Metal-Organic Frameworks as "Molecular Sponges": An Analysis of Their Strategic Role in the Context of Carbon Neutrality

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Abstract. Carbon neutrality has become a core strategic objective in the global fight against climate change, with countries actively pursuing its realization through diverse approaches such as carbon capture, utilization, and storage (CCUS). However, current technologies still face critical bottlenecks, including high energy consumption in CO2 capture, low conversion efficiency, and insufficient storage safety. Metal-organic frameworks (MOFs), as novel porous materials with high-efficiency adsorption, separation, and catalytic functions, have emerged as "molecular sponges" in the carbon neutrality technology system, providing a new paradigm to address core challenges in achieving carbon neutrality. Based on authoritative literature data, this study compares the performance differences between MOFs and traditional adsorbents/catalysts, outlines material design strategies and industrialization challenges, and ultimately constructs a strategic positioning framework for MOFs as "molecular sponges" in the carbon neutrality technology system. It focuses on analyzing their strategic applications in carbon capture, utilization, and storage, offering references for material innovation and system optimization in low-carbon technologies.

1 Introduction

Global climate change is becoming increasingly severe, and carbon neutrality has become the core strategy of all countries to deal with the climate crisis. A UN report released in November 2025 revealed that global greenhouse gas emissions in 2024 reached 57.7GtCO_2eq, marking a 2.3% increase from 2023 levels. This failure to meet the Paris Agreement targets has resulted in a temporary global temperature rise exceeding 1.5 ℃, as nations have been slow to implement carbon neutrality measures. Against this backdrop, carbon capture, utilization, and storage (CCUS) technology, serving as a pivotal bridge between energy transition and industrial emission reduction, is now becoming the cornerstone of carbon neutrality initiatives through its technological breakthroughs and large-scale implementation. However, traditional carbon capture technologies still exhibit critical limitations, primarily including high energy consumption, solvent degradation, equipment corrosion, and environmental impacts; CO_2 catalytic conversion remains constrained by low catalyst

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activity, poor product selectivity, and stringent reaction conditions [1]; CO_2 sequestration is widely questioned due to environmental safety concerns.This highlights the urgent need for new functional materials with high adsorption capacity, excellent selectivity, rapid kinetic response, good cycling stability, and green environmental friendliness, and can work with renewable energy systems.

Against the backdrop of unmet carbon neutrality milestones, MOFs have emerged as a standout material due to their unique structure and capabilities. Their "prefabricated architecture" and "customizable development" features have enabled rapid adoption across all phases of carbon neutrality efforts. With distinctive advantages in CO^2 adsorption, utilization, and storage—including porosity, flexibility, adsorption capacity, and recyclability—MOFs have earned the title of "molecular sponges" in the materials science community.

This paper focuses on the advantages of MOFs in practical carbon neutrality applications, exploring their pivotal role in replacing traditional carbon-neutral materials. Based on literature reviews, it synthesizes key advancements of MOFs in the carbon neutrality field from 2021 to 2025, evaluates their systemic potential and industrialization bottlenecks in real-world applications, and outlines future development directions. Through this analysis, the study aims to provide a clear technical roadmap for MOF industrialization to relevant interdisciplinary fields, enterprises, and governments, facilitating the transition of MOFs from laboratory innovations to large-scale carbon-neutral applications.

2 The structural basis of MOF and the characteristics of “Molecular Sponge”

The core appeal of MOFs lies in their dual characteristics: the rigidity and stability of inorganic materials, coupled with the structural flexibility and chemical modifiability of organic molecules, enabling "on-demand customization" of pore environments at the molecular level. Scientists achieve this through the integration of "structural design" and "functional realization" at the molecular scale, where modifications to "nodes" and "connectors" enable "modularization" of the material, allowing for virtually limitless expansion of MOF performance.

2.1 Structure and composition

The core structure of MOF is formed by metal nodes and organic ligands assembled through coordination bonds, resulting in a periodic porous network structure.

