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Metal-Organic Framework Gas-Phase Separation: Research Progress and Challenges in Structure-Mechanism-Application-Engineering

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Abstract. Metal-organic frameworks (MOFs) have the characteristics of high specific surface area, tunable pore channels and abundant active sites, and are important candidate materials for low-energy-consumption gas separation. This paper reviews the structural basis, action mechanisms and typical applications of MOF gas-phase separation, focuses on analyzing size sieving, thermodynamic adsorption, kinetic selective adsorption and the synergistic mechanism, and summarizes the research progress in CO_2/N_2, CO_2/CH_4, H_2 purification and hydrocarbon separation. On this basis, the influence of pore structure, framework characteristics, defect sites and stability on separation performance is discussed, and it is pointed out that industrial application is still restricted by factors such as stability, large-scale preparation, forming and processing, regeneration energy consumption and adaptability to complex working conditions. In the future, research on high-stability material design, green large-scale synthesis, low-energy regeneration and membrane/adsorption device engineering should be strengthened, so as to push MOF gas separation technology from the laboratory to practical application.

Keywords: Metal-organic frameworks, gas-phase separation, adsorption mechanism, molecular sieving, industrial application

1. Introduction

In the field of energy and chemical engineering, metal-organic frameworks (Metal-organic framework, MOF), which have the advantages of porous structure, high specific surface area and designable pore channels, show great application potential for the problems of high process energy consumption and low energy efficiency in separating hydrocarbons in the petrochemical field and the insufficient efficiency of carbon storage and utilization in carbon dioxide capture [1, 2].

In the 1990s, MOF was first applied to adsorption separation of the gas phase, and after that a large amount of research on MOF in this field was carried out [3-5]. Since the beginning of the 21st century, researchers have developed functionalized MOF materials for different gas separations, for example ZIF-8, because of its precisely controllable pore size and excellent chemical stability, can realize high-precision separation of small-molecule gases; MIL-53 has a flexible breathing effect and can carry out precise separation of complex gas-phase systems through pore channel regulation

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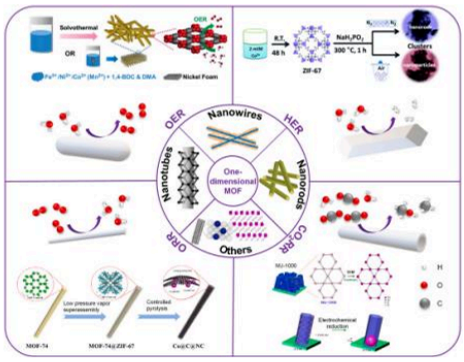
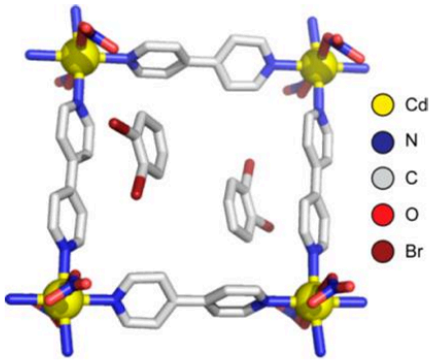
[6-8]. As the basic MOF systems were gradually improved, the research focus began to turn to functionalized modification for specific gas separation environments, relying on synthesis modification strategies such as ligand functionalization and ligand clipping to precisely regulate the pore size, active sites and framework stability of MOF materials, so as to make up for the application shortcomings of basic MOF such as weak stability and insufficient gas separation selectivity, and to make sure that MOF is further industrialized and applied in actual gas separation systems [9-11].

Based on this, starting from the crystal structure and topological characteristics of MOF, this paper systematically analyzes the regulation mechanism of core structural parameters such as pore geometry and active site distribution on gas-phase adsorption and separation behavior, focuses on typical industrial gas-phase systems such as CO_2/N_2, CO_2/CH_4, H_2 purification and hydrocarbon separation, and clarifies the adaptation mechanism and application form of MOF with different structures in each scenario; finally, combining the perspectives of materials science and engineering, it summarizes key influencing factors such as framework stability, defect effect and formability, and sorts out industrialization bottlenecks such as large-scale preparation, working condition adaptation and long-term cycling stability. This paper aims to systematically clarify the internal connection among the structure, performance and application of MOF, to lay out its research progress and development context in the field of gas-phase separation, and at the same time to provide theoretical basis and technical reference for the design of high-performance separation materials, industrial process optimization and engineering implementation.

