

# Metal Organic Frameworks: From Structural Engineering to CO<sub>2</sub> Capturing Applications

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## ABSTRACT

Carbon dioxide (CO<sub>2</sub>) emissions are a major driver of global climate change, creating an urgent need for efficient and scalable carbon capture technologies. Metal organic frameworks (MOFs) have emerged as a promising class of porous materials for CO<sub>2</sub> capture due to their tunable structures, ultrahigh surface areas, and chemically addressable adsorption sites. This narrative review synthesizes current research on MOFs for CO<sub>2</sub> capture, with a focus on how chemical composition and key structural features, including porosity, active sites, and framework stability, govern adsorption performance. Representative MOFs are discussed to illustrate structure performance relationships and to highlight design tradeoffs relevant to practical applications. In addition, current challenges and future research directions are examined, including material stability under realistic operating conditions, cost effective synthesis, and the integration of carbon capture with CO<sub>2</sub> utilization strategies. The objective of this review is to consolidate design principles for MOF based CO<sub>2</sub> capture and to provide a conceptual framework to guide the development and industrial implementation of high-performance MOF materials.

**Keywords:** Metal organic frameworks; carbon capture; chemical properties; applications; structure; climate change; carbon dioxide

## INTRODUCTION

Greenhouse gases play a fundamental role in regulating Earth's climate by trapping heat in the atmosphere. However, anthropogenic activities have substantially intensified this natural greenhouse effect, primarily through the large-scale emission of carbon dioxide (CO<sub>2</sub>), leading to accelerated global warming. Atmospheric CO<sub>2</sub> concentrations reached 426.9 ppm in May 2024, with the period from 2022 to 2024 representing the largest two-year increase in recorded

history (1). This rapid accumulation has been associated with increasingly frequent and severe extreme weather events, underscoring the urgency of mitigating CO<sub>2</sub> emissions to meet international climate targets that aim to limit global temperature rise to approximately 1.5–2 °C above preindustrial levels (2).

Carbon capture and storage (CCS) has been widely recognized as an indispensable strategy for addressing this challenge, as it enables the direct removal of CO<sub>2</sub> from both industrial emission sources and, potentially, the atmosphere. While renewable energy technologies are essential for long term decarbonization, they face significant limitations in reducing emissions from hard to abate sectors such as cement, steel, and petrochemical industries. In this context, CCS provides a complementary pathway that supports emission reduction while maintaining industrial productivity. In particular,

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capturing CO<sub>2</sub> from concentrated industrial streams, where CO<sub>2</sub> levels typically range from 20 percent to over 50 percent, is substantially more cost effective than direct air capture, in which CO<sub>2</sub> is present only in trace concentrations amid nitrogen and oxygen (3).

Conventional carbon capture approaches, including biological sequestration and geological storage, are constrained by challenges related to scalability, efficiency, and long-term stability. As an alternative, metal organic frameworks (MOFs), a class of synthetic porous crystalline materials with ultrahigh surface areas, have attracted increasing attention for CO<sub>2</sub> capture. Their modular construction from metal containing secondary building units and organic linkers enables precise control over pore size, surface chemistry, and adsorption sites, allowing MOFs to outperform traditional adsorbents such as activated carbons and zeolites in terms of selectivity and capacity. Despite rapid progress in this field, existing studies are often fragmented, and a comprehensive synthesis linking MOF structural design to CO<sub>2</sub> capture performance and practical applicability remains limited.

This narrative review aims to address this gap by evaluating the potential of MOFs for CO<sub>2</sub> capture through an integrated analysis of their chemical composition, structural features, and adsorption performance. By examining representative MOFs that exemplify structure performance relationships, this review seeks to clarify key design principles and to identify research directions that can facilitate the translation of MOF based CO<sub>2</sub> capture technologies from laboratory studies to industrial applications.

## THE CHEMISTRY OF MOFS

Metal organic frameworks are crystalline porous materials assembled from metal containing secondary building units and organic linkers. The modular combination of these components enables precise control over framework topology, pore architecture, and chemical functionality, which are critical factors governing gas adsorption behavior. By varying the identity of the metal centers and organic linkers, a wide range of MOF structures can be rationally designed to tailor interactions with target molecules such as carbon dioxide (4).