2.1.1 Diversity of metal nodes and organic ligands

Metal ions (e.g., Zn^{2+}, Cu^{2+}, Fe^{3+}) or multinuclear metal clusters such as $Zr_6O_4(OH)_4$ provide coordination sites, serving as the metal nodes of the framework. Metal Species, Coordination Number and Oxidation State of Metal Nodes Determine the Structural Rigidity, Electronic Properties and Functional Activity of MOFs. Organic molecules containing functional groups such as carboxyl, pyridine, and imidazole serve as organic ligands, which coordinate with metal nodes to form a framework support. The molecular structure, functional groups, and length of these ligands directly determine the pore size, shape, and surface chemical properties of the MOF [2]. The chemical diversity of metal ions and organic ligands is the fundamental reason for the structural tunability and broad functionality of MOF materials. The 'modular' assembly logic endows MOFs with extremely high design freedom, thus theoretically enabling the construction of millions of MOF structures. Table 1 lists the common metal ions and organic ligands in metal-organic framework (MOF) materials.

Table 1. Common Metal Ions and Organic Ligands in Metal-Organic Framework Materials.

Category	Specific Type	Common Representatives	Typical MOF Materials
Metal Ions	Alkaline Earth Metal Ions	Mg^{2+} , Ca^{2+} , Sr^{2+} , Ba^{2+}	Mg-MOF-74, Ca-MOF-5
	Transition Metal Ions (3d)	Fe^{3+} , Co^{2+} , Ni^{2+} , Cu^{2+} , Zn^{2+} , Mn^{2+}	MIL-100(Fe), ZIF-8(Zn), HKUST-1(Cu)
	Rare Earth Metal Ions (Lanthanides)	La^{3+} , Ce^{3+} , Nd^{3+} , Eu^{3+} , Tb^{3+}	UiO-66(Ce), Eu-MOF
	Precious Metal Ions	Pt^{2+} , Pd^{2+} , Au^{3+}	Pd-MOF-1, Au@MIL-101
Organic Ligands	Carboxylic Acid Ligands	Terephthalic acid (BDC), Trimesic acid (BTC), 2-Methylimidazole	ZIF-8 (2-Methylimidazole), MOF-5 (BDC), HKUST-1 (BTC)
	Heterocyclic Nitrogen Ligands	Imidazole, Pyridine, Triazole	ZIF Series, MIL-53
	Sulfonic Acid Ligands	Benzenesulfonic acid, Naphthalenedisulfonic acid	S-MIL-101, Sulfonic acid-functionalized UiO-66
	Mixed Ligands (Carboxylic Acid + Heterocyclic Nitrogen)	BDC + Imidazole, BTC + Pyridine	UiO-67-NH_2 , MIL-125-NH_2

2.1.2 Porous structure and specific surface on adsorption behavior

The pore structure of MOF materials is co-regulated by pore size, pore volume, pore channel array morphology, and active site distribution. The selectivity and adsorption strength of MOFs for adsorbate molecules primarily depend on the matching between MOF pore size and the kinetic diameter of the adsorbate molecules. Additionally, molecular sieving, equilibrium adsorption, and mass transfer equilibrium, as well as the advantages of high-efficiency mass transfer, collectively influence the adsorption behavior [3].

The specific surface area of MOFs is also one of the key parameters determining adsorption behavior. By regulating the number of adsorption sites, mass transfer efficiency, and the strength of host-guest interactions, it influences adsorption capacity, selectivity, and kinetic performance, synergizing with pore structure to achieve optimal adsorption performance. Firstly, the abundant active sites provided by high specific surface area significantly enhance the adsorption capacity. Secondly, specific surface area, pore structure, and pore size collectively regulate adsorption capacity and kinetics [4].

2.2 The connotation of the metaphor of "Molecular Sponge"

2.2.1 Static adsorption vs. dynamic regulation

The static adsorption properties, which are based on the "molecular storage space" formed by the regular pore structure and high specific surface area of MOFs, enable efficient capture of target molecules. This represents a fundamental difference from the "random adsorption" of traditional adsorbents (e.g., activated carbon).

The dynamic regulation characteristics demonstrate MOFs' responsiveness to external environmental factors (temperature, pressure, guest molecules, etc.), enabling precise switching of adsorption behavior through reversible deformation of the pore structure. Under varying conditions, MIL-53(Al) exhibits a compression-expansion process akin to a "sponge"; the adsorption capacity of X-dia-1-Ni increases dramatically, further highlighting the dynamic regulation properties of the "molecular sponge" [5].