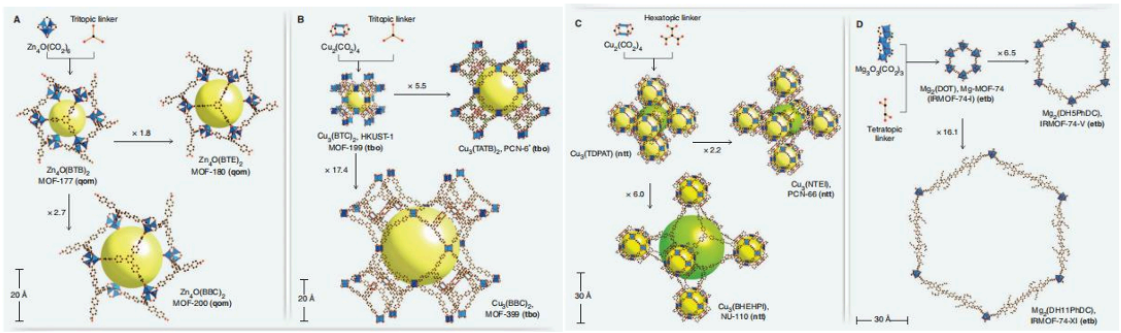
2. MOF structure and fundamentals of gas-phase separation



Schematic of 1D MOF structure [14]



Schematic of 2D MOF structure [15]



Multiple types of 3D MOF topologies [16]

Figure 1. MOF structures of different dimensions

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MOF is formed by self-assembly of metal ions or metal clusters and organic ligands through coordination bonds. Different building units and topological connections can form 1D, 2D and 3D pore channel structures, among which the 3D network usually has higher porosity and more sufficient mass transfer channels; the 1D narrow pore channel is more favorable for precise size sieving. Through ligand functionalization, metal node regulation and defect engineering, the pore size, polarity, open metal sites and framework flexibility can be further changed, so as to realize the coordinated regulation of adsorption capacity, diffusion rate and separation selectivity. As shown in Figure 1, the one-dimensional MOF nanomaterial, the two-dimensional square-grid MOF that can accommodate guest molecules and the three-dimensional MOF system with the same topology and enlarged pore cavity respectively illustrate the structural characteristics of MOF with different dimensions, and directly reflect the regulation effect of building units and topological connections on pore channel morphology and pore size [12-18].

Research on MOF in the field of gas-phase separation has accumulated for nearly 20 years, and the early development can be seen in Table 1. In recent years, MOF separation materials have gradually expanded from powder adsorbents to shaped particles, monolithic adsorbents, as well as MOF membranes and mixed-matrix membranes. Membrane materials, by virtue of tunable pore size and strong guest interaction, show good permeation-selectivity regulation potential in carbon capture and light hydrocarbon separation [19, 20].

Table 1. Early development of MOF in the field of gas-phase adsorption separation

Year	Research content	Highlight
2002	Reported the first MIL-53 material with breathing effect [21]	First discovered the reversible breathing effect of MOF, opening the prelude to research on flexible MOF materials
2004-2008	Successively reported the MIL-100, MIL-101 and MIL-88 series of isostructural flexible MOFs [22, 23]	Promoted the systematic development of flexible MOF
2008	Synthesized Co(BDP) and confirmed that it can realize controllable hydrogen adsorption and desorption [24]	Expanded the application of MOF in hydrogen storage and separation

3. Main action mechanisms of MOF gas-phase separation

MOF gas-phase separation mainly includes four types of mechanisms: size sieving, thermodynamic adsorption, kinetic selective adsorption and multi-effect synergy. The former relies on the matching of pore size and molecular size, the latter two respectively use the difference in gas-framework interaction and the difference in diffusion rate, and the synergistic mechanism takes into account selectivity, capacity and mass transfer rate through the coupling of multiple effects.

