

Post-Synthetic Modification Strategies for Enhancing CO₂ Capture Performance on Metal–Organic Frameworks: A Review of Progress, Challenges, and Future Opportunities

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ABSTRACT

Metal-Organic Frameworks (MOFs) are defined as porous materials utilized for the molecular adsorption, offering exceptionally high surface areas, tunable pore structures, and chemical versatility that make them promising adsorbents for post-combustion carbon capture. Nevertheless, pristine MOFs often exhibit limitations, such as insufficient CO₂ selectivity and high sensitivity to humidity and temperature. These limitations restrict their potential practical application. To overcome these challenges, post-synthetic modification (PSM) has emerged as an effective strategy for tailoring MOF properties after synthesis by introducing functional groups or active sites without disrupting the framework structure. The effects of different functionalization approaches on adsorption mechanisms are discussed, together with the advantages of PSM over alternative modification methods. In addition, this review emphasizes current challenges associated with industrial implementation, including systems complexity, long-term stability, and large-scale production. By summarizing recent advances and remaining limitations, we demonstrate the significant potential of post-synthetically modified MOFs for developing efficient, selective, and sustainable carbon capture technologies.

INTRODUCTION

The continuous rise in atmospheric carbon dioxide concentrations is one of the most concerning environmental challenges of our generation. Primarily originating from fossil fuel combustion and major industrial processes, the abundance of the CO₂ gas acts as a major driving force for global warming. In response, many researchers have focused on the development of efficient carbon capture and storage solutions. Among the available solutions, adsorption-based carbon capture has attracted substantial attention because of its potential for lower energy consumption and compatibility with post-combustion separation processes.

Sep 2026
Vol 11. No 7.

Oxford Journal of Student Scholarship
www.oxfordjss.org

Adsorption occurs when liquid or gas molecules accumulate and adhere to a liquid or solid surface. Unlike absorption, this process involves molecules being retained solely on the pore surfaces, rather than penetrating the internal structure of the material. The substance providing the surface is called the adsorbent, whereas the substance adhering to the surface is called the adsorbate. [1] Adsorption-based technologies use waste heat in order to utilize low-thermal-grade energy. Hence, energy usage is lowered on account of replacing energy-heavy mechanical compressors with thermal-driven cycles. [2]

The performance of an adsorbent is evaluated based on various criteria such as its selectivity and regeneration capability. Selectivity refers to the adsorbent's ability to adsorb a target molecule from a mixture of gases or substances over other components, whereas regeneration capability refers to the ability to reuse the adsorbent following the removal of the captured molecules. [1] Adsorption is classified into two categories based on the strength of the bonds formed:

Physisorption: Known as physical adsorption, this process occurs when the adsorbate binds to the surface of the adsorbent via weak interactions, such as Van Der Waals forces or other weak intermolecular forces. [3] Usually in physisorption, adsorbates can form multilayers when binding to the adsorbent.

Chemisorption: An adsorption is called a chemisorption, also referred to as chemical adsorption, when the interactions between the surface of the adsorbent and the molecules it attracts are made up of strong chemical bonds. Forming chemical bonds at the adsorbate surface can only occur for specific molecules; thus, this technique involves high selectivity for the adsorbates. [3] Chemisorption can proceed on the surface of the adsorbent without forming any multilayers.

Today, some of the most commonly used adsorbents involve zeolites, metal–organic frameworks (MOF), activated carbons, and metal oxides. Among them, MOFs have demonstrated the most outstanding capacity for storing CO₂. MOFs are crystalline solids that are built up from a combination of diverse inorganic and organic subunits. [4] Such a combination of unique substances allows them to maintain a three-dimensional and porous shape, causing it to be permeable to capture gas molecules such as hydrogen and nitrogen. However, unmodified MOFs are not sufficient alone for the maximum adsorption of target molecules. Some MOFs might require high pressures or temperatures that inhibit the regeneration of the adsorbent itself. To address this issue, MOFs are engineered using pre-synthetic and post-synthetic strategies and functional group incorporation into their pore structure. Furthermore, the hydrophobic surface of MOFs further enables the pores to be tuned for the maximum selective adsorption of the target molecules.

