

REVIEW



Reticular materials for sustainability: Advances in MOFs and COFs for carbon capture and water harvesting

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ABSTRACT

The urgent need to mitigate climate change and address freshwater scarcity has intensified research into advanced porous materials capable of capturing greenhouse gases and harvesting atmospheric water. Among these, reticular materials particularly Metal–Organic Frameworks (MOFs) and Covalent Organic Frameworks (COFs) have emerged as leading candidates due to their high surface area, tunable porosity, and chemical versatility. This review explores the structural foundations and functional differences between MOFs and COFs, comparing their performance in environmental sustainability applications. Special emphasis is given to their roles in carbon dioxide adsorption and atmospheric water harvesting, including insights into adsorption mechanisms, functionalization strategies, and real-world implementation. Moreover, recent advances in hybrid material design, AI-assisted material discovery, and the integration of these frameworks into scalable devices are discussed. Challenges related to synthesis scalability, cost, and long-term stability are also critically evaluated. Finally, the article highlights future research directions and the expanding potential of MOFs and COFs in other green technologies such as catalysis and solar fuels. Collectively, this review positions MOFs and COFs as transformative tools for a sustainable future, offering viable solutions to some of the most pressing environmental challenges.

KEYWORDS

Metal organic frameworks (MOFs); Covalent organic frameworks (COFs); Carbon capture; Atmospheric water harvesting

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Introduction

In order to maintain environmental sustainability, creative solutions are required to address the growing problems of resource scarcity and climate change. Significantly contributing to global warming and its related effects, including rising sea levels, extreme weather events, and biodiversity loss, are anthropogenic activities, especially the excessive use of fossil fuels, which have resulted in previously unheard-of levels of greenhouse gas emissions, most notably carbon dioxide (CO₂) [1].

At the same time, overuse, pollution, and shifting precipitation patterns are reducing the amount of clean water resources available. According to recent studies, drylands now make up around 40% of the planet's geographical area, which exacerbates water scarcity and jeopardizes agricultural output. The scientific community has been investigating cutting-edge materials that can alleviate resource constraints and mitigate the consequences of climate change in response to these environmental challenges [2]. These include reticular materials, particularly Covalent Organic Frameworks (COFs) and Metal–Organic Frameworks (MOFs), which have attracted a lot of interest. These crystalline, porous materials are perfect for gas adsorption, separation, and storage because of their high surface areas, adjustable pore sizes, and functionalized architectures [3].

Because of their robust adsorption capabilities and adaptable pore settings, metal-organic frameworks (MOFs), which are made of metal ions or clusters linked to organic

ligands, have exceptional adaptability in collecting CO₂. Because COFs are made up of just light components connected by covalent bonds, they have remarkable chemical and thermal durability as well as structural regularity, which makes gas storage and separation procedures more effective. Beyond carbon capture, these reticular materials have shown promise in water harvesting applications. Their ability to adsorb water vapor from the atmosphere and release it upon mild heating presents a sustainable approach to addressing water scarcity, particularly in arid regions [3,4].

This review aims to provide a comprehensive overview of the recent advancements in the design, synthesis, and application of MOFs and COFs for environmental sustainability. Emphasis will be placed on their roles in carbon capture and water harvesting, highlighting the underlying mechanisms, performance metrics, and potential for real-world implementation. By elucidating the capabilities and challenges associated with these materials, this article seeks to inform future research directions and promote the development of effective strategies to combat climate change and resource scarcity [5].

Overview of Reticular Materials: MOFs and COFs

Reticular materials, especially Metal–Organic Frameworks (MOFs) and Covalent Organic Frameworks (COFs), have gained substantial attention due to their unusual structures and properties, making them promising candidates for applications in storage of gases, separation, and environmental remediation [6].

