface area was so unbelievably high that it had to be a misprint. He was at BAFS and reproduced our work. The result was that they could

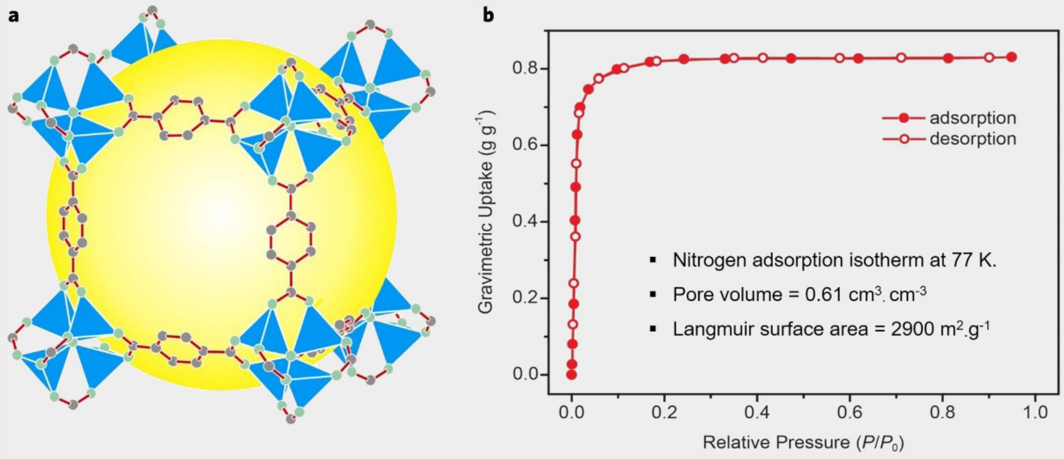


Figure 4. *(a) The MOF-5 structure consists of a cubic array of* $Zn_4O(CO_2)_6$ *units connected by phenylene links. Zn, blue tetrahedron; O, green; C, gray. The large yellow spheres represent the largest sphere that would fit in the cavities. (b)* N_2 *isotherm of MOF-5 measured at 77 K.*

in fact get something even more than 3,300 m^2/g. That marked the beginning of a very productive relationship with BASF, which demonstrated that metal-organic frameworks (MOFs) could be scaled up to multi-ton production. Before this collaboration, we made them at the milligram scale in the lab, and everyone regarded them as boutique materials—that is, not capable of large-scale manufacture. Through our partnership, BASF proved large-scale production was indeed possible, and they now produce at least a dozen MOFs on a multi-ton scale.

This is how MOF chemistry started, and now we can play with it because we know how to put building blocks together—how to stitch them with strong bonds. We are not limited to zinc; we can use almost any metal from the periodic table. We can vary the size and length of the linkers, install different functional groups on the linkers, and tune the connectivity: not just ditopic, but tritopic, tetratopic, and even up to 12-topic linkers. This lets us create many framework topologies beyond the primitive cubic and, above all, to functionalize the pores while precisely controlling their size and geometry. These capabilities opened a vast field, which I call it an "infinite open frontier." More than 10^{100} structures are theoretically possible—effectively limitless—and nearly 100 research groups in each of about 100 countries are working on these materials, studying not only their structures but also applications in clean energy, water treatment, biotechnology, and medicine.

In 2003, we defined this chemistry of linking molecular building blocks by strong bonds to make crystalline extended structures as "Reticular Chemistry." There are three components in this definition that are essential. First, the building blocks, which are the fundamental components of a reticular material. An infinite framework structure is obtained by stitching these building blocks together. Second, strong bonds that connect those building blocks. These strong bonds are especially important as we are aiming to synthesize materials for applications like water harvesting and CO_2 capture from air. These applications demand high chemical stability, so the material can be used repeatedly for years without creating additional waste. Third, the materials need to be crystalline. When we combine these three elements, the materials are achieved, and we call them metal-organic frameworks or MOFs. Meanwhile, we can also construct the framework without metals by stitching just organic compounds together with covalent bonds; these are called covalent organic frameworks (COFs). There is always an "O" in the name, so it becomes a pronounceable word—MOF or COF—instead of spelling out the letters. More recently, the power of this chemistry has been extended to molecular weaving, in which organic threads interlace to form three-dimensional woven structures that are not only porous but also flexible.

The strong bond building block approach has been quite fruitful, and it came about from interest in just designing beautiful structures. I didn't really set out as an assistant professor to solve anybody's problem and was just interested in making beautiful structures and trying to answer intellectual questions: How do I design structures in the way I just described, and why do they have such a high specific surface area? The crystal structure of MOF-5 after the complete removal of guest molecules is shown in