Among these strategies, post-synthetic modification has enabled a versatile approach for modifying the properties of MOFs after their synthesis. By introducing new functional groups, MOFs can be modified after the formation of the solid lattice. [5] Post-synthetic modifications are advantageous compared to other modification techniques due to having greater control over the types of functional groups that can be incorporated into the material without affecting its overall stability. [5] This review provides an overview of how post-synthetic modification strategies can be used to enhance CO₂ capture performance of MOFs.

By examining the relationships between adsorption performance and functionalization methods, current challenges and future directions for the development of efficient CO₂ capture technologies are also highlighted.

RESEARCH QUESTION

Given growing interest in tailoring MOFs through post-synthetic modification for carbon capture, this review seeks to address the following research question:

How have post-synthetic modifications improved the CO₂ capture performance of metal–organic frameworks, and what challenges and opportunities remain for their practical application?

REVIEW METHODOLOGY

This literature review was conducted by identifying resources relevant to post-synthetic modifications of MOFs for CO₂ capture. Literature was selected based on its relevance to the research question, guest incorporation, functionalization strategies, and their effects on CO₂ adsorption capacity and selectivity. Alongside foundational reviews, studies measuring framework stability were included, consisting of direct air capture, pre-combustion, and post-combustion gas capture. A total of 25 sources were selected because they provided the most directly relevant evidence for the scope of the review. The findings were synthesized to identify advances, limitations, and remaining opportunities for the practical applications of post-synthetically modified MOFs in CO₂ capture.

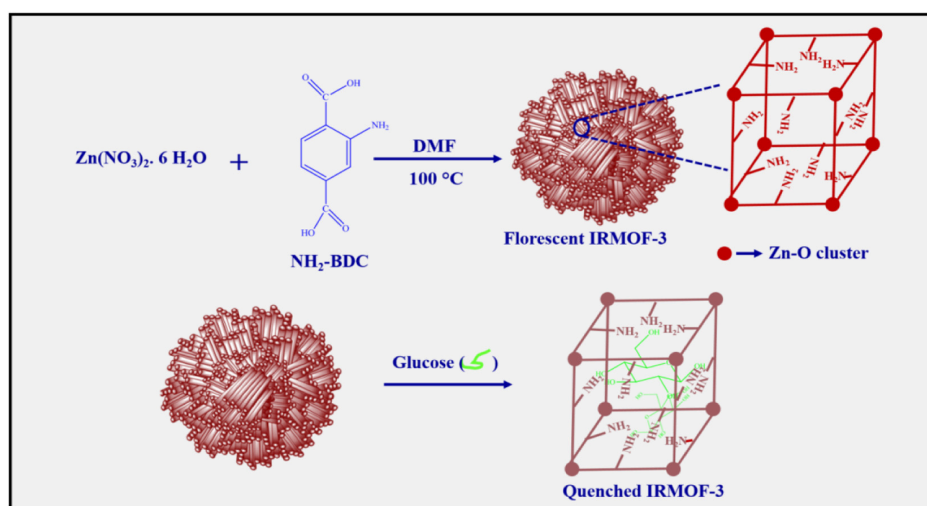
POST-SYNTHETIC MODIFICATIONS IN MOFs AND CO₂ CAPTURE

Post-synthetic modification (PSM) aims to resolve the limitations of conventional MOF synthesis by enabling structural and functional modifications after framework formation. [6] This strategy enhances the properties of MOFs that are often difficult or impossible to achieve through direct synthesis. Accordingly, PSM has become an optimal strategy for expanding the structural diversity and application potential of MOFs, involving various methods which will be further elaborated on in the following sections.