2.2.2 Molecular recognition, diffusion, and screening mechanism

The molecular recognition mechanism is achieved through specific interactions between active sites within MOF pores and guest molecules. The molecular diffusion mechanism directly determines diffusion rates and selectivity by regulating diffusion pathways, resistance, and molecular-pore interactions. The essence of molecular sieving lies in the synergistic design of pore structure and surface chemistry to selectively "release" or "retain" molecules with different sizes, shapes, or chemical properties [6].

2.2.3 Reversible adsorption, desorption, and self-repairing properties

Through the stability of the framework, the recoverability of active sites, and dynamic bonding effects, MOFs exhibit reversible adsorption-desorption and self-healing properties. The former reduces energy consumption for cyclic use, while the latter extends material lifespan, serving as the core guarantee for the recycling of "molecular sponges" [7].

The reversible adsorption-desorption capability of MOFs enables efficient desorption of adsorbed guest molecules while maintaining structural integrity and adsorption performance, allowing for cyclic reuse. Their self-healing property refers to the ability to recover structural integrity and performance through dynamic bonding or mild conditioning, similar to the elastic deformation recovery of sponges [8].

2.3 Design strategy of carbon management

Recent studies indicate that MOF functional customization revolves around three key principles: carbon species recognition, interface interaction enhancement, and full-chain synergy. The three core design strategies include ligand functionalization, precise metal node selection, and post-modification (PSM) co-regulation. These strategies can be combined or adjusted according to specific carbon neutrality applications to achieve optimal performance of MOFs in this field.

3 The strategic role of MOF in the path of carbon neutrality

The achievement of carbon neutrality targets relies on breakthroughs in the entire chain of technology of "carbon capture-utilization-storage". The core advantage of MOF materials lies in their ability to simultaneously achieve high selectivity in carbon capture, safety in storage, and high conversion efficiency, making them a key material system that connects various technological modules for carbon neutrality. Moreover, their unique properties demonstrate irreplaceable strategic value across all stages.

3.1 Carbon capture process

Carbon capture is a core front-end technology for carbon neutrality, designed to efficiently separate CO_2 from industrial flue gas, coal-fired power plant exhaust, or air, thereby reducing the concentration of greenhouse gases in the atmosphere. Through targeted design, MOFs achieve multidimensional optimization in CO_2 selectivity, adsorption capacity, cyclic stability, and regeneration energy consumption, gradually becoming a significant alternative to traditional adsorbents.

3.1.1 High selective adsorption representative material

To address diverse capture scenarios (high-concentration flue gas, low-concentration air, and humid environments), researchers have developed specialized MOF materials. Ni-DATZ-MOF-74 exhibits high selectivity with moisture resistance and structural stability, making it ideal for CO_2capture in humid conditions. SNNU-196-Nixun demonstrates recyclability while combining high adsorption efficiency with photocatalytic capabilities. CU-4 achieves high-selectivity capture through physical adsorption, featuring water stability and low regeneration energy consumption. MG-CL_2-MOF-74 is optimized for low-pressure CO_2 capture applications. UIO-66-$(OH)_2CO_2$ achieves high selectivity while balancing adsorption capacity, stability, and practical application potential [9].

3.1.2 Adsorption mechanism: physical adsorption, chemical adsorption and their synergistic effects

MOFs achieve efficient CO_2 capture through both physical and chemical adsorption mechanisms, with these synergistic processes enabling outstanding performance in carbon neutrality applications.

3.1.3 Analysis of regenerative energy consumption and cycle stability

Some MOF materials exhibit excellent thermal stability under mild conditions such as medium-low temperature heating, vacuum, or purging (e.g., UIO-66, MIL-120 series). The energy consumption for CO_2 desorption is only 30%-50% of that in traditional amine absorption methods. When combined with low-carbon energy sources like waste heat or solar power, certain MOFs further reduce desorption energy consumption.