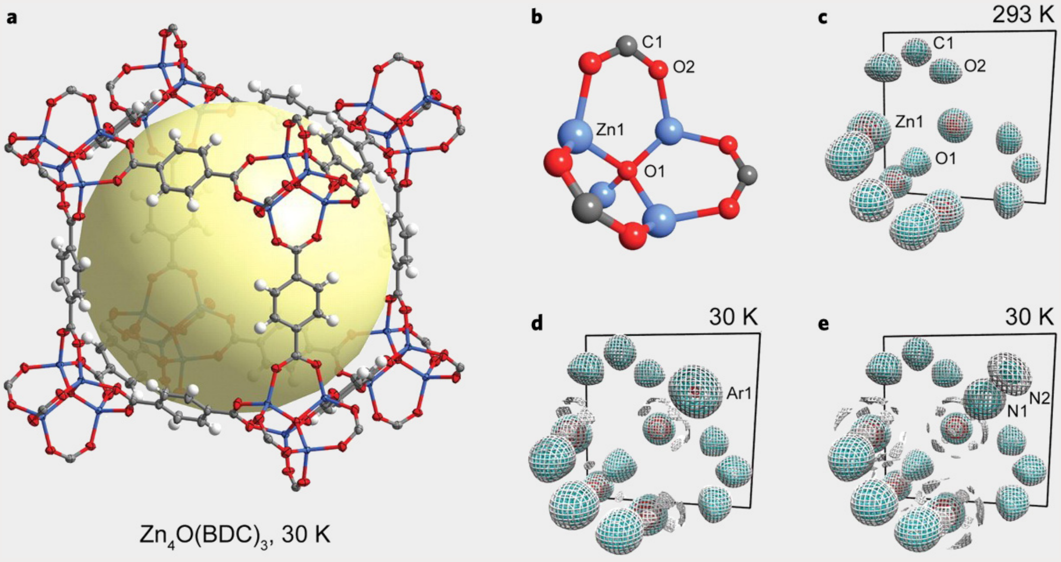


Figure 5. *(a) The MOF-5 structure consists of a cubic array of $Zn_4O(CO_2)_6$ units connected by phenylene links. (C, black; H, white; O, red; and Zn, blue), which define large pseudo cubic pores that can be completely evacuated. The yellow sphere represents the largest sphere that can occupy the pore without contacting the van der Waals surface of the framework. (b) A magnification of the corner of the pore schematically shows the location of adsorption site $\alpha(CO_2)_3$, located equidistant to the three carboxylates. (c) The corresponding three-dimensional electron density map of this site, determined from single-crystal XRD data obtained at 293 K from crystals loaded under either N_2 or Ar. At 30 K, regions of electron density assigned to adsorbed (d) Ar or (e) N_2 become prominent. Reprinted with permission from Ref. 10, Copyright © 2005, American Association for the Advancement of Science.*

Figure 5a–5c, allowing us to view the empty framework[10]. To understand why it has a high surface area, we determined where these gas molecules reside in the structure, because the positions they occupy represent the accessible surface onto which gas molecules can bind and therefore determine the overall surface area. The electron density of guest molecules, either nitrogen or argon, can be clearly identified from a single X-ray crystal diffraction pattern when the corresponding gases are introduced into the MOF pores at 30 K (Figure 5d and 5e). From the diffraction data, eight symmetry-independent adsorptive sites are identified. It turns out that not only the metal clusters act as adsorption sites, but the organic linkers—their faces and edges—do as well. In MOF-5, nearly every atom in the framework functions as an adsorption site, which explains its extraordinarily high specific surface area. I always try to think and view things from a different perspective. Let's say there is a grain of sand. If we manage to expose every atom in that grain, it would have an extraordinarily high surface area, because every atom would effectively become part of the surface. The moral of the MOFs story is that by building a scaffolding-like framework, you create a structure in which almost every atom can act as an adsorption site—and that is why MOFs exhibit such extremely high surface areas.

Here is another example of an MOF designed for ultrahigh surface area (Figure 6)[11]. The metal–oxide units (shown in pink) are linked by organic linkers. Note that a trigonal linker is used here, which provides many exposed faces and edges. The structure is porous, but the pores lack walls—the framework acts as a scaffold that maximally exposes the atoms, which explains its exceptionally high surface area. A gram of this material, no bigger than a coin, has the surface area of an entire football field—that's the real estate available for storing gases. You can imagine how exciting that is for tackling climate and related problems. When people discuss environmental problems, climate issues caused by carbon dioxide are at the forefront, and MOFs are ideally suited to serve as platforms for capturing CO_2.

The increasing concentration of CO_2 in the atmosphere causes global warming and is making our weather patterns more severe. This illustration represents a study of 153 events of natural disasters, including land heatwaves, ocean heatwaves, wildfires, and so on, and the great majority of them have been more severe than the average (Figure 7)[12]. In Malibu

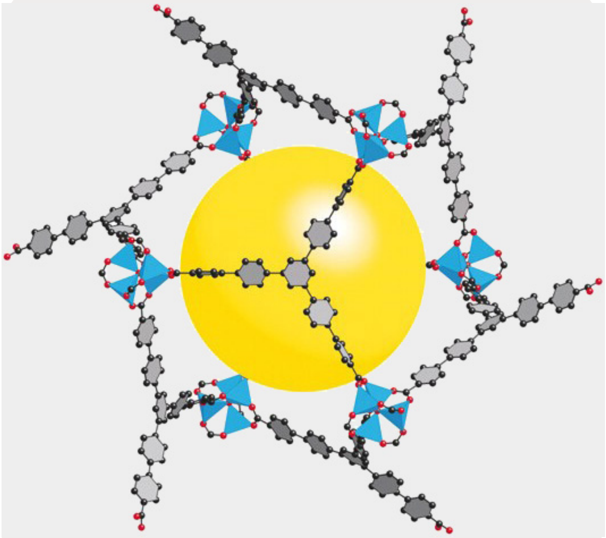


Figure 6. The MOF-200 structure consists of a cubic array of $Zn_4O(CO_2)_6$ units joined with 4, 4′, 4″-[benzene-1,3,5-triyl-tris(benzene-4,1-diyl)]tribenzoate (BBC). The yellow ball is placed in the structure for clarity and to indicate space in the cage. Zn, blue, tetrahedral; O, red; and C, black. Hydrogen atoms are omitted for clarity. Reprinted with permission from Ref. 11, Copyright © 2010, American Association for the Advancement of Science.