Secondary building units play a central role in defining MOF structure and functionality. Rather than isolated metal ions, these units consist of preorganized metal clusters that impose fixed coordination geometries and impart structural rigidity to the framework. Their coordination environments determine how organic

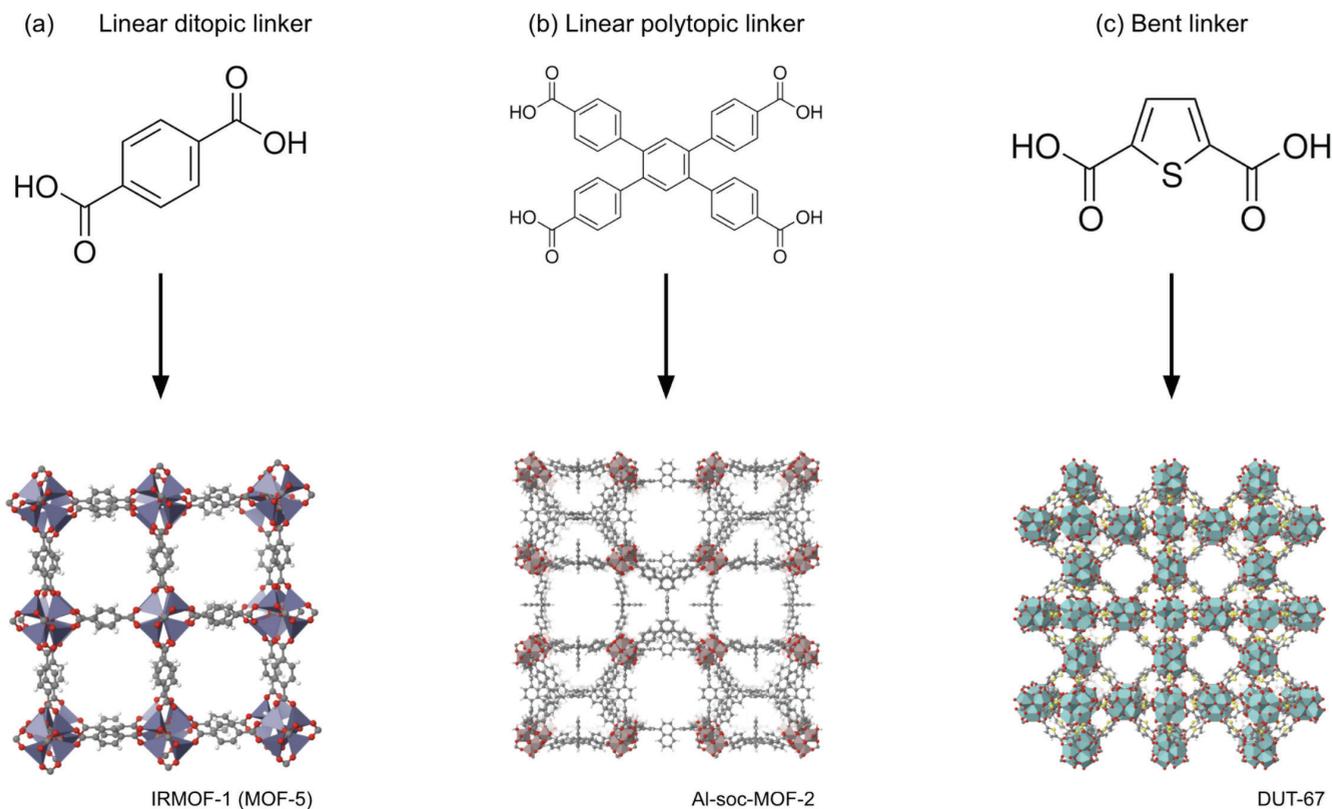
linkers connect, thereby shaping overall framework topology. In many MOFs, the removal of coordinated solvent molecules during activation generates open metal sites, which act as strong adsorption centers for CO<sub>2</sub> through enhanced electrostatic and Lewis acid interactions. This feature is particularly important for improving CO<sub>2</sub> uptake at low pressures relevant to post combustion capture conditions (5).

Organic linkers further regulate framework connectivity, pore size, and chemical environment. Linkers with two coordination sites typically connect adjacent secondary building units to form extended linear or planar motifs, while linkers containing three or more coordination sites enable the construction of fully three-dimensional frameworks with higher connectivity. Beyond connectivity, linker geometry strongly influences pore accessibility and diffusion pathways, while linker functionalization can introduce specific chemical interactions with CO<sub>2</sub> molecules. As a result, linker selection represents a key design lever for balancing adsorption capacity, selectivity, and framework stability (6).