3.1. Size sieving mechanism

Size sieving is based on the matching relationship between the kinetic diameter of the gas and the size of the pore window. When the pore size is between the sizes of the two components, small molecules can enter the pore channel while large molecules are excluded, so a higher selectivity is obtained. KAUST-7 can use rigid ultramicropores to realize propylene/propane sieving, IPM-101

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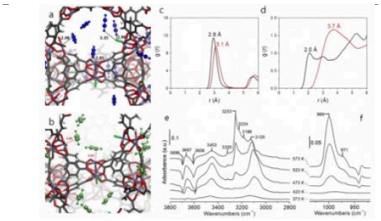
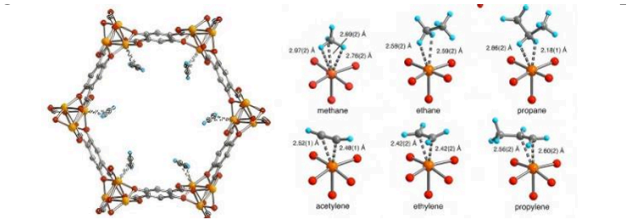
can be used for n-butane/isobutane separation, and the SIFSIX series can improve CO_2 sieving performance through ultramicroporous structures [25-28]. This mechanism has high selectivity, but has high requirements on pore size precision and framework stability.

3.2. Thermodynamic adsorption mechanism

Thermodynamic adsorption depends on the difference in affinity between different gases and the MOF framework, and mainly involves electrostatic interaction, hydrogen bonding, van der Waals force and coordination interaction. This mechanism is suitable for systems with similar sizes but different polarity, polarizability or coordination ability. Open metal sites and functional groups such as amino and hydroxyl can enhance the adsorption of target molecules, for example MIL-100(Cr) for acetylene, Ag@Ni-DOBDC for Xe and M-MOF-74 for unsaturated hydrocarbons all show strong selectivity [29-32]. The left side of Figure 2 shows the GCMC simulation configuration, radial distribution function and in situ infrared spectra of MIL-100 (Cr) adsorbing acetylene and ethylene, explaining the microscopic interaction and adsorption thermodynamic behavior of the two molecules with the framework; the right sub-figure shows the crystal structure of M-MOF-74 and the solid-state coordination configuration of its open Fe^{2+} sites binding light hydrocarbons, revealing the coordination adsorption selectivity of open metal sites. Adsorption enthalpy and Henry coefficient can be used to evaluate adsorption affinity in the low-pressure region, but too strong adsorption may also increase regeneration energy consumption.



Adsorption thermodynamics of ethylene and acetylene [29]



Coordination adsorption of open Fe^{2+} sites with light hydrocarbons [32]

Figure 2. Thermodynamic adsorption mechanism

3.3. Kinetic selective adsorption mechanism

Kinetic selective adsorption uses the difference in diffusion rate of different molecules in the pore channel to achieve separation. Influencing factors include molecular size, pore opening size, diffusion energy barrier and framework dynamic behavior. Typical forms include diffusion energy barrier difference, gating effect, hopping diffusion and "molecular trapdoor". ZIF materials can amplify the diffusion difference of propylene/propane; flexible MOF can induce pore opening and closing through temperature or pressure; Zr-PMA and MOF-Pytpy respectively show hopping diffusion and dynamic gating behavior [33-36]. This mechanism is especially suitable for mixed gases with close sizes and similar thermodynamic properties.

3.4. Synergistic mechanism

The synergistic mechanism works through two or more effects among size sieving, thermodynamic adsorption and kinetic diffusion acting together, so as to break through the limitation of a single mechanism in capacity, selectivity or rate. For example, $ZnAtzPO_4$ uses a narrow pore window to form ethane diffusion resistance, and at the same time preferentially adsorbs ethylene by means of

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pore wall sites; ZNU-2-Si realizes propyne/propylene separation through the synergy of strong adsorption sites and diffusion energy barrier [37, 38]. Therefore, multi-mechanism coupling has become an important design direction for high-performance MOF separation materials.