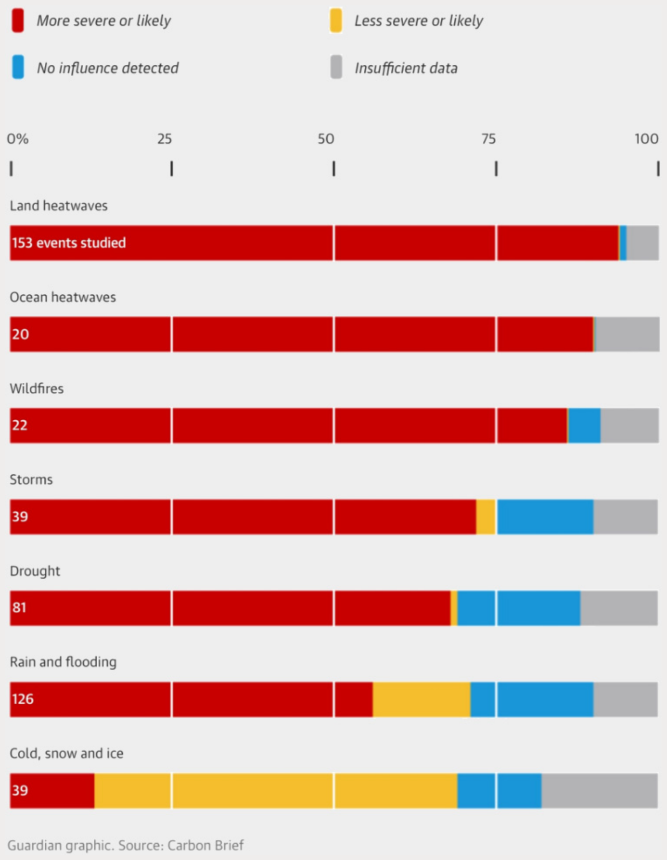
in 2018, roughly one quarter of the city burned, and in 2022, 4.3 million acres burned across California. Water is another pressing problem. For example, the water levels of Hoover Dam kept decreasing in the recent 40 years. I recently visited the dam and observed a very low water level, which is alarming because the reservoir supplies nearly 20 million people with water. All of the above environmental crises are closely linked to the rapid rise in atmospheric CO_2 concentrations, which has driven global warming, worsened droughts, and triggered a cascade of related environmental problems.

Therefore, we design and synthesize reticular materials for carbon capture, in particular carbon capture from air, which is a more difficult problem than that from flue gas. If the material takes CO_2 from air where its concentration is about 400 ppm, it will work better in a power plant, where CO_2 concentration is much higher (4% or 15%), to prevent CO_2 from going into the air. In simple terms, a carbon dioxide capture system works like this: adsorbent material is loaded into the device; air enters from one side, carbon dioxide is removed as the air passes through the adsorbent, and carbon-dioxide-free air exits the other side. The requirements for practical carbon-capture materials are demanding. First, materials must exhibit high selectivity for CO_2 over other gases in mixed streams (e.g., N_2, O_2, H_2O, and trace contaminants) to enable efficient capture from air or flue gas. Second, they must be chemically robust—displaying both hydrolytic stability in humid environments and oxidative stability in the presence of O_2, and other reactive species—to retain performance under real operating conditions. Third, long-term cyclability is essential: the sorbent should preserve capacity and kinetics over many adsorption–desorption cycles (effectively years of operation) without significant degradation. Fourth, low regeneration energy is required so that captured CO_2 can be released with minimal energetic penalty. Finally, the synthesis and processing routes must be scalable and cost-effective, permitting manufacture at a multi-ton scale for meaningful deployment. There are lots of materials coming to our mind, like aqueous amines and metal hydroxides, but unfortunately, none of them meet all the above criteria. Here, I'll show you how reticular materials, both MOFs and COFs, can potentially solve this CO_2 problem.

Here is an MOF, which is called MOF-808. MOF-808 is made from zinc oxide units that are linked by trimesic acid. To enhance its CO_2 capture performance, glycine units, which contains -NH_2 groups as CO_2 adsorption sites, are functionalized in pores of MOF-808 (Figure 8a)[13]. We study the CO_2 capture mechanism in MOF-808 pores using solid-state NMR. It turns out that under dry conditions the dominant products are carbamates, whereas in the presence of water the equilibrium shifts toward carbamic acid and bicarbonate (Figure 8b). Based on this mechanism, two amine groups are required to capture one CO_2 molecule under dry conditions, while in humid conditions the stoichiometry becomes one amine per CO_2, meaning the theoretical CO_2 uptake can be doubled in a humid atmosphere.