I (a) Covalent Post-Synthetic Modification:

Most common PSM strategies involve covalent modification, which refers to the chemical transformation of the organic linker (ligand) of a MOF while conserving the original framework topology. [5] Among the various functional groups available for modification, amine (-NH₂) groups are the most extensively studied because they are highly reactive and can undergo a wide range of organic reactions under relatively mild conditions. In this approach, amino-functionalized MOFs are treated with suitable chemical reagents, such as acid anhydrides, resulting in the introduction of new functional groups without disrupting the crystallinity or porosity of the framework. [5]

The feasibility of covalent PSM was first demonstrated using IRMOF-3, an extensively studied MOF, due to the presence of pendant amino groups that remain chemically accessible after framework formation. [5] In a study, Wang and Cohen successfully modified the amino groups of IRMOF-3 through acylation with acetic anhydride, converting the free amines into amide functionalities while retaining the crystal structure and porosity of the framework, demonstrating that conventional organic reactions could be performed within the confined environment of a MOF without compromising its structural integrity. As a consequence of this, covalent PSM is proved to be a practical strategy for optimizing pore functionality after synthesis. [5], [7] Building upon this concept, a wide variety of organic transformations have since been employed to expand the chemical diversity of MOFs. For instance, the amino groups of IRMOF-3 have been reacted with various acid anhydrides to introduce alkyl and aromatic amide functionalities, enabling systematic tuning of the pore surface chemistry. [7] Such modifications alter the chemical environment within the pores while maintaining the original framework topology, depicting one of the principal advantages of covalent PSM over direct solvothermal synthesis. [5]



[22] Note. Reproduced from "IRMOF-3: A fluorescent nanoscale metal organic frameworks for selective sensing of glucose and Fe (III) ions without any modification," by A. Kumar, A. R. Chowdhuri, A. Kumari, and S. K. Sahu, 2018, Materials Science and Engineering: C, 92, p. 915. Copyright 2018 by Elsevier.

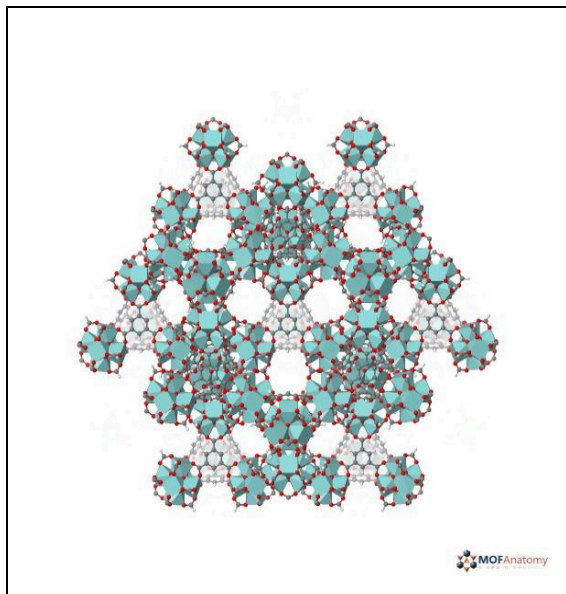
Beyond IRMOF-3, covalent PSM has been successfully applied to other amino-containing MOFs with enhanced chemical stability. For instance, MIL-53(Al)-NH₂ was transformed into isocyanate using the organic chemicals diphosgene and thiophosgene. [7] These reactive intermediates were subsequently converted into urea, thiourea, carbamate, and thiocarbamate derivatives through reactions with amines and alcohols, greatly expanding the range of accessible functional groups within the framework. [7] Likewise, DMOF-1-NH₂ underwent post-synthetic conversion of amino groups into azides, followed by Cu(I)-catalyzed azide-alkyne cycloaddition to produce materials with high conversion efficiencies, demonstrating the compatibility of modern organic synthetic methodologies with MOF chemistry. [7] These studies established covalent PSM as a versatile tool for engineering the internal surface chemistry of MOFs. By modifying the organic linker after framework assembly, researchers can introduce

functional groups that are incompatible with conventional solvothermal synthesis while sustaining crystallinity and permanent porosity. Consequently, covalent PSM has become a key strategy for tailoring MOFs in applications requiring precise control over adsorbent-adsorbate interactions, such as CO₂ capture.