The structural role of organic linkers extends beyond simple framework assembly. Linear linkers such as 1,4 benzenedicarboxylate tend to promote ordered networks with well-defined pore channels, whereas non linear or bent linkers favor the formation of more complex architectures with irregular cavities and discrete metal organic polyhedra. These differences in topology directly affect pore size distribution and surface chemistry, which in turn influence gas transport and adsorption behavior. Functional groups such as amino, halogen, or alkyl substituents can be introduced onto linkers to further tune host guest interactions and enhance CO<sub>2</sub> affinity under practical operating conditions (7).

Although MOFs are sometimes classified according to dimensionality, such as one dimensional, two dimensional, or three-dimensional connectivity, this distinction is less important for CO<sub>2</sub> capture performance than the resulting pore structure and chemical environment. Frameworks with higher dimensional connectivity generally exhibit improved structural robustness and interconnected porosity, which are advantageous for maintaining adsorption capacity under repeated adsorption desorption cycles. Consequently, modern MOF design increasingly emphasizes topology control and chemical functionality rather than simple dimensional classification (8).

Figure 1 illustrates how linker geometry influences framework topology and pore architecture, highlighting



**Figure 1.** The geometry and connectivity of organic linkers strongly influence the topology and functionality of metal organic frameworks. Linear linkers with two coordination sites tend to form ordered frameworks with regular pore channels, while linkers with higher connectivity enable more complex three-dimensional architectures. Nonlinear linker geometries promote irregular cavities and discrete metal organic polyhedra. Adapted from publicly available structural data in Ref. (9).

the structural diversity achievable through rational linker design and its implications for gas adsorption behavior.

## KEY STRUCTURAL FEATURES FOR CARBON CAPTURE

Porosity is one of the most critical structural determinants governing the carbon capture performance of metal organic frameworks. A porous framework enables gas molecules to diffuse through the internal structure and interact with chemically active adsorption sites, thereby facilitating CO<sub>2</sub> uptake and storage. Unlike simple surface adsorption, porosity in MOFs arises from the deliberate assembly of metal containing secondary building units and organic linkers, making it highly tunable but also strongly dependent on framework topology and coordination geometry.

An important design strategy for controlling porosity in MOFs is the isorecticular principle (7), in which

the overall crystal topology of a parent framework is preserved while the organic linkers are systematically modified. By extending or functionalizing linkers while maintaining the same connectivity, pore size, shape, and surface area can be adjusted in a predictable manner. This approach enables precise tuning of pore metrics that are essential for matching the molecular dimensions of CO<sub>2</sub>. Given that the kinetic diameter of CO<sub>2</sub> is approximately 0.35 to 0.51 nm (10), frameworks with pore apertures in the range of about 3.5 to 5.5 Å are generally considered favorable for selective CO<sub>2</sub> adsorption, as they balance diffusion accessibility with strong host guest interactions.

Beyond moderate pore sizes, some MOFs exhibit ultrahigh porosity, characterized by exceptionally large void fractions and internal surface areas. In the context of carbon capture, ultrahigh porosity refers to frameworks in which a substantial proportion of the crystal volume is accessible void space, resulting in high total pore volume and adsorption capacity. Such structures typically possess

