MATEC Web of Conferences **420**, 04005 (2026) https://doi.org/10.1051/matecconf/202642004005
MPCNE 2026

Metal–Organic Frameworks for Atmospheric Water Harvesting: From Material Design to Practical Applications

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Abstract. Atmospheric water harvesting (AWH) is a promising approach to alleviating water shortages in arid and water-scarce regions. Metal-organic framework materials (MOFs) have become leading adsorption materials in the AWH field due to their controllable pore structure and strong affinity for water molecules at low relative humidity. This article provides an overview of the development history of MOFs for AWH, with a focus on the most advanced materials such as MOF-303 and MOF-801. Their structural characteristics, water adsorption mechanism and regeneration behaviours were systematically discussed. The latest improvement strategies such as multi-ligand substitution and ligand extension design, were highlighted to demonstrate the rational regulation of channel hydrophilicity, water absorption capacity and energy efficiency. In addition, a brief review was conducted on the development of green synthetic routes and their potential applications in desert water supply, urban and industrial systems, as well as medical and military scenarios. Finally, the key challenges and future development directions of the MOF-based AWH system in large-scale application were summarized.

1 Introduction

1.1 Global water scarcity

About two-thirds of the world's population is affected by water shortage, making it one of the most serious challenges facing humanity [1]. The distribution of water resources on Earth is very uneven. Freshwater makes up only about 2.5% of all water. Less than 0.01% of this water is found in lakes and rivers as surface water.

There are usually two types of water shortage. One is the scarcity of material resources. Secondly, the economy is affected by water shortage. If there is not enough water, there will be a shortage of materials. Where there is water but no water, the economy will stagnate. This is usually caused by weak infrastructure or limited water resources [1]. Urbanization and climate change have together exacerbated water resource pressure. The global urban population facing water shortages is predicted to increase from 933 million in 2016 to 1.693-

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2.33 billion in 2050. Among them, India is expected to be the most serious in terms of the growth of water-scarce population [2].

Traditional water supply methods, such as large-scale reservoirs and seawater desalination, are often restricted due to high costs, geographical conditions and the impact on the local environment [2]. These restrictions have created an urgent need for new water extraction alternatives, eventually leading to interest in atmospheric water extraction (AWH) technology

1.2 Insufficient in conventional technologies

The development of MOFs for AWH has gone through a clear path. From early materials with poor water stability to highly professional structures with ability of efficiently absorb water under drought conditions. The earlier generation of MOFs, such as HKUST-1, MOF-5 and MOF-74, they decompose when in contact with water and can only adsorb water >60%RH. The conditions for using them for AWH are very strict. Subsequent research has led to mid-generation water-stable MOFs, such as MIL-101, UiO-66, Co2Cl2(BTDD), and Ni2Br2BTDD. They can adsorb water in the range of 20~60%RH. Although these materials shown a better water stability, their adsorption humidity range still fails to meet the AWH requirements in arid environments (15~40% RH). The real breakthrough occurred in the development stage of low-RH water-absorbing MOFs, which is crucial for AWH. The MOFs representatives include MOF-801, MOF-303 and MOF-LA2-1, etc. They can absorb water at 20%RH and have a large water absorption capacity [1, 3].

1.3 Advantages of metal–organic frameworks

Under this background, the research direction is gradually shifting towards AWH. The metal-organic framework in MOFs has multiple advantages, making it highly suitable for AWH. MOFs have a high specific surface area and porosity due to their porous structure, thus they can achieve adjustable pore sizes for efficient water adsorption. They are regarded as the most promising materials for AWH under low RH conditions. In addition, MOFs can collect water from the air using only solar energy even in desert areas, and the water produced is drinkable and does not require any treatment [1]. Recent studies have shown that MOF-801 maintains long-term effectiveness in multiple adsorption cycles without significant efficiency loss, indicating that MOFs also have good cycling stability [4].