I (b) Guest Incorporation Modification:

In the course of the delivery of large molecules, researchers often face challenges given that their encapsulation and transport are considerably more difficult than those of small molecules. To address this problem, physisorption has emerged as a straightforward post-synthetic incorporation strategy. In this approach, pre-synthesized MOFs with sufficiently large pore apertures are immersed in a solution containing the desired biomolecule, allowing the guest molecules to diffuse into the pores and become retained through non-covalent interactions such as hydrogen bonding, electrostatic interactions, hydrophobic interactions, or coordination with open metal sites. [8] The framework itself remains unchanged, resulting in the preservation of the crystalline structure of MOFs.

The incorporation of ionic liquids also serves as a vital guest incorporation technique to alter MOF pore capacity. Ionic liquids incorporated into MOF materials (known as IL/MOF composites) enable abundant ionic sites, thereby providing interactions such as hydrogen bonding, interaction, and acid-base interaction. [9] Popular post-synthesis methods like wet impregnation can be used upon fabricating IL/MOF composites, optimizing the properties of the framework. [9] Ultimately, IL/MOF composites serve as potential adsorbents for gas capture processes. Previous studies have scrutinized the adsorptive performances of poly(ionic liquid) (PIL)/MOF composites alongside core-shell IL/MOF structures and obtained that PIL/MOF composites have a much higher CO₂ affinity due to their large surface area, introducing them as better adsorbents for CO₂ capture. [10] A representative example of ionic liquid incorporation into MOF-808 was reported by Ahmad et al., who assembled ionic liquid molecular layers (ILMLs) onto the external surface of MOF-808 nanoparticles through a solution-mediated assembly method. The ionic liquid used formed nanometer-scale layers (approximately 1.7-1.8 nm thick) that acted as an adhesive interface for CO₂ adsorption while upholding the intrinsic porosity of MOF-808. [11] Electrostatic attractions between the ionic liquid anions and the Zr₆ metal nodes were confirmed by FTIR analysis, whereas PXRD patterns demonstrated that the crystallinity of MOF-808 remained intact following the post-synthetic modification. [11] As a result, the ILML@MOF-808 composite exhibited nearly a threefold increase in CO₂ adsorption capacity compared with pristine MOF-808. [11]



[23] Note. From MOF-808, by MOF Anatomy, n.d., MOF Anatomy (<https://mofanatomy.com/mof/mof-808>). Copyright [Year] by MOF Anatomy.

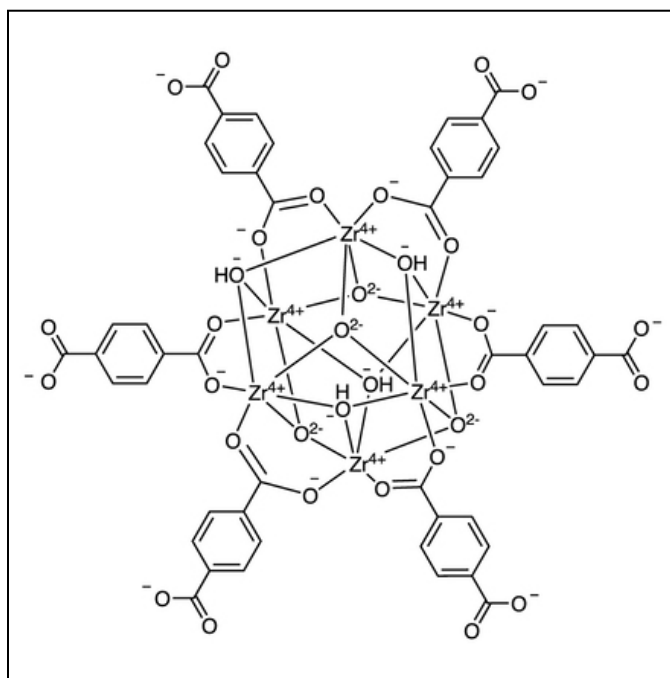
THE PRACTICAL APPLICATIONS OF MOFs IN CO₂ CAPTURE