How does MOF-808 perform in air, where CO_2 concentration is as low as 400 ppm? Here is the result (Figure 9)[14]. When air flows through the material, the downstream CO_2 concentration drops down to zero, indicating all CO_2 contained in the air is adsorbed. The carbon dioxide adsorption capacity of MOF-808 increases with relative humidity (RH), reaching $1.205\ \mathrm{mmol} \cdot \mathrm{g}^{-1}$ under 50% RH, which would exceed the required capacity if the material could sustain ~100,000 cycles. In the present experiments, however, the material could not be cycled more than ~500 times: although it is stable in water and acid, it is not stable under basic conditions.

To address this stability issue, we turn to COFs. Since 2005, continuous efforts have aimed to synthesize



Guardian graphic. Source: Carbon Brief

Figure 7. *Event-attribution results for natural hazards showing the proportion of studies reporting that human-induced climate change has made impacts more severe or likely (red), less severe or likely (yellow), no influence detected (blue), or where data are insufficient (grey). Source: Carbon Brief.*

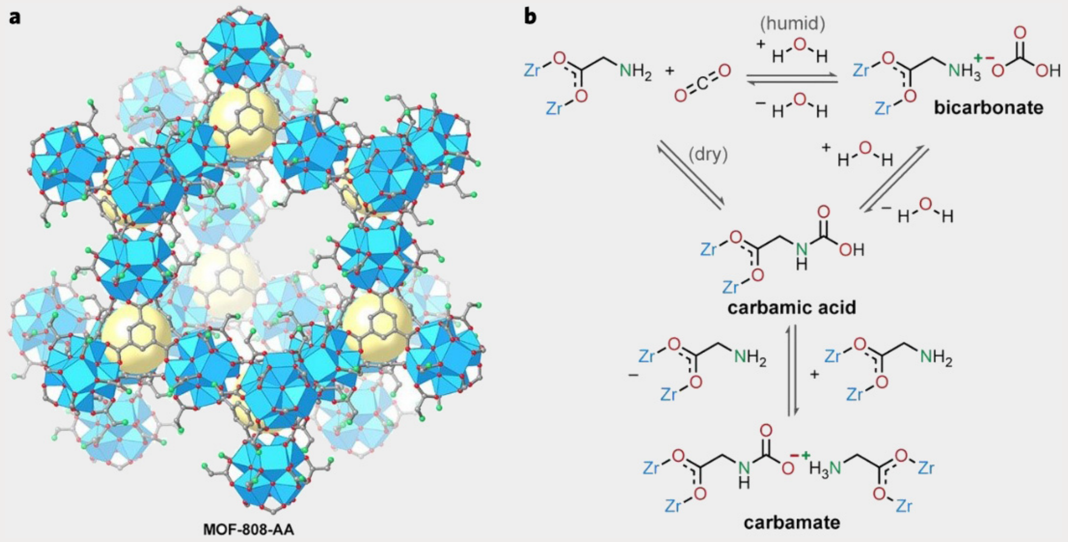


Figure 8. *(a) Structure of MOF-808-AA. Zr atoms are represented as light blue polyhedra, while other atoms are represented as spheres. C, gray; O, red; N, green. H atoms are omitted, and the yellow spheres highlight the small tetrahedral pores for clarity. (b) Proposed CO_2 adsorption mechanism of MOF-808-AA. Reprinted with permission from Ref. 13, Copyright © 2022 American Chemical Society.*

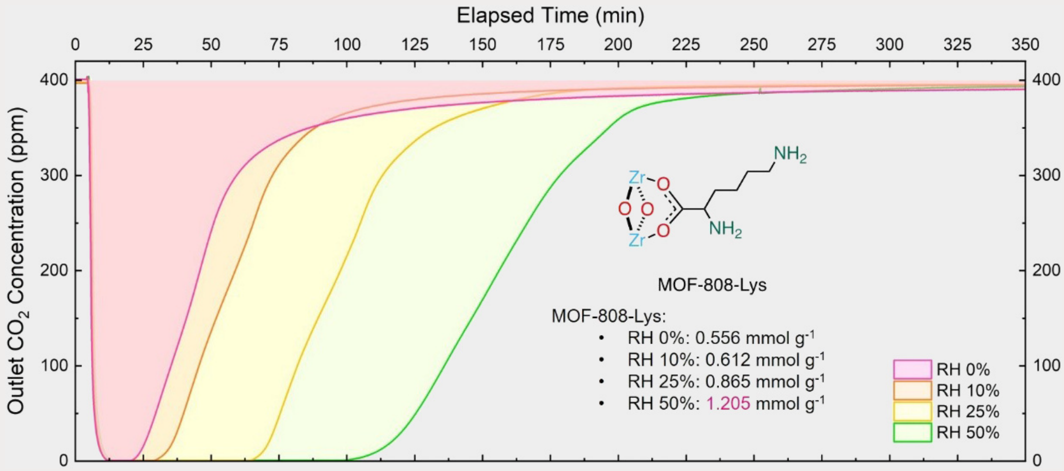


Figure 9. *Dynamic breakthrough measurements at 25°C with 0, 10, 25, and 50% RH for (a) MOF-808-Lys. In the plot of the outlet CO_2 concentration, the CO_2 uptake can be derived through numerical integration of the marked area. Reprinted with permission from Ref. 14, Copyright © 2024 American Chemical Society.*