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MOFs are crystalline materials formed by the coordination of metal ions or clusters with organic ligands, resulting in extended three-dimensional networks. The metal nodes, often referred to as secondary building units (SBUs), and the organic linkers can be systematically varied, allowing for precise control over the framework's topology and functionality. This modularity enables the design of MOFs with tailored pore sizes and chemical environments. In contrast, COFs are entirely organic crystalline materials constructed through the covalent bonding of light elements such as carbon, hydrogen, boron, nitrogen, and oxygen. The strong covalent bonds confer high thermal and chemical stability to COFs. Their structures can be designed in two or three dimensions, offering tunable porosity and functionality. Schematic illustration comparing their topologies is shown in (Figure 1) [7].

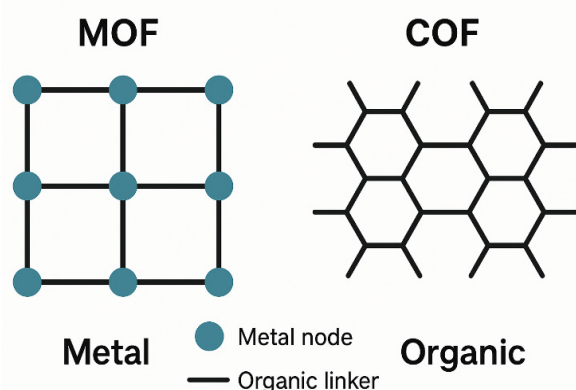


Figure 1. Visual comparison of MOFs (metal nodes + linkers) and COFs (entirely organic) frameworks.

Properties

Both MOFs and COFs exhibit exceptional porosity and surface areas. MOFs have reported surface areas ranging from 1,000 to 10,000 m²/g, depending on their specific structure and composition. COFs also demonstrate high surface areas, with some 2D COFs exceeding 2,500 m²/g and 3D COFs reaching over 4,000 m²/g [7,8].

The stability of these materials is a critical factor for practical applications. MOFs, while structurally versatile, can be sensitive to moisture and certain chemical environments due to the nature of their metal-ligand coordination bonds. However, advancements in MOF design have led to more robust frameworks capable of withstanding harsh conditions. COFs, with their covalent linkages, generally exhibit superior thermal and chemical stability, maintaining their structural integrity in various solvents and across a wide pH range [9].

Comparative analysis

While both MOFs and COFs offer high porosity and tunable structures, their differences lie in composition and stability. MOFs, containing metal nodes, often provide active sites beneficial for catalysis and gas adsorption but may suffer from lower stability in aqueous or acidic environments. COFs, being metal-free, offer enhanced stability and are less prone to

degradation under similar conditions. However, the absence of metal centres in COFs can limit their catalytic activity, which can be addressed by incorporating functional groups or metal complexes into the framework. Therefore, MOFs and COFs are complementary materials in the realm of porous frameworks. Their distinct structures and properties make them suitable for a range of applications, and ongoing research continues to explore their potential in environmental sustainability efforts and highlighting the tunability and scalability aspects of both systems (Table 1) [10,11].

Table 1. Comparison of key features between MOFs and COFs including building blocks, porosity, and application domains.

Feature	MOFs	COFs
Building Units	Metal nodes + organic linkers	Fully organic linkers
Porosity	High	Very high
Thermal Stability	Moderate	High
Tunability	Excellent	Moderate to Excellent
Scalability	Emerging	Challenging
Key Applications	Gas storage, separation, catalysis	Water harvesting, sensing, electronics

MOFs and COFs for Carbon Capture

Mechanism of CO₂ adsorption

Because of their high surface areas, tunable porosity, and functional versatility, reticular materials metal-organic frameworks (MOFs) and covalent organic frameworks (COFs) in particular have emerged as promising candidates for effective capture technologies in response to the increasing concentration of atmospheric carbon dioxide (CO₂). MOFs and COFs primarily capture CO₂ through physisorption, which involves weak van der Waals forces, but their structures can be engineered to enhance interactions with CO₂ molecules [12].

In MOFs, the presence of open metal sites (OMSs) facilitates stronger interactions with CO₂. For instance, the activation of MOFs by removing coordinated solvent molecules exposes OMSs, which act as Lewis's acid sites, enhancing CO₂ adsorption through electrostatic interactions. A study on a cobalt-based MOF, DZU-6, demonstrated that the introduction of OMSs increased CO₂ capacity by over 40% compared to its non-activated counterpart [13].