Researchers have enhanced the adsorption performance of MOFs pertaining to the introduction of functional groups and the incorporation of guest molecules. Hence, the ability to modify the physiochemical properties of MOFs through post-synthetic modification has broadened their practical applications in the CO₂ capture field. This section discusses representative studies that carefully selected post-synthetic modifications to improve adsorption capacity, selectivity, and cyclic stability. Out of the various frameworks available, it is crucial to select experimental groups that respond to the desired modifications. In order to address these, IRMOF and UiO-66 were chosen to demonstrate direct air capture and pre-combustion and post-combustion air capture as desired. As UiO-66 exhibits an exceptional large surface area, its extension points for 1,4-benzenedicarboxylic acid coordination allow significant stability. [20] Conversely, IRMOF (such as IRMOF-1/MOF-5) was selected due to its prototype status, exceptionally high surface area, and highly systematic pore tunability [21]. The ability to predictably alter pore dimensions and surface chemistry within the IRMOF family provides a benchmark for investigating fundamental gas adsorption mechanisms and molecular transport kinetics.

II (a) Direct Air Capture (DAC):

Direct air capture (DAC) functions as a promising strategy for reducing the atmospheric CO₂ concentration directly, thereby relieving the transportation cost in carbon sequestration. [12] The carbon captured through this system can be directly used as industrial raw materials for the production of various other high-value-added products, truly reducing the atmospheric CO₂ pressure. [12] Having said that,

most solid adsorbents exhibit poor CO₂ capture capacity, as a consequence of which hinders the practical applications of DAC. Consequently, it is essential to develop more efficient adsorbents with high CO₂ capture capacity in humid air. Quasi-MOFs, a type of MOF synthesized by removing a portion of the organic ligand, act as promising candidates in order to capture CO₂ under dry conditions. Nonetheless, its working principles under humid conditions are still being explored, utilizing post-synthetic modification with H₂O. [12] Accordingly, the frameworks UiO-66 and Quasi-UiO-66 were examined independently and were synthesized by introducing different amounts of organic compounds. To improve the performance of these frameworks under realistic atmospheric conditions, the researchers included structural defects into UiO-66 through the controlled removal of organic linkers, obtaining quasi-UiO-66 with additional open coordination sites available for post-synthetic modification. [12], [13] The defective frameworks were subsequently functionalized with water molecules, enabling the formation of hydrogen-bonding networks that promoted stronger interactions between CO₂ and the adsorbent under humid conditions. Characterization techniques, including powder X-ray diffraction (PXRD), FTIR, and nitrogen adsorption measurements, confirmed that the structural integrity of frameworks was retained following the post-synthetic modification while introducing additional adsorption sites. [12] Compared to pristine UiO-66, the modified quasi-framework exhibited a substantially greater CO₂ adsorption capacity under humid conditions, demonstrating that controlled defect engineering combined with post-synthetic modifications can effectively overcome one of the major limitations of conventional MOFs in direct air capture applications. These findings emphasize the importance of tailoring both the defect density and surface chemistries of MOFs to enhance their affinity toward the low concentrations of carbon dioxide present in ambient air while maintaining sufficient stability for repeated adsorption-desorption cycles. [12], [13]



[24] Note. From UiO-66, by Tokyo Chemical Industry Co., Ltd., n.d., TCI

II (b) Pre-combustion CO₂ Capture:

Pre-combustion CO₂ capture is commonly used in industry, aiming to combust fuels. During the process, CO₂ is removed before burning the fuel, a technique widely applied in gasification plants. CO₂ concentration in pre-combustion is typically higher (15-40%) than that of post-combustion (10-15%). In this approach, fuel is first converted into syngas containing CO and H₂. The CO is then reacted with steam to produce CO₂ and H₂. The carbon dioxide is separated, leaving hydrogen as the fuel. Compared to post-combustion capture, pre-combustion systems generally operate under elevated pressures and higher CO₂ concentrations, making adsorption thermodynamically more favorable. However, slightly selective CO₂/H₂ separation, long-term framework stability, and rapid regeneration remain essential requirements for industrial applications. [14]