4. Application of MOF in typical gases

4.1. CO_2/N_2 separation system

In industrial flue gas the volume fraction of CO_2 is usually about 10%-15%, and traditional amine liquid absorption has problems of high regeneration energy consumption, corrosion and solvent loss. MOF can enhance CO_2 adsorption through ultramicropore sieving, open metal sites or polar functional groups, and use flexible pore channels to regulate the diffusion process. NH2-MIL-53(Al) can use the amino group interaction and the framework breathing effect to improve CO_2/N_2 selectivity; functionalized UiO-66 mixed-matrix membranes can also improve permeability and selectivity at the same time, as shown in Figure 3, PXRD, nitrogen adsorption, FTIR and thermogravimetric characterization are used to compare the crystal phase, pore structure and thermal stability of UiO-66 and its functionalized derivatives, reflecting the regulation effect of the functional group modification strategy on the physicochemical properties of MOF [39-43]. Materials such as the MUV series further reflect the advantage of the synergy of kinetics and weak interaction [44, 45]. But H_2O, SO_2 and NOx in real flue gas will cause competitive adsorption or framework damage, and long-term stability is still the key to engineering.

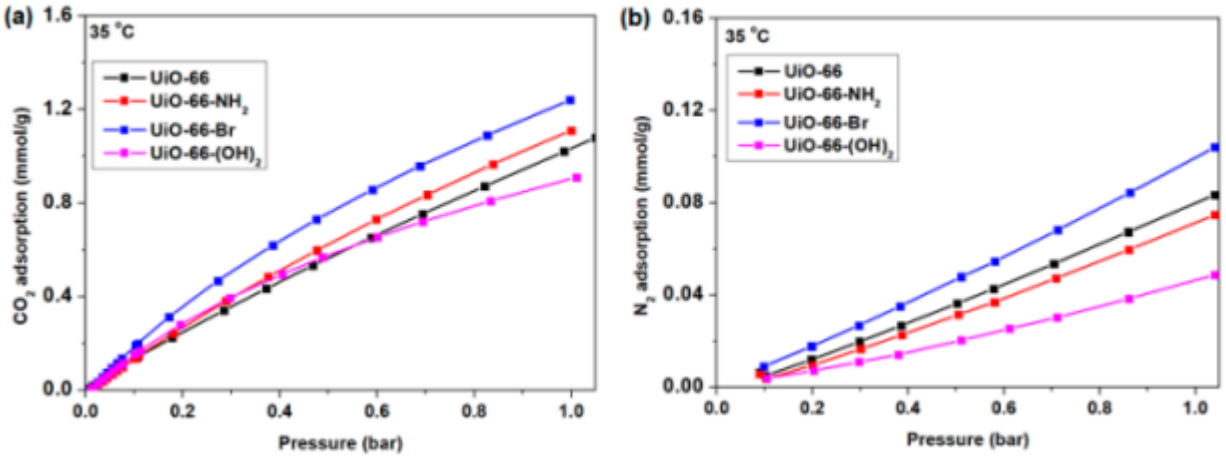

Figure 3. Single-component adsorption isotherms of different functionalized UiO-66 materials for CO_2 and N_2 at 35 °C [42]

4.2. CO_2/CH_4 separation system

CO_2/CH_4 separation is an important link in natural gas upgrading and biogas purification. Because the kinetic sizes of the two are close, and the actual feed gas often contains water vapor, heavy hydrocarbons and H_2S, a single separation mechanism often cannot meet the requirements of complex working conditions. SIFSIX-3-Zn can combine narrow pore sieving with the electrostatic interaction of fluorine sites, Mg-MOF-74 relies on open metal sites to enhance CO_2 adsorption, and Zr-MOF mixed-matrix membranes can improve the permeation-selectivity balance of the membrane

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[46, 47]. The current limitations mainly include material cost, reproducibility of large-scale synthesis, forming and processing, and cycling stability.