COFs, being entirely organic, rely on the incorporation of functional groups to enhance CO₂ affinity. Recent research introduced metal ion-doped Schiff-base COFs, where CO₂ molecules insert between the metal ion and the nitrogen atom of the imine bond, resulting in improved CO₂ sorption capacity [13].

Functionalization and selectivity

Functionalization of MOFs and COFs is pivotal in enhancing CO₂ selectivity and capacity. Amine-functionalized MOFs have shown remarkable improvements in CO₂ capture. For example, Mg₂(dobpdc) functionalized with diamines exhibited step-shaped adsorption isotherms and high CO₂ uptake, even in the presence of water vapor. Similarly, amine-modified ZIF-8 demonstrated enhanced CO₂ capture capacity, highlighting the

potential of simple functionalization techniques [14,15].

In COFs, the integration of specific functional sites into the pore walls allows for customized interfaces for CO₂ capture. For instance, the incorporation of nitrogen-containing groups enhances interactions with CO₂ molecules, improving adsorption capacity [15]. Several MOFs have been identified for their exceptional CO₂ capture capabilities. CALF-20, composed of zinc ions coordinated with triazolate and oxalate ligands, exhibits selective CO₂ adsorption over water and maintains stability under harsh conditions, making it suitable for industrial applications. UiO-66, with its zirconium-based framework, offers exceptional chemical and thermal stability, making it versatile for gas storage and separation [16].

In the realm of COFs, COF-999 stands out for its efficient CO₂ capture from ambient air. Its structure, featuring olefin linkages and post-synthetically modified with covalently attached amine initiators, allows for high CO₂ adsorption capacity and stability over multiple cycles [14,16].

Industrial relevance and examples

The practical application of MOFs and COFs in industrial CO₂ capture is gaining momentum. CALF-20 has demonstrated exceptional stability under conditions mimicking industrial flue gases, including exposure to steam and wet acid gases, positioning it as a promising material for large-scale CO₂ capture.

Furthermore, the scalability and robustness of these materials are being explored for integration into existing carbon capture systems and underscoring the urgency for carbon capture technologies (Figure 2). The tunable nature of MOFs and COFs allows for customization to specific industrial requirements, enhancing their applicability in various sectors, including cement production and power generation. In summary, the advancements in the design and functionalization of MOFs and COFs have significantly enhanced their CO₂ capture capabilities. Their structural versatility, combined with high selectivity and stability, underscores their potential as viable solutions for mitigating CO₂ emissions in industrial settings [17].

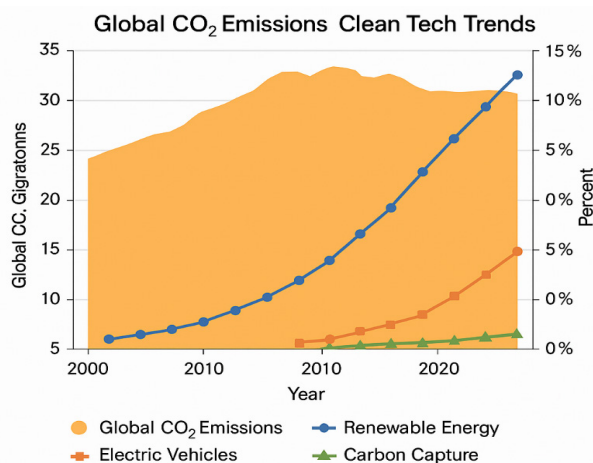


Figure 2. Trends in CO₂ emissions alongside adoption of renewables, EVs, and CCS technologies.
(Data Source: Compiled from IPCC and IEA reports).

MOFs and COFs for Water Harvesting

The escalating global demand for clean water has intensified research into innovative solutions for water scarcity. Atmospheric Water Harvesting (AWH) emerges as a promising approach, leveraging materials capable of adsorbing water vapor from the air and releasing it upon mild heating. Among these materials, Metal Organic Frameworks (MOFs) and Covalent Organic Frameworks (COFs) have garnered significant attention due to their tunable porosity, high surface areas, and functional versatility [18].