To satisfy these demands, amine functionalization has proven to be effective concerning the strong affinity between amine groups and CO₂ molecules. Usman et al. reported that incorporating amino-functionalized linkers into aluminum-based frameworks, such as [Al(OH)(NH₂bdc)], significantly enhanced CO₂ selectivity over competing gases, including methane and nitrogen. The introduction of amino groups reduced the number of non-selective adsorption sites while simultaneously increasing the polarity of the framework, strengthening the interaction between the quadrupole moment of CO₂ and the modified pore surface. [14] As a result, methane adsorption became negligible at pressures below 2 bar, whereas CO₂ adsorption and selectivity increased substantially.

Further improvements were achieved by modifying the chemical functionality of organic linkers. Sulfone-containing frameworks exhibited stronger framework-CO₂ interactions than pristine aromatic ligands due to the high polarity of the sulfone group, while pyridine-functionalized MOFs incorporating 4-(trifluoromethyl)pyridine (py-CF₃) demonstrated CO₂/N₂ selectivities exceeding those of conventional activated carbons and zeolites under low pressure conditions. [14] In addition to the nature of functional groups, the length of grafted amide chains also influenced adsorption performance. MOFs functionalized with shorter alkyl amide substituents exhibited higher CO₂ uptake (4.65 mmol g⁻¹) than those containing longer butyl chains (2.95 mmol g⁻¹), indicating that excessive chain length can partially obstruct pore accessibility, thereby reducing adsorption capacity. [14] These studies demonstrated that post-synthetic functionalization increases the affinity of MOFs toward carbon dioxide capture as well as enabling the adsorption behavior to be tailored according to the operating conditions encountered in pre-combustion capture processes.

II (c) Post-combustion CO₂ Capture:

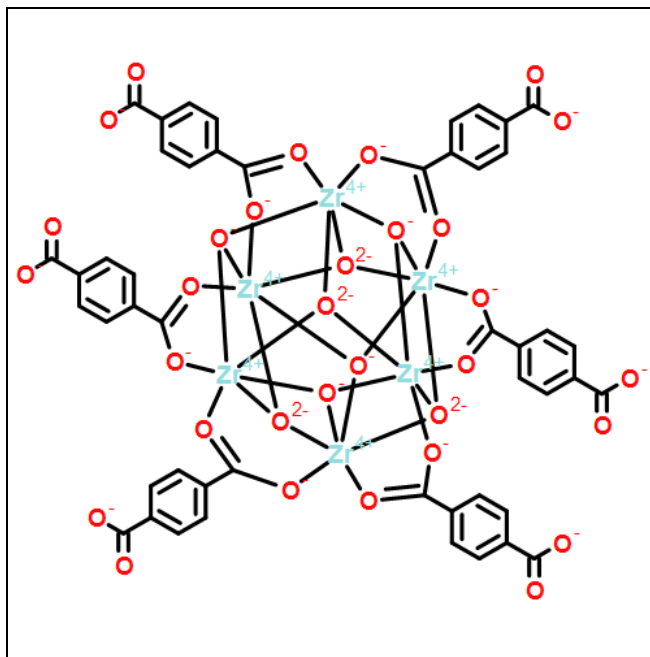
Post-combustion CO₂ capture is currently the most mature carbon capture strategy and is considered the most practical for retrofitting existing fossil fuel-fired power plants and industrial facilities, as it requires minimal modifications to the combustion process itself. [15] In this approach, CO₂ is separated from flue gas after fuel combustion, where it typically exits at low partial pressures (approximately 10-15%)

alongside nitrogen, water vapor, oxygen, and trace impurities. [10] These operating conditions present significant challenges for conventional adsorbents, as low CO₂ concentrations and high humidity often reduce adsorption capacity and selectivity. Consequently, considerable attention has been directed toward post-synthetically modified MOFs.