robust COFs. Today we can crystallize COFs with carbon–carbon and carbon–nitrogen linkages, among the strongest bonds in chemistry. One example is COF-701, reported by our group in 2019 (Figure 10)[15]. COF-701 exhibits exceptional chemical stability under extreme conditions, including concentrated HCl, saturated KOH, and even highly corrosive reagents such as n-butyllithium. Such stability is precisely what is required for materials intended for long-term use in power plant environments. In 2024 we achieved a breakthrough in direct air capture (DAC) using COFs. We developed a material, COF-999, which increased the CO_2 adsorption capacity to 2.05 mmol $\cdot$ g^{-1} and retained this capacity over extended cycling[16]. We subjected COF-999 to a 20-day cycling test using ambient air from Berkeley to simulate real-world conditions. Over the 20-day period the material's uptake varied with changes in RH, and on the first and last days—when RH was the same—the CO_2 adsorption capacity was essentially identical, demonstrating excellent cycling stability (Figure 11). Based on these results, we believe COF-999 is a promising candidate for DAC of CO_2. In the area of CO_2 capture from flue gas, a colleague of mine at the University of Calgary has developed a MOF with a CO_2 capacity of 2–4 mmol $\cdot$ g^{-1} that, since 2021, has been cycled more than 450,000 times[17]. Although it is not suitable for DAC, it performs well with high-CO_2 flue streams and has already been commercialized for that application. BASF has announced to scale this material up to several hundred tons per year, and it is currently in use at multiple cement plants in Canada.

The next thing that I want to discuss in detail is water. This image shows projected water stress through 2040 (Figure 12)[18]. By 2040, even regions we now consider humid are expected to face water stress because of excessive groundwater extraction and resulting shortages of clean water. Materials that can harvest water from air—especially at low RH in arid regions—could help alleviate this crisis. Note that even if every person on Earth were given 50 L of water, the total would still represent less than 1% of the moisture in the atmosphere. The challenge is that extracting water from air at low RH is energy intensive. For example, in a city at 30°C with 20% RH, directly condensing water from the air requires cooling the air to about 4°C, which consumes a great deal of energy. Our idea is to synthesize an MOF that adsorbs and concentrates water from arid air into its pores. The MOF is then placed in an enclosed box and exposed to sunlight; as the box warms, the MOF releases the stored water, which then condenses. Because the MOF concentrates water in its pores, releasing it requires much less energy than directly condensing water from arid air. In this example, releasing the water from the MOF requires only a temperature change on the order of 4°C (Figure 13)[19].

MOF-303 is one of the representative materials we developed for water harvesting. It was characterized by single-crystal X-ray diffraction, which provided the atomic positions of every atom in the unit cell. MOF-303 is built from rod-like aluminum-oxide secondary building units together with aligned pyrazolate linkers; these components generate pores lined with alternating hydrophilic and hydrophobic pockets. When water

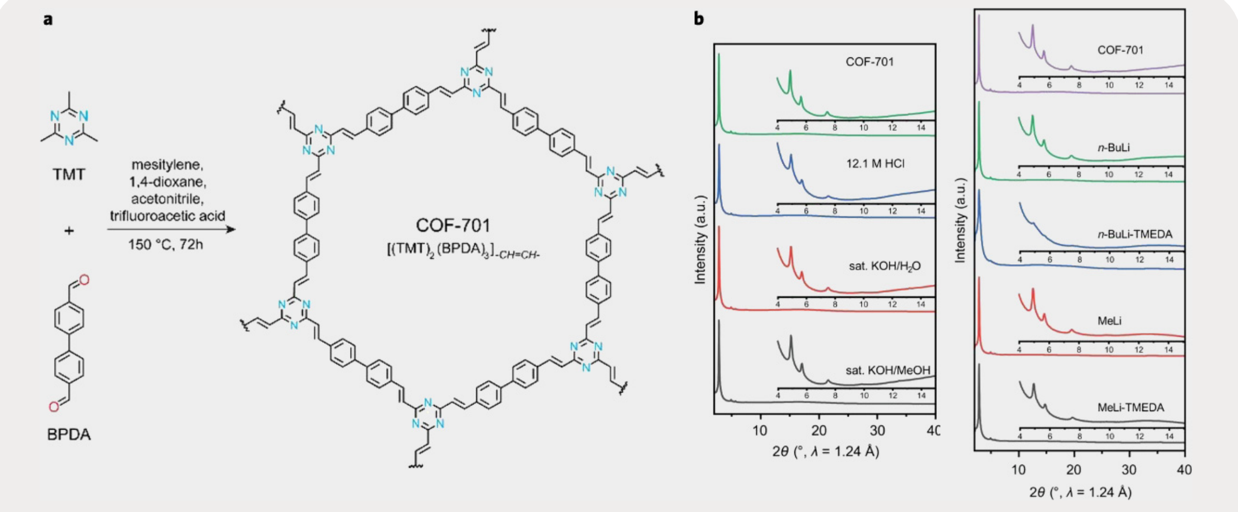


Figure 10. (a) Synthesis of COF-701 by Aldol Condensation between TMT and BPDA. (b) Chemical stability test of COF-701 with Brønsted acid and base and organolithium reagents. WAXS patterns of treated materials with zoomed insets. Reprinted with permission from reference 15, Copyright © 2019 American Chemical Society.