4.3. H_2 separation/purification system

Industrial hydrogen production is often accompanied by impurities such as CO_2, CH_4 and N_2, and hydrogen purification directly affects subsequent storage, transportation and fuel cell operation. Because H_2 has small size, fast diffusion and weak polarity, MOF separation is more suitable for adopting pore size regulation and kinetic sieving strategies. ZIF-8 can use the pore window to amplify the diffusion difference between H_2 and larger impurity molecules, while UiO-66 has both tunable pore channels and structural stability; materials such as Mg_2(dobdc) can also achieve indirect purification by preferentially adsorbing impurities [48-50]. MOF-based mixed-matrix membranes still face problems such as filler-polymer interface defects, particle agglomeration, and insufficient stability under high temperature, high pressure and water- and sulfur-containing working conditions [51, 52].

4.4. Hydrocarbon separation system

The separation of olefins/alkanes and hydrocarbon isomers is a high-energy-consumption link in the petrochemical industry, and traditional cryogenic distillation has large energy consumption. MOF can realize low-energy separation by means of size sieving, diffusion difference and open metal sites. KAUST-7 can sieve propylene/propane, ZIF-8 can amplify the diffusion difference between the two, MgMOF-74 and FeMOF-74 preferentially adsorb unsaturated hydrocarbons through open metal sites, and UiO-66 and MIL-53 can use pore channel confinement to identify some hydrocarbon isomers [53-56]. The current difficulties mainly lie in precise pore size regulation, multi-mechanism synergistic construction and competitive adsorption in multi-component systems.

5. Factors influencing MOF gas-phase separation

The separation performance of MOF is jointly affected by pore size and pore channel structure, framework rigidity and flexibility, defects/active sites and stability, and these factors directly determine adsorption capacity, diffusion rate and separation selectivity.

5.1. Pore size and pore channel geometry

Pore size and pore channel geometry determine the accessibility, diffusion path and mass transfer resistance of gas molecules. The 1D narrow pore channel is convenient for building a sieving window close to the molecular scale, and has high selectivity, but the diffusion path is single and easily affected by blockage; the 3D connected pore channel has lower mass transfer resistance and higher flux. Multi-level structures such as cage-narrow window can also strengthen adsorption and sieving at the same time, so pore size precision and pore channel connectivity need to be designed in coordination [57-59].

5.2. Framework characteristics

Framework rigidity and flexibility determine the stability of the pore window under actual working conditions. Rigid MOFs such as UiO-66 and NU-1000 can maintain a relatively stable sieving pore size; flexible MOF can produce a gating effect under the induction of temperature, pressure or guest

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molecules. Moderate flexibility is beneficial for improving dynamic selectivity, but excessive flexibility may cause pore size fluctuation and even structural instability, so adjusting framework rigidity by means such as metal doping is of great significance. Figure 4 is a schematic diagram of the heterobimetallic regulation mechanism of the $Zn_{(100-x)}Cox(Bim)(OAc)$ nanosheet membrane; as the Co doping ratio increases, the number of Co-N coordination bonds increases and the framework rigidity improves, while the sieving performance of the material evolves, which verifies the coordinated regulation effect of the metal doping strategy on framework rigidity and sieving ability [60-62].