2 Evolution of water-harvesting MOFs

The formation of MOF is a clear and gradual process for water in the atmosphere. These early materials usually exhibit low water stability and gradually form specialized structures that effectively absorb water during droughts. The first generation of MOFs, such as HK-1, MOF-5, and MOF-74, either came into direct contact with water to separate it or only removed water when the relative humidity exceeded 60%, which would greatly limit the formation. Then the water stability of MOFs was studied, including IL-101, UiO-66, Co_2Cl_2 (BTDD), and Ni_2Br_2 (BTDD), which operated under a humidity of 20-60% of the frame water. Although these materials are relatively stable, their absorption of moisture is insufficient to filter 15% to 40% of water in a dry environment with relatively high humidity. A breakthrough has been made in the water absorption of Von MOF at low water temperatures, which is crucial for the collection of atmospheric water. The colours of this stage are MOF-801, MOF 303 and MOF-LAL-1. At a relatively high air humidity of 20%, a strong suction force suction force. This transformation process clearly indicates that the research on hydrotherapy for volatile water deposits conducted within the MOF framework is aimed at low humidity, rapid circulation and well-considered structural design, with moderate application [3].

3 AWH representative high-performance MOFs

3.1 MOF-303

3.1.1 Fundamental characteristics of MOF-303

MOF-303 is an Aluminium-based metal organic framework and is widely regarded as one of the most advanced materials for atmospheric water collection under low relative humidity conditions. Structurally, the MOF-303 is composed of infinitely extended rod-shaped secondary building units (SBUs), which are made up of AlO_6 octahedra, sharing cis-trans angles alternately and interconnected through $PZDC^2$ poisons. This arrangement forms distinct hydrophilic pockets in the pores. In MOF-303, polar organic linkers are the main water adsorption sites. Their orderly arrangement forms hydrophilic pockets, which strongly bind the first water molecule to enter and then serve as nucleated seeds for subsequent adsorption. This molecular design distinguishes MOF-303 from earlier MOFs, which mainly relied on inorganic junctions to absorb water. Hanikel et al. demonstrated that the water absorption process of MOF-303 is gradual. Single crystal X-ray diffraction indicates that the initial water molecules are tightly bound in hydrophilic capsules, then form isolated clumps, then develop into interconnected chains, and finally evolve into a three-dimensional water network bound to hydrogen. The nucleation process of this network formation explains the unique S-shaped adsorption isotherm of MOF-303. In terms of performance, the MOF-303 has an extremely high-water absorption capacity in low relative humidity conditions and is particularly suitable for arid environments [5]. MOF-303 can achieve a water uptake of 0.7 L kg^{-1} at 10% relative humidity and 27 °C. Importantly this high performance is accompanied by remarkable durability. The same study reports that MOF-303 retains approximately 97% of its initial capacity after 2000 adsorption–desorption cycles, indicating excellent long-term cycling stability [1].

3.1.2 Recent improvements on MOF-303

Recent studies on MOF-303 have focused on preserving its low-relative-humidity water uptake mechanism while introducing structural modifications to optimize water capacity and energy efficiency. At present, two representative improvement strategies have been developed. The first uses multivariate linker substitution to tune pore hydrophilicity, represented by MOF-333. The second extends the linker of MOF-303 to generate a framework with a larger pore volume, represented by MOF-LA2-1.

The first approach involves multivariate control of pore hydrophilicity. A multivariate strategy was introduced to precisely regulate the hydrophilic environment within the pores without altering the overall topology of MOF-303. In this method, the original pyrazole-based linker ($PZDC^{2-}$) is progressively replaced by the less hydrophilic fumarate-derived linker (FDC^{2-}), forming the solid-solution framework MOF-333 {[Al(OH)(FDC)]}. This substitution removes the initial adsorption step observed in MOF-303, where the low-pressure adsorption feature gradually disappears with increasing FDC content. By adjusting the PZDC/FDC ratio, the relative humidity at which the steep adsorption step occurs can be continuously tuned. In addition, this multivariate synthesis method shows high chemical robustness and reproducibility. Elemental analysis and NMR demonstrate that the linker composition in the final materials closely matches the feed ratios. MOF-333 also exhibits reduced regeneration temperature and regeneration heat, while maintaining its water uptake capacity after more than 2000 adsorption–desorption cycles [5].