Atmospheric water harvesting

AWH operates on the principle of adsorption-desorption cycles. During the adsorption phase, porous materials capture water molecules from ambient air. Subsequently, mild heating induces desorption, releasing the water for collection. The efficiency of this process hinges on the material's affinity for water, adsorption capacity, and regeneration energy requirements and to target regions facing the greatest water stress (Figure 3). [19].

Global Water Scarcity

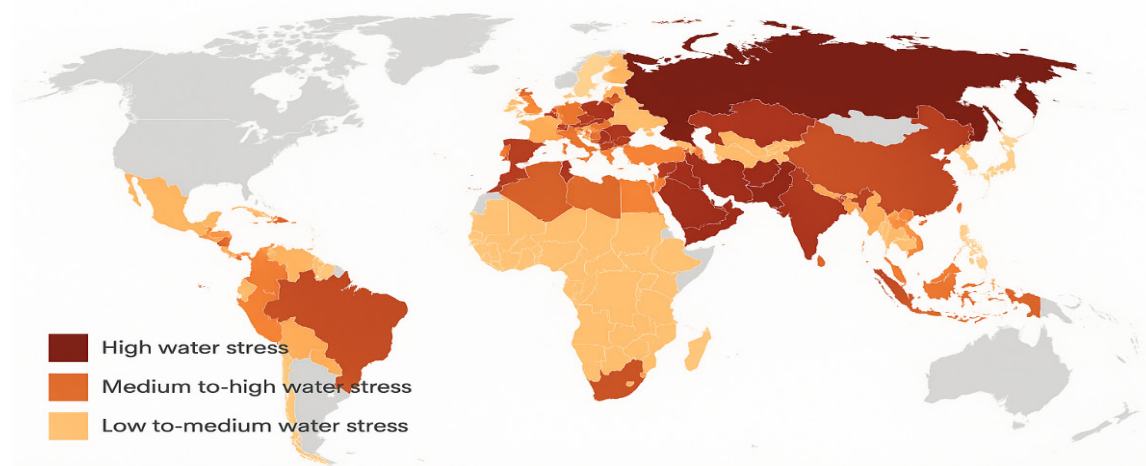


Figure 3. World map showing geographic distribution of water stress and scarcity levels.
(Source: Adapted from UN Water Reports and WRI Aqueduct Water Risk Atlas.)

MOFs and COFs offer advantages in AWH due to their customizable structures. By tailoring pore sizes and incorporating hydrophilic functional groups, these materials can be optimized for specific humidity conditions, enhancing water uptake and release efficiency [19,20].

Case studies

MOFs:

MOF-801, a zirconium-based framework, has demonstrated exceptional water adsorption capabilities. At 20% relative humidity (RH), it achieves a water uptake of 0.28 g/g, increasing to 0.4 g/g at 90% RH. Its robust structure ensures stability over multiple cycles, making it suitable for AWH applications [21].

MOF-303 has been tested in arid environments, such as the Mojave Desert, operating efficiently at 10% RH and 27°C. It produced an average of 0.7 L of water per kg of MOF per day, showcasing its potential for real-world applications [20,21].

COFs:

With a temperature fluctuation between 30°C and 60°C, the 2D covalent organic framework COF-309 shows a water absorption capacity of 0.52 g/g in isobaric circumstances. Its endurance is demonstrated by the fact that it remains stable for at least 170 adsorption-desorption cycles [22].

An S-type water vapor adsorption isotherm with a steep step in the 30%–40% RH range is presented by COF-432, another noteworthy COF. It may be regenerated at a low temperature of 35°C and achieves a water uptake of roughly 0.25 g/g at 40% RH [23].

MOF/COF design for high and low humidity climates

Designing MOFs and COFs for specific humidity conditions involves strategic modifications:

Low humidity environments: Incorporating hydrophilic functional groups, such as sulfonate or amine groups, can enhance water uptake at low RH levels. For instance, sulfonated COFs have shown steep water sorption at RH as low as 5%, making them suitable for arid regions [20,22].