Zirconium-based MOFs possess exceptional hydrolytic stability compared to conventional MOFs. Hu et al. investigated the post-synthetic ionization of UiO-66(Zr)-(COOH)₂, a water-stable framework containing pendant carboxylic acid groups that are amenable to chemical modification. [16] Rather than altering the framework structure itself, the researchers employed a simple neutralization reaction by treating the MOF with aqueous solutions of LiOH, NaOH, and KOH, producing the ionized derivatives UiO-66(Zr)-(COOLi)₂, UiO-66(Zr)-(COONa)₂, and UiO-66(Zr)-(COOK)₂. This post-synthetic modification introduced alkali metal cations into the framework while preserving its crystallinity and porous architecture, providing additional adsorption sites capable of interacting more strongly with CO₂ molecules. [16]

The adsorption performance of the modified frameworks was evaluated through CO₂ and N₂ adsorption isotherms at 273 K and 298 K, under pressure conditions up to 1 bar, to simulate the flue gas. [15] As a result, UiO-66(Zr)-(COOK)₂ demonstrated an 83% increase in gas selectivity, as calculated through using Ideal Adsorbed Solution Theory (IAST), whereas UiO-66(Zr)-(COONa)₂ exhibited a selectivity of 99.6%, being among the highest experimentally reported values obtained from binary mixed-gas breakthrough measurements at the time of publication. These improvements were attributed to the enhanced electrostatic interactions between the incorporated alkali metal cations and the quadrupole moment of CO₂, resulting in stronger framework-guest interactions without sacrificing the framework's hydrolytic stability. [15]

These findings demonstrate that post-synthetic modification can significantly improve the performance of MOFs under post-combustion operating conditions. By strengthening the framework-CO₂ interactions without compromising structural stability, ionized zirconium-based MOFs exhibit the high selectivity and moisture tolerance required for industrial flue gas treatment. Consequently, post-synthetic modification represents an effective strategy for addressing the adsorption limitations associated with post-combustion carbon capture while maintaining the durability necessary for repeated adsorption-desorption cycles. [15]



[25] Note. From UiO-66 (Zr), by CD Bioparticles, n.d., CD Bioparticles (<https://www.cd-bioparticles.com/>). Copyright [Year] by CD Bioparticles.

II (d) A Comparison of Post-Synthetic Modifications Applied to UiO-66

Table 1 below summarizes the post-synthetic modifications applied to the metal organic framework, UiO-66, discussed in the previous section.

Table 1
Comparison of Post-Synthetic Modifications Applied to UiO-66

MOF	PSM	Experiment Method	Experimental Findings	Reference
UiO-66	N/A Pristine framework used as a reference	PXRD, FTIR, and N ₂ adsorption; CO ₂ adsorption measurements under humid conditions	- Served as the reference framework - Substantially lower CO ₂ adsorption capacity	[12], [13]
Quasi-UiO-66	Controlled removal of organic linkers to introduce structural defects, followed by H ₂ O post-synthetic modification	PXRD, FTIR, and N ₂ adsorption; CO ₂ adsorption measurements under humid conditions	- Substantially higher CO ₂ intake under humid conditions, compared to pristine UiO-66 - Additional H ₂ O-derived adsorption sites introduced.	[12], [13]
UiO-66(Zr)-(COOH) ₂	Pendant R-COOH groups retained as functional sites; used as a precursor for ionization	Treatment with aqueous alkali-metal hydroxides; CO ₂ /N ₂ adsorption isotherms at 273 and 298 K up to 1 bar	- Reference framework for alkali-metal ionization - Retained hydrolytic stability and porous structure	[16]
UiO-66(Zr)-(COOLi) ₂	Ionization of pendant -COOH groups with LiOH, introducing lithium ions	Aqueous LiOH treatment followed by CO ₂ /N ₂ adsorption measurements	- Improved CO ₂ adsorption relative to UiO-66(Zr)-(COOH) ₂	[16]
UiO-66(Zr)-(COOK) ₂	Ionization of pendant -COOH groups with KOH, introducing potassium ions	Aqueous KOH treatment followed by CO ₂ /N ₂ adsorption and IAST analysis	- 83% increase in gas selectivity - Stronger CO ₂ -framework interactions and retained hydrolytic stability	[16]
UiO-66(Zr)-(COONa) ₂	Ionization of pendant -COOH groups with NaOH, introducing sodium ions	Aqueous NaOH treatment, CO ₂ /N ₂ adsorption, and binary mixed-gas breakthrough measurements	- 99.6% selectivity in CO ₂ /N ₂ - Among the highest experimentally reported at the time	[16]