The second improvement strategy aims to increase the total water uptake of MOF-303 by expanding pore volume while retaining the favourable arrangement of hydrophilic pockets. This is achieved by introducing a vinyl group into the original PZDC linker to form the extended linker $PZVDC^{2-}$, yielding MOF-LA2-1. By employing a linker-extension strategy, MOF-LA2-1 is obtained, exhibiting an approximately 50% increase in water uptake relative to the state-of-the-art atmospheric water harvesting material MOF-303.PXRD results confirm successful is reticular expansion, while water adsorption isotherms show a significantly increased total water uptake. Although the adsorption step shifts to higher relative humidity, the material remains suitable for arid environments. In addition, MOF-LA2-1 exhibits lower regeneration heat and regeneration temperature and maintains stable performance after 150 temperature-swing cycles [6].

3.2 MOF-801

3.2.1 Fundamental characteristics of MOF-801

MOF-801 is a zirconium-based metal–organic framework and is another material widely regarded as one of the state-of-the-art sorbents for atmospheric water harvesting under low relative humidity conditions. Structurally, MOF-801 is constructed from $Zr_6O_4(OH)_4$ inorganic clusters coordinated with fumarate ligands, forming a robust framework with excellent water stability that is suitable for repeated adsorption–desorption cycling. One of the key features of MOF-801 is its multi-cavity pore structure. MOF-801 contains three types of pores. Their apertures are about 4.8 Å, 5.6 Å, and 7.4 Å. This structure leads to a stratified water adsorption process. Water molecules are first adsorbed in the smaller cavities. They then move into the larger cavities as adsorption continues. From a physicochemical point of view, the hydroxyl groups on the $Zr_6O_4(OH)_4$ cluster are very important. These hydroxyl groups increase the hydrophilicity of MOF-801 under low humidity conditions. Water molecules can easily interact with these sites. Hydrogen bonds are formed between water molecules and the hydroxyl groups. This helps water molecules adsorb at the early stage. Even when the relative humidity is as low as about 20%, adsorption can still occur. At a stable relative humidity of 20%, MOF-801 shows a water uptake of around 25 g of water per 100 g of adsorbent. This makes it one of the best-performing materials reported in this field. This behaviour is mainly caused by the cooperative filling of multiple cavities. Water clusters can grow step by step. At the same time, the adsorption heat does not increase significantly. Another important feature of MOF-801 is its equilibrium isosteric heat of adsorption (Qst). The value is around 60 kJ mol^{-1}. This heat is high enough to allow water adsorption at low humidity. However, it is still low enough for water to be released under relatively mild regeneration temperatures [3].

3.2.2 Two methods comparison (solvothermal vs green room temperature synthesis)

Previous studies have reported two different synthetic pathways of MOF-801, namely the conventional solvothermal synthesis (SS-MOF-801) and the green room-temperature synthesis (GS-MOF-801). In the solvothermal method, MOF-801 was synthesized using a mixed solvent of N, N-dimethylformamide (DMF) and formic acid, and then heated to 130 °

C in an autoclave. The obtained product undergoes multiple solvent exchange steps and is then activated at high temperatures. The material obtained through this process is called SS-MOF-801. Although this method can reliably produce highly crystalline MOF-801, it involves the use of toxic organic solvents and requires a relatively high energy input.

In contrast, green synthesis uses water instead of DMF and is carried out at room temperature. After standing for 48 hours, the formation of MOF-801 was manifested as the appearance of a cloud-like suspension. After several post-treatment steps, the final product was vacuum-dried at 150°C for 7 hours and was recorded as GS-MOF-801. This route significantly reduces solvent toxicity and energy consumption, making it more in line with the principles of sustainable material synthesis.

The adsorption performance of GS-MOF-801 was directly compared, and it was found that it had obvious advantages. Both adsorbents require thermal activation, and the optimal activation temperatures for SS-MOF-801 and GS-MOF-801 are 90℃. Under this condition, the maximum water absorption rate of the GS-MOF-801-90 adsorbent was 41.1 g / 100 g, which was 12% higher than that of the SS-MOF-801-90. This improvement is mainly attributed to the fact that the specific surface area of GS-MOF-801 is much larger, approximately 89% higher than that of its solvothermal synthesized counterpart. In addition, GS-MOF-801 may contain structural defects of higher density and a greater number of hydrophilic functional groups, providing more active adsorption sites for water molecules. Therefore, it still maintains strong adsorption performance under low relative humidity conditions. Even at a relative humidity of 30%, GS-MOF-801 exhibits a significant water absorption rate of 31.5 grams per 100 grams. These results further prove that the green synthetic MOF-801 is highly suitable for atmospheric water collection in arid and low-humidity environments [4].