Under normal conditions, MOFs exhibit excellent structural stability and recyclability. However, in practical applications such as increased humidity or exposure to acidic gases, MOFs may suffer structural degradation and lose their recyclability. Leveraging the customizable nature of MOFs, researchers have achieved cyclic stability in complex scenarios and are progressively developing MOFs adaptable to diverse applications [10].

3.1.4 Comparison with traditional amino adsorbents and activated carbon

Table 2 compares the performance of MOF materials, traditional amine-based adsorbents, and activated carbon in carbon neutrality.

Table 2. Performance Comparison of MOF Materials, Traditional Amine-based Adsorbents and Activated Carbon in Carbon Neutrality.

Evaluation Index	**Metal-Organic Framework Materials**	**Traditional Amine-based Adsorbents**	**Activated Carbon**
CO_2 Adsorption Capacity	High; typically 2–8 mmol/g (e.g., Mg-MOF-74 can reach 8.6 mmol/g); pore size and structure are adjustable to match CO_2 molecular size	Moderate; 1–3 mmol/g; mainly relies on chemical reaction between amine groups and CO_2	Low to moderate; 0.5–2 mmol/g; limited by specific surface area and pore structure
Adsorption Selectivity (CO_2 /N_2)	Excellent; selectivity coefficient is usually >100; functional modification of ligands can further improve the affinity to CO_2	Good; selectivity coefficient is 50–100; chemical adsorption has strong specificity to CO_2	Poor; selectivity coefficient is generally <50; physical adsorption is non-selective
Adsorption Mechanism	Physical adsorption dominated, supplemented by chemical adsorption; pore filling effect and coordination interaction with metal sites are the main driving forces	Chemical adsorption; amine groups (-NH_2) react with CO_2 to form carbamate or bicarbonate	Physical adsorption; van der Waals force and capillary condensation are the main driving forces
Regeneration Performance	Good; low regeneration energy consumption (80–120 kJ/mol CO_2); can be regenerated by temperature swing adsorption (TSA) or pressure swing adsorption (PSA) without significant structure damage	Poor; high regeneration energy consumption (150–300 kJ/mol CO_2); amine groups are prone to volatilization and degradation after multiple regeneration cycles	Good; low regeneration energy consumption (60–100 kJ/mol CO_2); simple regeneration process, but adsorption capacity will decrease slightly after long-term use
Stability	Medium; water vapor and acidic gases may cause framework collapse; modified MOFs (e.g., UiO-66) have enhanced stability	Poor; amine groups are easy to hydrolyze and oxidize; need to be used in dry environment	Excellent; chemical stability is high; resistant to acid, alkali and high temperature; can be used in complex industrial environments
Cost	High; synthesis requires high-purity metal salts and organic ligands; complex preparation process; large-scale production is limited	Medium; raw materials are cheap and easy to obtain; mature synthesis process; suitable for industrial application	Low; wide source of raw materials (e.g., coal, coconut shell); simple preparation process; low production cost
Application Scenarios in Carbon Neutrality	Suitable for high-purity CO_2 capture in flue gas, natural gas purification and direct air capture (DAC)	Mainly used for CO_2 capture in power plant flue gas; suitable for large-scale fixed-source emission scenarios	Applicable to low-concentration CO_2 adsorption in industrial waste gas; can be used in combination with other technologies

3.2 Carbon sequestration-storage and transportation phase

MOFs play a pivotal role in carbon sequestration by serving as the key intermediate link in the carbon neutrality chain, enabling high-density, secure storage and low-loss, efficient transportation of CO_2, H_2, and CH_4.

3.3 Carbon conversion process

Carbon conversion, as a key technological pathway to achieve the "carbon neutrality" goal, centers on converting captured CO_2 into high-value chemicals or fuels, thereby realizing the dual objectives of "carbon reduction" and "carbon resource utilization." Through catalytic and hydrogenation processes, CO_2 can be transformed into CH_3OH, CH_3CH_2OH, CH_4, olefins, CO, etc.

4 Systemic synergy of MOF in carbon neutrality system

The integrated application of multiple green technologies represents the sole pathway to carbon neutrality. By leveraging MOF's unique properties and combining green development strategies with resource optimization, researchers are exploring deep system integration with carbon-neutral solutions. Through precise allocation of zero-carbon and recyclable energy and material flows, this approach reduces energy consumption and environmental impact across the entire industrial chain, providing critical support for the large-scale adoption of MOF in carbon-neutral initiatives.