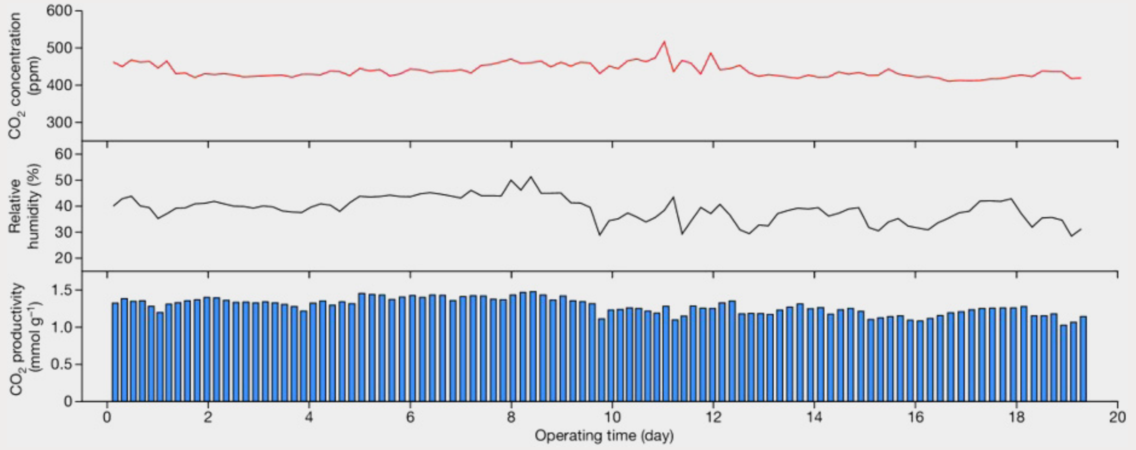


Figure 11. CO_2 capture productivity of COF-999 after each adsorption cycle (blue), corresponding ambient outdoor CO_2 concentration (red) and RH (black). All data were measured for 20 continuous days of operation using outdoor air. Reprinted with permission from Ref. 16, Copyright © 2024, Springer Nature.

molecules move through the pores and encounter this grid of hydrophilic and hydrophobic pockets, the first molecules occupy the hydrophilic sites; once those sites are saturated, additional water bridges the hydrophobic pockets via hydrogen bonding (Figure 14)[20]. To release the captured water, the MOF can be exposed to sunlight so that heating drives desorption (passive water harvester), or it can be regenerated electrically (active water harvester). Our first generation of water harvester is an electrified device—you plug it in, air enters through an inlet and passes over the MOF, which adsorbs water. When the MOF is heated, the released water condenses and is collected at the bottom as ultra-pure water. The device is about the size of a small microwave oven and contains only 200 g of MOF, yet it can produce 5 L of water per day. The MOF is designed to last for the lifetime of the electronics (about 5–6 years). We tested the product water: it contains no detectable metals or organic contaminants and is therefore very pure. In addition, we are developing and testing multiple prototypes. One design, which is called "rain in a box," works on the same principle as the

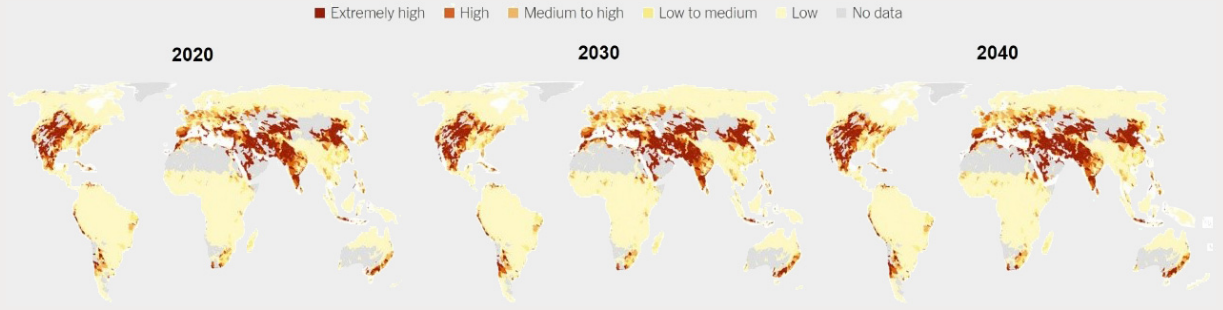


Figure 12. Projected water stress through 2040. Source: New York Times.