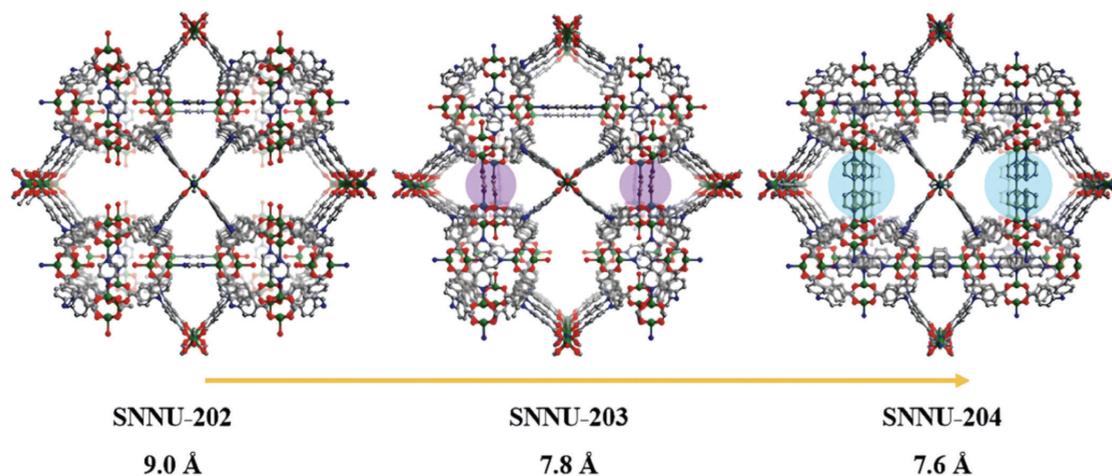
Brunauer Emmett Teller surface areas that far exceed those of conventional porous materials, allowing them to adsorb large quantities of gas molecules (10). While ultrahigh porosity can significantly enhance gravimetric CO<sub>2</sub> uptake, it may also introduce tradeoffs related to framework stability and selectivity, highlighting the need to balance pore volume with structural robustness (Figure 2).

Thermal and chemical stability represent another essential requirement for practical carbon capture applications, particularly under industrial operating conditions. While many MOFs remain stable under ambient laboratory environments, exposure to elevated

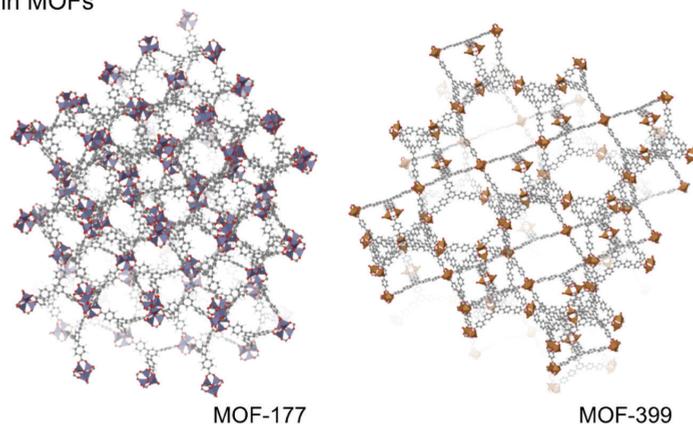
temperatures, non neutral pH conditions, moisture, and reactive flue gas components can lead to framework degradation. High stability is typically associated with strong coordination bonds, such as metal oxygen or metal nitrogen linkages, and with robust metal clusters that resist hydrolysis and ligand displacement. Frameworks capable of maintaining crystallinity and porosity under acidic or basic conditions, high humidity, and prolonged thermal stress are therefore more suitable for real world CO<sub>2</sub> capture processes (4).

In addition to adsorption from the gas phase, MOFs have also been explored as solid absorbents in gas scrubbing processes, where selective mass transfer

(a) The isoreticular principle: the accurate control of porosity



(b) Ultra-high porosity in MOFs



**Figure 2.** Porosity control in metal organic frameworks. (a) Schematic illustration of the isoreticular principle, in which the overall framework topology is preserved while systematic modification of organic linkers enables precise tuning of pore size and geometry. Representative structures are shown to demonstrate progressive changes in pore dimensions. (b) Examples of metal organic frameworks exhibiting ultrahigh porosity, highlighting the large internal void space characteristic of frameworks with exceptionally high surface area and pore volume. Adapted from publicly available structural data in Ref. (9).

occurs between a gas mixture and a liquid phase. Their tunable pore environments and chemically addressable internal surfaces enable tailored interactions with CO<sub>2</sub>, offering advantages over conventional absorbents such as amine solutions, activated carbons, and zeolites. Collectively, the combination of tunable porosity and robust thermal and chemical stability positions MOFs as state-of-the-art materials for advanced gas separation and carbon capture technologies (10).

Building on these structural design principles, the following section focuses on representative MOF systems that exemplify how porosity and stability can be deliberately engineered to achieve high performance CO<sub>2</sub> capture under near ambient and industrially relevant conditions.