4.1 Synergy with renewable energy

The intermittent and unstable nature of renewable energy sources (e.g., solar, wind, and hydro) remains a key challenge for large-scale deployment. Through functional customization, MOFs can synergistically optimize energy capture, storage, and carbon conversion, thereby establishing an integrated 'energy-carbon cycle' system.

4.1.1 Synergy of CO_2 capture and conversion scenarios

In the electrocatalytic hydrogen production process using MOF materials, replacing grid hybrid input with clean energy sources like solar and wind power significantly reduces the Global Warming Potential (GWP). The utilization of solar thermal energy provides a sustainable heat source for the Direct Air Conversion (DAC) system, while also substantially enhancing its carbon-negative effect.

4.1.2 Direct synergy in the electrolysis system

Electrolysis systems (e.g., water electrolysis for hydrogen production, CO_2 reduction via electrolysis) serve as core platforms for renewable energy storage and conversion. Through electrode structure optimization and active site regulation, MOFs and their derivatives have significantly enhanced the efficiency and stability of electrolysis processes [11].

4.2 Integration with carbon capture, utilization and storage systems

CCUS full-chain optimization requires addressing the interconnection bottlenecks across all stages—capture, transportation, utilization, and storage. Through Process Integration (PI) design and Life Cycle Assessment (LCA) optimization, MOF achieves reduced energy consumption and minimized environmental impact. Its outstanding stability and regenerability also meet the stringent demands of real-world operating conditions.

4.2.1 Process integration and life cycle assessment (LCA) analysis

Typically, after capturing CO_2, the process requires desorption, purification, compression, and transportation to enable further utilization or storage. This phase accounts for approximately 60%–80% of the total energy consumption in the CCUS process. The core of MOF integration in CCUS systems lies in achieving material transfer and minimizing energy loss between stages through functional material design. Life cycle assessment (LCA) provides a scientific basis for evaluating the environmental benefits of such integrated systems.

4.2.2 Stability and regenerability of MOF materials under actual operating conditions

The complexity of real-world operating conditions imposes stringent requirements on the stability of MOF materials, while excellent regenerability is key to reducing operational costs. In industrial flue gas capture scenarios, Mg-MOF-74-N_2 achieves a CO_2 capacity of 3.67 mmol/g, with its adsorption capacity remaining unchanged after 10 adsorption-desorption cycles. ZnH-MFU-41 demonstrates remarkable performance in capturing CO_2 from simulated flue gas environments generated by steel production. After 508 cycles over 150 hours, it retains over 96% of its initial adsorption capacity while maintaining stable selective adsorption of CO_2 among flue gas pollutants.

4.3 Industrialization challenges and prospects

The safety and environmental concerns of MOFs, along with the high energy consumption required for their production per unit mass, have significantly hindered their transition to higher technological maturity levels. With breakthroughs in advanced preparation techniques, the bottlenecks faced by MOFs in large-scale applications within carbon-neutral systems—such as cost, scalable production, recyclability, and toxicity—are being progressively overcome, offering broad prospects for industrialization.

4.3.1 Breakthroughs in cost, scale, recyclability, and toxicity issues

Zn-MOF $\{[Zn_5(tz)_6(HCOO)_4]_2H_2O\}$ achieves hundred-gram-scale production through a combination of inexpensive metal salts and simple ligands, reducing the cost to approximately $14.05 per kilogram, thereby laying the foundation for low-cost applications. New industrial transformation methods such as Twin-Screw Extrusion, Continuous Flow Synthesis, andDry-Gel Conversion have achieved large-scale production of $Cu_3(BTC)_2$, ZIF-8, MIL-140A, MIL-100(Fe), and Al-fumarate. Industrial-scale reuse has been achieved for materials such as ZnH-MFU-4l and CALF-20. Current research has achieved the substitution of water, ionic liquids, and bio-based solvents, as well as the transition to solvent-free preparation methods. Additionally, metal precursors such as acetates, carbonates, and hydroxides are employed, with by-products predominantly being environmentally friendly CO_2 and H_2O or weak acids [12].