4 Potential applications

4.1 Practical application

The use of MOF for atmospheric water collection has been practically applied for the first time in a desert environment. From laboratory-scale experiments to field tests in some of the world's driest deserts, researchers have used multiple generations of equipment to assess the kilogram scale of MOFs. The tested MOF has demonstrated its ability to effectively collect water in desert conditions, producing more than 1 L of water per kilogram per day. This achievement is of great significance as it marks the first time in human history that a device has successfully produced potable water directly from desert air. It shows that MOFs can operate under extremely low relative humidity conditions, a capability not achieved by other classes of materials. This work therefore, validates the feasibility of MOF-based systems as practical, decentralized solutions for water supply in desert regions [7].

4.2 Developing applications

4.2.1 Urban and industrial applications

In addition to independent atmospheric water collection equipment, MOF technology has also been integrated into urban and industrial VC systems. This has become an important emerging application. In the past few years, the application of metal-organic frameworks (MOFs) in atmospheric water collection, heating, ventilation, air conditioning (CVC), and indoor humidity control has attracted increasing research interest. This type of integration allows water to be collected and the climate to be controlled simultaneously within a building.

In this way, the problems of water shortage and energy efficiency can be solved. Compared with the traditional desiccants used in CVS systems, mof has obvious advantages. Studies show that mof has better adsorption performance than traditional materials such as silica gel and zeolite. In an aAWH system driven by CVACC, mofs can capture moisture in the airflow. It also helps to reduce the potential heat load. This reduces the energy consumption of the entire system. This application is particularly suitable for cities and industrial areas. These environments are usually densely populated and rely on continuously operating CVC systems. Therefore, the MOF-HVAC system can operate stably and effectively. They also need to support distributed water supply. This is particularly useful in areas with relatively low humidity. In addition, the absorption of water may be caused by solar energy or low-mass heat dissipation. Although there are still issues such as large-scale production and long-term stability, the combination of mof and CVC systems has great potential. It offers a promising approach to distributed water recycling and effective climate control for urban and industrial facilities [8].

4.2.2 Healthcare applications

The atmospheric water collection system based on MOFs also shows strong development potential in medical, disaster relief and military applications. In these cases, obtaining clean water is of vital importance. The AWH system based on MOF is particularly suitable for areas where cheap water sources are unavailable, or where other critical factors such as safety and security are dominant, as well as conditions frequently encountered in disaster areas and military operations. In disaster relief situations, immediate access to drinking water can support medical care and increase the survival rate of patients. Personalized AWH systems can also be valuable for individual soldiers or small units, as war fighters may survive for up to three weeks without food but only a few days without water. Supplying water to remote military bases involves high logistical risk and cost; therefore, reducing water resupply can provide significant tactical advantages [9].

4.3 Future applications

MOF-based atmospheric water harvesting is now increasingly influenced by artificial intelligence and machine-learning techniques. The main reason is the huge chemical space of MOFs. There are potentially millions of different MOF structures. Because of this, traditional trial-and-error methods are not practical anymore.Using experiments alone takes too much time and cost. As a result, AI-driven and data-based methods have become necessary. These methods help researchers find high-performance MOFs that are suitable for large-scale production. Machine learning works by learning structure–property relationships related to atmospheric water harvesting. It often combines large MOF databases with predictive models. With this approach, thousands of existing and hypothetical MOFs can be screened in a short time. This process is much faster than experimental testing. Machine learning can also help optimize key performance factors. These include water adsorption capacity, adsorption–desorption kinetics, and hydrolysis stability. All of these factors are important for industrial applications. Improving them makes MOFs more realistic for real AWH systems. In addition to screening structures, machine learning is also useful in other stages. It can assist in optimizing synthesis conditions. It can also support post-synthesis characterization. This helps researchers make better decisions earlier in the design process. Overall, machine learning provides a faster and more efficient path for MOF development. It reduces experimental costs and shortens development time. Therefore, machine learning shows strong potential in supporting the rational design of next-generation MOFs and the development of efficient and scalable atmospheric water harvesting systems [10].