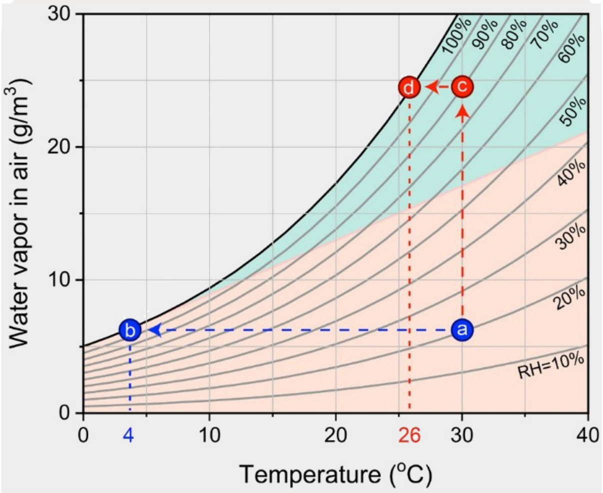


Figure 13. Modified psychrometric chart illustrating how air of low RH (a), must be cooled to low temperature (b) to be saturated with water (i.e., dew point), while at high RH (c) such cooling is minimal (d). The use of MOFs essentially takes low RH air (a) and makes it high RH (c) and thus saturates desert air with water more efficiently than direct cooling. The green region is where direct cooling may be used to generate water from air, but not in the pink region, where MOFs are ideally suited to turn desert air of lower levels of moisture into "tropical air." Reprinted with permission from Ref. 19, Copyright © 2020 American Chemical Society.

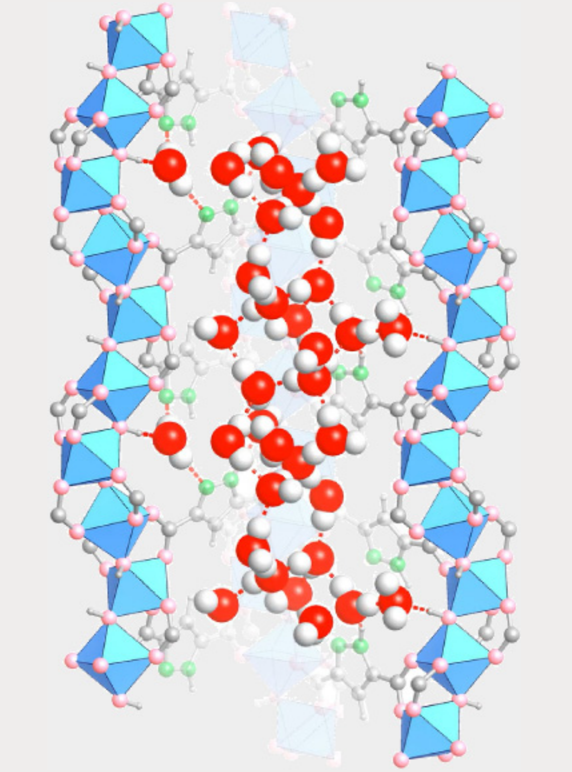


Figure 14. H_2O binding structures in MOF-303. O, red; N, green; C, gray; Al, blue octahedron. Hydrogen bonding is illustrated in a red dotted line. Reprinted with permission from Ref. 20, Copyright © 2021, American Association for the Advancement of Science.

electrified device but is intended to deliver even more water—in this case you can actually see rain forming and water being collected.

Students testing these prototypes even traveled to Death Valley to demonstrate that the MOF performs under extreme conditions. The MOF was packed in a "pancake" configuration: at night the device is opened so water in the air can saturate the MOF, and during the day the device is closed and the MOF is warmed up by sunlight, releasing water that then condenses and is collected—without any external energy input (Figure 15)[21]. With one ton of MOF operated passively in this way, about 2,250 L of water can be collected per day; if the system is operated actively (electrically driven), the yield can reach

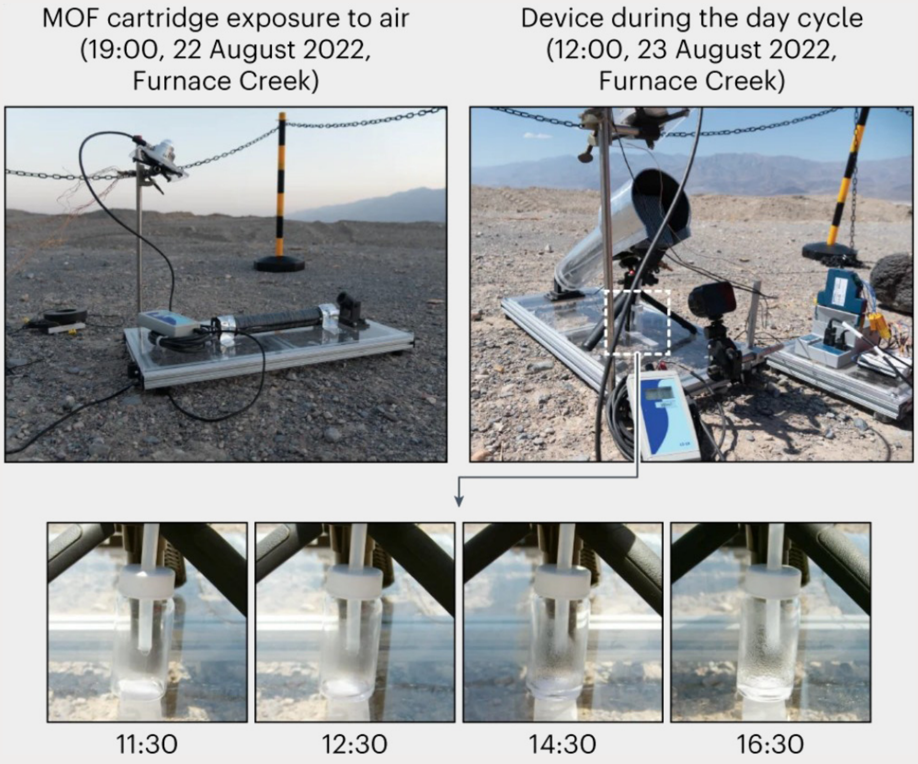


Figure 15. Photographs of the device setup, including the power station (500 Wh), pyranometer and data acquisition (DAQ) systems, and water collected at different times during the 10th June test in Death Valley. Reprinted with permission from Ref. 16, Copyright © 2023, Springer Nature.