4.3.2 Advanced preparation techniques

In the context of carbon neutrality, achieving green and large-scale production with low energy consumption is essential. Companies that have achieved mass production and their representative products include BASF, MOF Technologies, and Framergy. The mechanochemical synthesis route offers significant advantages, such as extremely low solvent usage, high raw material safety, minimal environmental impact, and a cost advantage of only 1/5.7 compared to solvothermal synthesis. This approach demonstrates greater sustainability and represents the direction for advanced large-scale MOF production [13].

5 Challenges and future prospects

MOFs demonstrate significant potential in carbon neutrality, but scaling up laboratory innovations to industrial deployment faces multiple challenges. These challenges extend beyond material properties to encompass system integration, environmental impacts, and interdisciplinary collaboration. Identifying and addressing these barriers is crucial to unlocking the strategic value of MOFs as “molecular sponges”. This discussion examines core challenges and future development pathways through authoritative literature and practical case studies.

5.1 Stability and selective attenuation under actual operating conditions

The outstanding experimental performance of most MOFs is severely compromised in practical applications, with significant degradation in adsorption capacity, selectivity, and cyclic stability. The critical challenge lies in bridging the gap between laboratory-scale demonstrations and industrial-scale implementation, which represents the most substantial obstacle to MOFs' integration into carbon neutrality initiatives.

5.2 Development of multifunctional MOF composite systems

A single MOF struggles to simultaneously meet multiple demands such as high adsorption capacity, rapid kinetics, strong stability, and catalytic activity, making the construction of multifunctional composite systems an important trend. Through strategies like MOF/carbon material composites, MOF/porous SiO_2 composites, MOF/metal oxide composites, MOF-on-MOF composites, and MOF/MXene composites, the performance of materials in three major directions—carbon capture, catalytic conversion, and energy storage—has been significantly enhanced [14].

5.3 Life cycle carbon footprint and recycling strategies

A comprehensive analysis of the carbon footprint throughout the MOF lifecycle reveals that the preparation stage consumes high energy, while the usage and recycling stages exhibit lower energy consumption compared to traditional CO2 adsorption technologies. However, there remains a gap between these energy consumption patterns and the requirements for carbon neutrality. In recent years, with the advancement of green MOF preparation techniques, shifts in adsorption mechanisms, and increased recycling cycles, the carbon footprint advantages have become increasingly evident.

To enhance the recycling efficiency of MOFs, reduce environmental risks, and achieve their circular utilization, methods such as loading MOFs into porous carriers for recovery, chemical recycling regeneration, pyrolysis conversion into porous carbon or metal oxide derivatives for recovery, and preparation of composite materials for recycling have been adopted [15].

5.4 From material research to interdisciplinary collaboration

Based on a review of relevant literature from 2021 to 2025, the development of MOFs in the field of carbon neutrality—from material research to interdisciplinary collaboration—should follow these pathways.

5.4.1 Multidisciplinary collaborative design for R&D breakthroughs

Through the synergy of theories and technologies in materials science, artificial intelligence, computational science, and environmental science, we achieve end-to-end collaboration spanning theoretical innovation, R&D efficiency enhancement, and comprehensive lifecycle support.

Collaboration with environmental engineering enhances environmental considerations during the process, focusing on the preparation of low-energy-consumption and low-pollution materials and resource recycling to reduce environmental impact. Collaboration with the energy sector promotes the utilization of new energy sources and advances in energy storage and battery technologies, improving the performance of photocatalytic and electrocatalytic reactions to achieve the complete replacement of traditional energy sources. Chemical engineering collaborates to develop green and low-cost MOF synthesis methods, enabling large-scale production and application of MOFs. Collaboration with computer science and artificial intelligence facilitates the design and screening of MOF materials, as well as performance prediction and simulation, thereby shortening the "trial-and-error period".

5.4.2 Engineering transformation phase: cross-domain collaborative breakthrough

This phase requires cross-disciplinary collaboration among chemical engineering, environmental science, and policy departments to overcome scaling challenges through three dimensions: process optimization, end-to-end pollution control, and policy pilot integration, achieving integrated transformation that is "technically feasible, environmentally friendly, and policy-aligned." By collaborating with chemical engineering science, we will accelerate the enhancement of synthetic process capacity and the realization of industrial-scale production. Through coordination with environmental science and other disciplines, we will establish a comprehensive recycling system design for the entire production process. Furthermore, real-time sharing of pilot-scale data with policy departments will expedite the formulation of technical standards.