5 Conclusion

5.1 Challenges

Atmospheric water extraction assisted by MOF still faces challenges. One of the most fundamental challenges lies in the inherent trade-off between the strong adsorption of water molecules at low relative humidity and the release of adsorbed water at low temperatures. When a strong interaction is formed between the material and water molecules, the desorption process of water molecules will be significantly restricted, which means that it is often difficult to achieve the release of these strongly bound waters at lower temperatures in practical operations [3]. In other words, materials that can adsorb water at extremely low humidity often require a higher regeneration temperature, which significantly increases the energy consumption of the entire water extraction cycle [11].

Another key challenge involves the reaction conditions required for MOF synthesis, which strongly affect its scalability and environmental sustainability. Many high-performance MOFs are still mainly prepared by solvothermal methods, and this synthetic route usually requires the use of toxic organic solvents, accompanied by high reaction temperatures and long reaction cycles. These synthetic conditions have raised concerns regarding cost, safety and environmental impact during the transition from laboratory-scale to industrial production [11].

Furthermore, although MOFs exhibit excellent water adsorption performance, the practical application of MOF-assisted AWH is still limited by material costs, synthesis complexity, and large-scale manufacturing capabilities. Complex synthetic routes not only limit production capacity but also introduce batch-to-batch differences, thereby affecting adsorption performance and cycling stability [3]. Achieving the target aperture distribution and functional group density usually requires strict control of the synthesis parameters. Even if the synthesis parameters change only slightly, it may cause significant differences in crystal structure, defect distribution and water adsorption performance [11].

5.2 Conclusion

Collecting water from the atmosphere is regarded as a possible way to reduce global water shortages. In recent years, it has attracted more attention. This is especially true in arid and water-scarce areas. In these areas, traditional water supply technologies often fail to function well. This article reviews the development of AWH metal-organic frameworks. It mainly focuses on MOF-303 and MOF-801. These materials have been extensively studied and possess high performance. This article discusses their structural design principles, adsorption behaviours and application potential. Over time, the development of AWH MOF has undergone significant changes. The early MOFs had very poor stability in water. Their water absorption is not intentional. On the other hand, newer MOFs are specifically designed to absorb water with lower relative humidity. Many structural strategies are widely used. This includes hydrophilic pockets, laminated interstitial structures, displacement of multiple binders and expansion of binders. These designs help to control the thermodynamics and kinetics of adsorption. Therefore, AWH based on MOF has shifted from accidental water absorption to a more reasonable material design. This also allows for low-humidity operation and rapid cycling. MOF-303 is a typical example. There are ordered hydrophilic points in its structure. Water molecules first bind to these sites. After that, water masses gradually formed. This process enables MOF-303 to acquire a high-water absorption capacity even at very low relative humidity, around 10%. Recent studies also indicate that there is still room for adjustment in the performance of MOFs. For example, the interstitial hydrophilicity can be modified by various methods, as shown in MOF-333. The volume of pores can also be increased through the expansion of binders, such as MOF-LA2-1. These strategies allow for the adjustment of the position of the adsorption stage, the total water absorption capacity and the regeneration energy. Meanwhile, structural stability can still be maintained. MOF-801 has different adsorption behaviours. It has multiple cavities and clusters rich in Zr hydroxyl groups. These characteristics lead to the synergistic adsorption of isothermal equilibrium water. Therefore, MOF-801 is suitable for low-temperature regeneration. The synthesis of materials is also very important. This affects scalability and sustainability. MOF-801 can be synthesized by the solvothermal method or the green ambient temperature method. Compared with the solvothermal method, the green method reduces solvent toxicity and energy consumption. It can also produce materials with good adsorption performance at low humidity. In terms of application, AWH based on MOF is no longer confined to laboratory testing. It is gradually moving towards practical application. For instance, desert water collection equipment, integrated CVS systems, and portable units for military operations and disaster relief. In addition, data-driven methods such as machine learning are being used more and more. These tools help to speed up screening and material design. Overall, MOF materials remain one of the most promising platforms for collecting atmospheric water in the future.

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