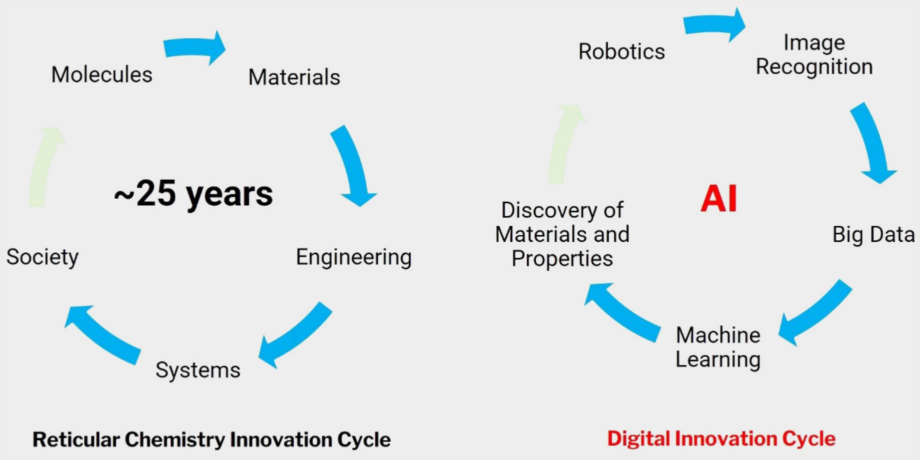


Figure 16. The illustration of AI-assisted “Digital Innovation cycle.”

roughly 25,000 L per day. The latest version of the device is about the size of a small refrigerator and delivers 22 L per day while consuming less than 0.4 kWh per day. That energy use corresponds to an approximate cost of \$0.12 in California and about \$0.06 in Texas. The device can already harvest water from air at very low cost, and we are continuing to optimize the system. Our latest-generation MOF for water harvesting is called MOF-LA2-1. Compared with MOF-303, extending the organic linker by two carbon atoms increases water uptake by approximately 50%[22]. The modified linkers create a more hydrophobic pore environment, allowing adsorbed water to be released at lower temperatures and thus making the whole process more energy-efficient.

Next, I will describe our work with AI. In the case of MOFs, it took roughly thirty years to progress from molecules to materials and finally to engineered devices, and they are now nearing commercial implementation. For example, as I have mentioned above, a colleague of mine in Canada is already employing an MOF material in a cement plant. Can AI accelerate commercialization? There is no reason it cannot. We are developing an alternative workflow, which we call the "Digital Innovation Cycle" or "Digital Discovery Cycle"—that leverages robotics and image-recognition systems driven by machine learning to generate large datasets, apply machine-learning analyses, and identify the experimental conditions likely to yield the next generation of materials (Figure 16). By following the Digital Discovery Cycle, we can produce materials that were not previously obvious—at least to me—indicating that AI is contributing novel insights. In the meantime, we have initiated experiments with ChatGPT, using simple conversational prompts to train it for tasks such as text mining, image mining, research supervision, molecular editing, and other research-group–level functions. To date, these activities have been conducted in collaboration with human researchers. We collected 250 papers describing MOF syntheses and trained ChatGPT to extract synthesis parameters—starting materials, solvents, temperatures, and other routine details. The system completed this extraction in under 2 weeks, while performing the same task manually would likely have required several months. This approach is promising because it puts all the facts in front of the researcher. As a result, decisions can be made based on facts rather than solely on chemical intuition, which is fallible and not always evidence-based.

One project we are pursuing with ChatGPT aims to accelerate the synthesis and crystallization of new MOFs and COFs. In the water-harvesting example noted above, I showed that adding two carbon atoms to the organic linker increased the MOF's water uptake by 50%. The idea itself is straightforward, but demonstrating it requires first synthesizing and crystallizing the modified MOF. Even the most talented students can take a long time to obtain crystals because they explore a limited reaction space guided by intuition and experience. Using ChatGPT, however, a wider reaction space was scanned, and students were able to crystallize the MOF in under 2 weeks[23]. This improvement in efficiency is substantial, and currently I assign almost 50% of my group to work on AI/ChatGPT. In addition to helping us synthesize new MOFs and COFs, we can train ChatGPT to review the literature and pose intelligent, multistep questions—and to provide not only the questions but also the answers.

To conclude, we have achieved atomic and molecular-level precision in extended, periodic two- and three-dimensional structures—an advance I hope will contribute to solving the climate problem. I believe AI for reticular chemistry is not only an important first step in engaging emerging scholars with research but also reduces barriers for scholars worldwide to participate in the field.

PUBLISHER'S NOTE

An amendment has been made to the last name of the second author due to an oversight on the authors' part. It has been updated on 24 October 2025.

CONFLICT OF INTEREST

The authors declare no competing interests.

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