## REPRESENTATIVE MOFS FOR CO<sub>2</sub> CAPTURE

Table 1 summarizes representative metal organic frameworks that exhibit efficient CO<sub>2</sub> capture performance under near ambient conditions. These materials were selected to illustrate how distinct structural features, including open metal sites, cooperative adsorption sites, and framework stability, translate into practical adsorption performance.

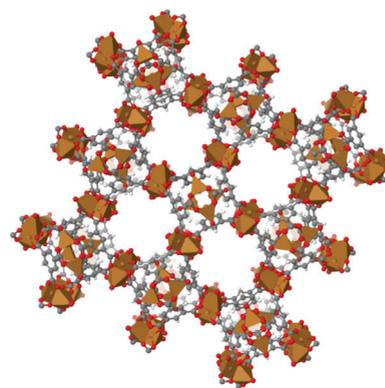
### HKUST-1: Copper-Based Framework for CO<sub>2</sub> Adsorption

HKUST-1, also known as MOF-199, is a prototypical copper-based framework featuring open metal sites that play a central role in CO<sub>2</sub> adsorption. These open Cu<sup>2+</sup> sites are generated by removing coordinated terminal ligands, such as water or dimethylformamide, through

**Table 1.** Representative metal organic frameworks for CO<sub>2</sub> capture under near ambient conditions. Operating pressure, temperature, and adsorption capacities are reported using consistent units. Variations in the reported CO<sub>2</sub> uptake values for FJI-H14 arise from differences in operating temperature, reflecting the temperature dependence of adsorption thermodynamics. (Table adapted from Ref. (5))

MOF absorbent	Operating pressure (bar)	Operating temperature (K)	CO <sub>2</sub> capture capacity (mmol g <sup>-1</sup> )
HKUST-1	1	298	4.1
FJI-H14	1	298–351	12.5–6.5
Bio-MOF-11	1	298	4.1

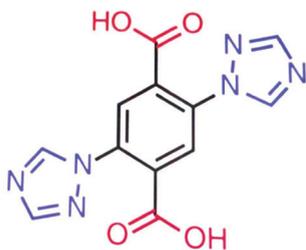
thermal activation or vacuum treatment. The resulting Lewis acidic sites interact strongly with CO<sub>2</sub> molecules, leading to high adsorption affinity at low pressures. At 298 K and 1 bar, HKUST-1 exhibits a CO<sub>2</sub> uptake of approximately 4.1 mmol g<sup>-1</sup>, while higher pressures can further increase adsorption capacity. The adsorption isotherm typically displays Type I behavior, indicating strong adsorption at low partial pressures and making HKUST-1 suitable for CO<sub>2</sub> capture from flue gas streams (11) (Figure 3).



**Figure 3.** Crystal structure of HKUST-1, highlighting the presence of open copper sites that facilitate strong interactions with CO<sub>2</sub> molecules. Adapted from publicly available structural data in Ref. (9).

### FJI-H14: Multi-Site MOF for CO<sub>2</sub> Capture

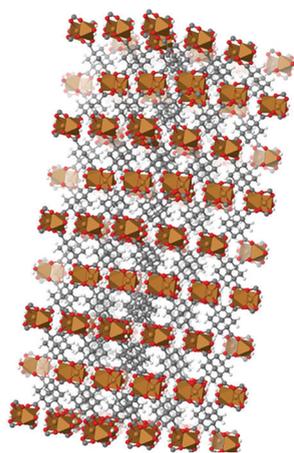
FJI-H14 is a Cu(II) based metal organic framework that incorporates both open metal sites and Lewis basic sites within its structure, enabling cooperative adsorption mechanisms. The coexistence of multiple active sites enhances CO<sub>2</sub> binding strength and results in high CO<sub>2</sub>/N<sub>2</sub> selectivity under mixed gas conditions. At lower temperatures, FJI-H14 exhibits higher adsorption capacity due to the exothermic nature of CO<sub>2</sub> adsorption, while increasing temperature reduces uptake as equilibrium shifts toward desorption. Under simulated post combustion flue gas conditions, FJI-H14 demonstrates robust adsorption performance and high selectivity, underscoring the importance of synergistic site design for efficient carbon capture. Despite its strong adsorption characteristics, extremely high operating temperatures may compromise coordination stability, emphasizing the need to balance adsorption strength with structural robustness (12) (Figure 4).