High humidity environments: Adjusting pore sizes to facilitate capillary condensation can improve water uptake in humid conditions. MOFs with larger pore diameters have demonstrated increased water adsorption capacities at higher RH levels [21].

By tailoring the chemical functionality and pore architecture, MOFs and COFs can be optimized for diverse climatic conditions, enhancing their applicability in AWH systems [23].

Energy efficiency and regeneration cycles

The practicality of AWH systems depends on the energy required for regeneration and the material's stability over multiple cycles.

Energy efficiency: Materials like MOF-303 and COF-432 can be regenerated at relatively low temperatures (35°C–60°C), reducing energy consumption. This low-temperature desorption is advantageous for integrating AWH systems with renewable energy sources, such as solar power [23,24].

Regeneration cycles: Durability is crucial for long-term application. COF-309 maintains performance over at least 170 cycles, while MOF-801 exhibits consistent water harvesting capabilities over extended periods without significant degradation [24,25].

These attributes underscore the potential of MOFs and COFs in developing sustainable and energy-efficient AWH systems, offering viable solutions to global water scarcity challenges [25].

Challenges and Opportunities

Scalability of synthesis

Traditional synthesis methods for MOFs and COFs, such as solvothermal and hydrothermal techniques, often involve lengthy reaction times, high energy consumption, and the use of hazardous solvents, limiting scalability. Recent developments have introduced alternative methods like mechanochemical synthesis and flow chemistry. Mechanochemical synthesis offers a solvent-free approach, reducing environmental impact and cost. Flow chemistry enables continuous production, enhancing scalability and consistency in product quality. However, these methods require further optimization to achieve the desired crystallinity and porosity essential for effective performance [26].

Cost and stability concerns

The economic feasibility of MOFs and COFs is influenced by the cost of raw materials, synthesis processes, and post-synthetic modifications. The use of expensive metal precursors and organic linkers can escalate production costs. Additionally, the stability of these frameworks under operational conditions, such as varying temperatures, humidity, and exposure to chemicals, is critical. Strategies to enhance stability include the incorporation of robust linkages and functional groups that can withstand environmental stresses. Developing cost-effective and stable MOFs and COFs remains a priority for their practical application [27].

Integration into real-world systems

Translating the exceptional properties of MOFs and COFs into functional devices necessitates their integration into systems like filters, membranes, and sensors. Challenges in this domain include maintaining structural integrity during processing, ensuring compatibility with other materials, and preserving porosity and active sites. Techniques such as electrospinning and hot-pressing have been explored to fabricate MOF/COF-based composites. However, these methods may lead to partial blockage of active sites or structural degradation. Innovative fabrication approaches that retain the intrinsic properties of MOFs and COFs while enabling seamless integration are essential for their successful deployment [28].

Conclusions

The pursuit of environmental sustainability has brought Metal–Organic Frameworks (MOFs) and Covalent Organic Frameworks (COFs) to the forefront of materials science due to their exceptional porosity, tunability, and selectivity. This review highlights the crucial roles these reticular materials play in two key green technologies: carbon capture and atmospheric water

harvesting. MOFs and COFs have demonstrated high efficiency in selective CO₂ adsorption and water uptake under varying humidity conditions, making them viable candidates for mitigating climate-related challenges.

Despite their promise, challenges remain in terms of scalability, long-term stability, and integration into practical systems. However, advances in hybrid materials, combined with artificial intelligence and high-throughput screening, are accelerating the discovery and deployment of more robust and cost-effective frameworks. Furthermore, their growing use in related green technologies like catalysis and solar fuel production suggests a wide-ranging potential beyond what is currently realized.

MOFs and COFs represent a transformative class of materials capable of addressing critical environmental concerns. Continued innovation, particularly at the intersection of chemistry, materials engineering, and data science, will be essential for unlocking their full potential and transitioning them from lab-scale innovations to real-world applications.

Disclosure statement

No potential conflict of interest was reported by the authors.

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