OPPORTUNITIES & CHALLENGES

The structural exhaustivity of MOFs has established them as one of the most promising classes of porous polymers for applications spanning gas storage and separation, catalysis, drug delivery, and energy conversion. Their molecular architecture, formed by the assembly of metal nodes and organic linkers, allows precise control over pore size and framework topology. [6] Post-synthetic modification strategies have significantly expanded the functional diversity of MOFs by enabling the incorporation of catalytic

sites, ionic liquids, polymers, and other guest species without compromising the crystallinity of the parent framework. This degree of tunability provides opportunities to design application-specific materials with enhanced selectivity, adsorption capacity, and catalytic performance. [17]

Among these opportunities, carbon capture has received considerable attention on account of the urgent need for efficient greenhouse gas mitigation technologies. Functionalization of MOFs with amine groups, ionic liquids, and other CO₂-philic species has substantially improved adsorption capacity for CO₂ selectivity while maintaining the high surface area and porosity characteristic of these materials.[14] Likewise, the incorporation of catalytically active metals or functionalized ligands through post-synthetic modification has transformed MOFs into adaptable heterogeneous catalysts capable of promoting a broad range of organic transformations under relatively mild conditions. In biomedical applications, their tunable pore architecture enables the encapsulation and controlled release of therapeutic agents, proteins, and nucleic acids, highlighting their potential as advanced drug delivery platforms. [18]

Despite these remarkable advances, several challenges continue to hinder the large-scale development of MOFs. One of the primary limitations is their chemical and hydrolytic stability. [17] Although frameworks such as the MOF-808 families exhibit resistance toward moisture and chemical degradation, many MOFs constructed from lower-valent metal ions experience structural collapse upon prolonged exposure to humid or acidic environments. [18] Mechanical stability also remains a concern during industrial processing, where pore collapse and reduced adsorption performance may occur. [19]

The scalability and economic feasibility of MOF synthesis present additional obstacles as well. Conventional solvothermal syntheses often require expensive organic linkers, toxic solvents (like N-N dimethylformamide), elevated temperatures, and extended reaction times, increasing both production costs and environmental impact. [18] While continuous-flow synthesis, mechanochemical approaches, and greener solvent systems have emerged as promising alternatives, further optimization is required to produce MOFs economically at industrial scales without sacrificing crystallinity or performance. [17], [19]

Another critical challenge lies in balancing functionality with porosity. Although post-synthetic modification introduces desirable chemical properties that enhance adsorption or catalytic activity, excessive functionalization may partially block pore channels, confining the gas to diffuse through the material. [17]

CONCLUSION

All in all, this review demonstrates that post-synthetic modification is an effective strategy for enhancing the CO₂ capture performance of metal–organic frameworks. Techniques including amine functionalization, ionic liquid incorporation, and linker modification have been proven to improve adsorption capacity, selectivity, and framework functionality while preserving structural integrity.

However, challenges such as framework stability, scalability, and regeneration efficiency continue to limit industrial implementation. Addressing these limitations presents significant opportunities for future research. Looking forward, future research should focus on the rational design of robust, scalable, and multifunctional MOFs capable of operating under realistic conditions. Advances in computational screening and machine learning-assisted discovery are expected to accelerate the identification of framework compositions with tailored properties. Integrating MOFs into mixed-matrix membranes and hybrid porous materials offers promising opportunities to overcome current challenges while expanding their practical applicability. Continued development of environmentally benign synthesis routes and durable framework chemistries will be crucial for translating the exceptional laboratory performance of MOFs into commercially viable technologies across environmental, energy, and biomedical sectors.

ACKNOWLEDGEMENTS

Thank you to Lumiere Education and Raja Oubelhas from Chalmers University of Technology for the development of this research paper.

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