5.4.3 System deployment phase: global synergy of policy and science

The transition of MOF materials from industrial production to large-scale deployment in global carbon neutrality scenarios is not an isolated effort by any single country or sector. It requires a three-dimensional framework of "policy guidance, financial empowerment, and global collaboration." By leveraging international policy tools to steer technological development, innovative financial mechanisms to stimulate market vitality, and transnational collaboration networks to address challenges in technology transfer and regional adaptation, MOF technology can achieve efficient global implementation, providing scalable technical support for carbon neutrality goals. The key to this phase lies in breaking down national and disciplinary barriers, transforming MOF's technological potential into globally shareable emission reduction capabilities.

6 Conclusion

As global carbon neutrality initiatives advance, the low-carbon technology ecosystem is evolving from single-focused emission reduction to a multidimensional "reduction-negative-carbon-circularity" synergy, where MOFs (Metal-Organic Frameworks) demonstrate strategic significance. First, MOFs bridge technological gaps: They provide novel pathways to overcome bottlenecks in traditional carbon management. In Direct Air Carbon Capture (DAC) systems, MOFs 'low-concentration adsorption and low-temperature regeneration capabilities could drastically reduce unit costs, paving the way for large-scale negative-carbon applications. In carbon utilization, MOFs' single-atom catalytic site control resolves poor product selectivity in conventional catalysts, shifting carbon conversion from "low-value utilization" to "high-value recycling." Second, MOFs drive systemic synergy: They establish critical bridges between renewable energy and carbon management. Solar-powered MOF adsorption-desorption cycles reduce regeneration energy consumption, while MOF-based photovoltaic systems achieve closed-loop operation of "solar capture-CO2 capture-carbon conversion." Enhanced electrocatalytic capabilities enable complete replacement of traditional energy sources with high-value CO2-based chemicals or fuels. This "energy-carbon management" synergy improves renewable energy efficiency and reduces carbon emissions, aligning with the integrated development trend of future low-carbon systems. Third, MOFs support diverse applications: Their modular design allows adaptation to carbon source requirements across various scales and types. This technology achieves full compatibility across diverse scenarios—from large industrial emitters (e.g., power plants, steel mills) to small and medium-sized facilities (e.g., cement plants, biomass power plants)—addressing the limitations of existing CCUS technologies, which are often centralized and require high entry barriers. In emerging applications like marine carbon sequestration and hydrogen storage/transportation, the salt resistance and extreme environment resilience of MOF@polymer composite membranes and MOF@inorganic oxide composites further expand the application boundaries of low-carbon technologies.

However, it is crucial to recognize that the large-scale application of MOFs (Metal-Organic Frameworks) still faces challenges including cost constraints, long-term stability issues, environmental footprint, insufficient interdisciplinary collaboration, and underdeveloped policy support and market mechanisms. Future development should shift from focusing solely on new material synthesis to a comprehensive innovation approach integrating "performance, process, system, and sustainability." This involves: developing green, continuous synthesis processes to reduce costs; building multifunctional composite systems to enhance adaptability in complex operating conditions; conducting life cycle assessments to ensure net carbon reduction benefits; fostering deep collaboration across chemical, engineering, and policy domains to accelerate technology transfer; improving government decision-makers' awareness and attention, expanding international technical cooperation, and expediting the promotion of demonstration projects.

In summary, MOFs (Metal-Organic Frameworks), as "molecular sponges," have demonstrated full-chain value from "carbon capture" to "carbon conversion" and "carbon storage (transportation, storage)" in the carbon neutrality pathway. However, unlocking their strategic potential requires deep interdisciplinary integration, sustained engineering progress, and global policy support alongside market mechanism refinement. With technological innovation and collaborative mechanisms improving, MOFs are poised to become "pillar materials" in the global carbon neutrality process, providing critical support for accelerating net-zero emission targets.

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