**Figure 4.** Structural representation of FJI-H14, illustrating the coexistence of open metal sites and Lewis basic sites that contribute to cooperative CO<sub>2</sub> adsorption. Redrawn based on Ref. (11).

### Bio-MOF-11: Stable and Recyclable Cobalt-Based MOF

Bio-MOF-11 is a cobalt based framework that relies primarily on Lewis basic sites to enhance CO<sub>2</sub> adsorption through acid base interactions. In addition to its inherent adsorption capability, Bio-MOF-11 exhibits good structural compatibility with guest species, allowing post synthetic modifications such as cation exchange to further optimize performance. At 298 K and 1 bar, Bio-MOF-11 displays a CO<sub>2</sub> uptake of approximately 4.1 mmol g<sup>-1</sup>. After cation exchange, the framework maintains comparable adsorption capacity while showing improved thermal stability and cycling performance. These characteristics make Bio-MOF-11 a promising candidate for repeated CO<sub>2</sub> capture under operational conditions where durability and recyclability are critical (13) (Figure 5).



**Figure 5.** Crystal structure of Bio-MOF-11, illustrating its porous framework and adsorption sites relevant to CO<sub>2</sub> capture. Adapted from publicly available structural data in Ref. (9).

### SYNTHESIZING STRUCTURE PERFORMANCE RELATIONSHIPS

The representative MOFs discussed above demonstrate that CO<sub>2</sub> capture performance is not an intrinsic material property, but rather the result of deliberate structural engineering. Across different framework platforms, adsorption behavior emerges from the interplay between pore architecture, active site chemistry, and framework stability. These examples collectively illustrate how targeted design strategies translate fundamental structural features into practical carbon capture performance.

Comparative analysis reveals clear structure performance tradeoffs that guide rational MOF design. Frameworks dominated by open metal sites, such as HKUST-1, exhibit strong adsorption affinity at low pressures but may be limited in maximum uptake and long-term durability under harsh operating conditions. In contrast, frameworks incorporating multiple cooperative adsorption sites, exemplified by FJI-H14, achieve higher capacities and selectivities, albeit with increased sensitivity to temperature and coordination stability. MOFs emphasizing framework robustness and recyclability, such as Bio-MOF-11, prioritize long term operational stability over peak adsorption capacity, highlighting the importance of durability in repeated capture cycles.

These tradeoffs underscore that optimal MOF design depends on the intended capture scenario. For post combustion flue gas treatment, materials combining strong adsorption sites with sufficient thermal and chemical stability are favored. In contrast, applications involving atmospheric or humid gas streams require enhanced framework resilience and tolerance to moisture, even at the expense of reduced gravimetric capacity. Consequently, no single MOF architecture is universally optimal; instead, performance arises from balancing adsorption strength, selectivity, stability, and scalability.

Overall, the structure performance relationships identified in this review emphasize that effective CO<sub>2</sub> capture materials must integrate controlled porosity, tailored active sites, and robust framework chemistry. These principles provide a foundation for guiding future MOF development toward application specific optimization rather than maximizing isolated performance metrics.

## CONCLUSION

This narrative review has examined the chemistry, structural design, and application of metal organic frameworks for CO<sub>2</sub> capture, with an emphasis on how porosity control, active site engineering, and framework stability collectively determine adsorption performance. By analyzing representative MOF systems, this work highlights the central role of rational structural design in translating fundamental material properties into practical carbon capture capabilities.

Beyond adsorption and storage, the future of MOF based carbon capture lies in the integration of capture and utilization. Rather than serving solely as passive sorbents, MOFs can be engineered or functionalized to act as heterogeneous catalysts that convert captured CO<sub>2</sub> into value added chemicals and fuels. Such multifunctional platforms offer a pathway toward closed loop carbon management, in which CO<sub>2</sub> becomes a resource rather than a waste product.

At the same time, large scale deployment of MOF technologies will depend on advances in cost effective synthesis, long term stability, and recyclability under realistic operating conditions, including humid and chemically complex gas streams. Addressing these challenges will require interdisciplinary efforts that bridge materials chemistry, catalysis, and process engineering. Continued progress along these directions has the potential to accelerate the transition from laboratory scale demonstrations to industrial implementation, contributing meaningfully to global carbon mitigation strategies.

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## CONFLICT OF INTEREST

The author declares that there are no conflicts of interest regarding the publication of this article.

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