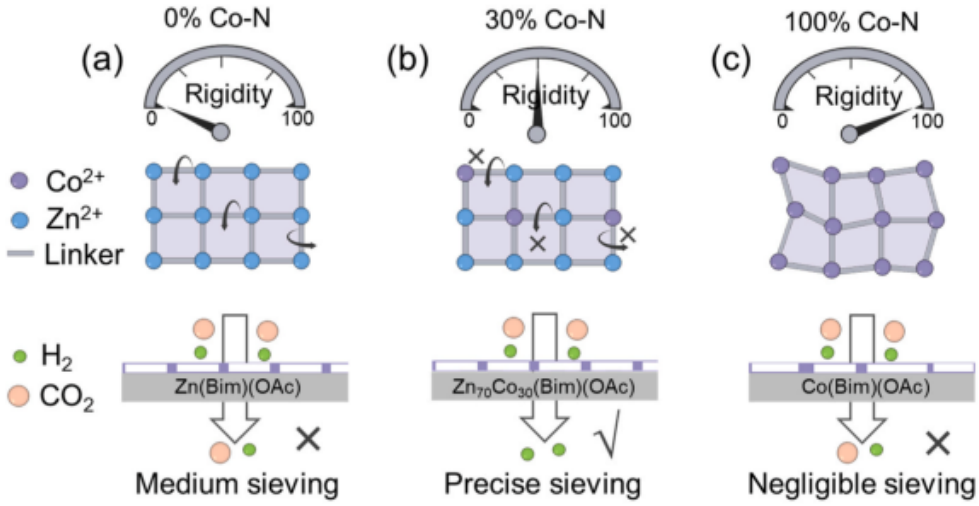

Figure 4. Schematic of the regulation of Co^{2+} doping on framework rigidity and its effect on H_2/CO_2 molecular sieving performance [60]

5.3. Defects and active sites

Defect engineering can expose open metal sites through ligand deletion, metal vacancies and other ways, increase adsorption sites and improve local pore channel connectivity. An appropriate amount of defects is beneficial for improving capacity and diffusion performance, but too many defects will destroy the long-range order of the crystal and reduce specific surface area, structural stiffness and mechanical stability. Therefore, the defect concentration needs to be balanced between activity and stability [63, 64].

5.4. Stability

Stability is the prerequisite for MOF to move from the laboratory to industrial application, and includes hydrothermal, chemical, thermal and cycling stability. Its essence depends on the metal-ligand bond strength, ligand rigidity and framework connection density. Zr-, Al- and Cr-based MOF usually have good water resistance and heat resistance; facing corrosive gases such as NH_3 and SO_2, the tolerance can also be improved by hydrophobic modification, surface protection and other methods [65, 66].

6. Main challenges facing MOF gas-phase separation

The industrialization of MOF is first restricted by stability and formability. Some materials are prone to framework hydrolysis, crystal form transformation and deactivation of active sites under water

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vapor, high temperature, acid and alkali or corrosive gases; at the same time, high porosity is often accompanied by low mechanical strength, and cracks and pore channel collapse may occur during tableting, granulation or packing, causing separation performance degradation [67]. Therefore, material evaluation needs to shift from ideal single-component conditions to real working conditions such as water-containing, multi-impurity, high-pressure and long-term cycling.

Cost and large-scale preparation are also core bottlenecks. High-purity organic ligands and organic solvents will significantly increase the cost of raw materials, recovery and environmental protection; scale-up synthesis may also lead to inconsistent crystallization and uncontrolled defects due to uneven heat and mass transfer. The use of cheap or bio-based ligands, aqueous/solvent-free synthesis, continuous manufacturing and raw material recycling is an important direction for reducing cost [68-70]. At the same time, traditional thermal regeneration has high energy consumption and may cause framework damage, and it is urgent to develop milder and lower-energy regeneration methods.

7. Conclusion and outlook

MOF relies on tunable pore structure and diversified active sites, and can realize processes such as CO_2 capture, natural gas upgrading, H_2 purification and hydrocarbon separation through size sieving, thermodynamic adsorption, kinetic selective adsorption and the synergistic mechanism, and has obvious potential in reducing the energy consumption of traditional separation. But high capacity and high selectivity under laboratory conditions are not equivalent to industrial applicability, and stability, resistance to interference from complex gases, large-scale preparation, forming and regeneration are still the keys determining its application prospect.

Future research should shift from "performance first" to the coordinated design of "performance-stability-cost-engineering": first, develop high-stability frameworks such as Zr, Al and Cr and hydrophobic, pillaring and surface protection strategies; second, promote aqueous, solvent-free and continuous green synthesis, improve batch consistency and reduce cost; third, develop low-energy regeneration, particle forming, MOF membrane and mixed-matrix membrane technologies; fourth, combine molecular simulation and machine learning to establish structure-performance prediction relationships, and accelerate material screening and process optimization. With the coordinated progress of materials and engineering technology, MOF is expected to be the first to achieve large-scale application in some high-value-added or high-energy-consumption gas separation scenarios.

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