

Metal–Organic Frameworks (MOFs) for Selective Gas Capture and Storage

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ABSTRACT

Metal–Organic Frameworks (MOFs) have emerged as one of the most extensively studied porous materials for selective gas capture and storage owing to their ultrahigh surface area, tunable pore geometry, and chemically functionalizable frameworks. Over the last decade, Indian research groups have made significant contributions toward understanding adsorption mechanisms, synthesizing moisture-stable materials, and developing multifunctional MOFs suitable for energy and environmental applications. This expanded research paper provides a detailed academic analysis of MOFs for selective gas capture with emphasis on Indian investigations involving carbon dioxide capture, methane storage, hydrogen adsorption, and membrane-based separation. It discusses synthesis strategies, structural characterization, adsorption thermodynamics, computational modeling, and performance evaluation approaches used by Indian scientists. The results reveal that linker modification, open metal sites, and hybrid composites markedly improve adsorption selectivity and capacity under practical conditions. The discussion highlights technological challenges related to scalability, stability, regeneration energy, and industrial translation while outlining future opportunities for sustainable carbon management and clean-energy storage systems.

Keywords- Metal–Organic Frameworks; Gas Capture; Carbon Dioxide Adsorption; Porous Materials; Indian MOF Research.

I. INTRODUCTION

Metal–Organic Frameworks (MOFs) represent a unique class of crystalline porous solids formed by self-assembly between inorganic metal nodes and organic ligands, resulting in highly ordered frameworks possessing exceptional surface area and adjustable pore chemistry [3,12]. The modular nature of MOFs allows researchers to tune structural parameters at the molecular level, making them ideal candidates for selective adsorption of gases.

The increasing concentration of greenhouse gases, especially carbon dioxide, has intensified global research into efficient gas separation technologies. Conventional adsorbents such as zeolites, silica gels, and activated carbons often lack structural flexibility, limiting their selectivity and adsorption efficiency. MOFs overcome these limitations through programmable framework design and controllable chemical functionality [6].

Indian scientific communities have actively participated in MOF research, focusing on environmentally relevant applications such as carbon capture from flue gas, methane storage for energy applications, and hydrogen adsorption for clean fuel technologies [1]. Research outputs from IITs, IISc, CSIR laboratories, and central universities have significantly expanded knowledge of adsorption mechanisms and material engineering.

The adsorption process inside MOFs depends on pore size distribution, framework polarity, and interaction strength between gas molecules and adsorption sites. The ability to introduce open metal sites and functional groups enables strong host–guest interactions, particularly for polarizable gases such as CO₂ [5].

Indian researchers have explored amine-functionalized and nitrogen-rich MOFs to improve CO₂ affinity. These frameworks demonstrate enhanced adsorption enthalpy and selectivity compared with non-functionalized counterparts, particularly under low-

pressure conditions relevant for post-combustion carbon capture [4].

Moisture stability remains one of the most significant barriers to practical MOF deployment. Early frameworks degraded under humid conditions, motivating Indian researchers to investigate zirconium- and aluminum-based MOFs known for strong metal-oxygen bonds and hydrolytic stability [9].

Hydrogen and methane storage are increasingly important due to India's transition toward sustainable energy systems. High surface area MOFs with optimized pore volume show promising adsorption capacities under moderate pressure and temperature conditions [11].

Another major contribution from Indian studies involves integrating computational chemistry with material synthesis. Density functional theory and molecular simulations provide insights into adsorption energies, diffusion pathways, and framework flexibility, thereby accelerating material optimization [8].

Indian research has also expanded toward membrane-based gas separation where MOFs are embedded into polymer matrices to create mixed-matrix membranes. These systems combine the mechanical flexibility of polymers with the selective adsorption capabilities of MOFs [7].

Beyond adsorption, multifunctional MOFs capable of catalyzing reactions involving captured gases have been explored. Such systems enable simultaneous capture and conversion of CO₂ into useful chemicals, representing a promising direction for circular carbon technologies [2].

Green synthesis routes have gained attention in Indian laboratories aiming to reduce solvent usage, energy consumption, and environmental impact associated with MOF preparation [10]. This aligns with broader sustainability goals in chemical manufacturing. Collectively, Indian studies have demonstrated that MOFs are not only scientifically versatile but also technologically promising materials capable of addressing critical challenges in gas capture, storage, and environmental sustainability.

II. METHODOLOGY

The synthesis of MOFs in Indian research primarily relies on solvothermal or hydrothermal methods in which metal salts and organic linkers react under controlled thermal conditions to produce crystalline frameworks [1]. Parameters such as temperature, solvent type, reaction duration, and precursor ratio are systematically optimized to obtain desired structural characteristics.

In several studies, modulators are introduced during synthesis to control crystal size and defect concentration, which directly influence adsorption behavior. Fine-tuning these synthesis parameters enables enhanced pore accessibility and improved gas uptake performance.

Post-synthetic activation is a crucial step in MOF preparation. Indian researchers commonly employ solvent exchange followed by vacuum drying to remove guest molecules trapped inside pores, thereby maximizing accessible surface area for gas adsorption [5].

Structural characterization is carried out using powder X-ray diffraction to confirm phase purity and crystallinity, while electron microscopy reveals particle morphology and size distribution [9].

Thermogravimetric analysis is frequently employed to evaluate thermal stability and decomposition behavior, ensuring materials can withstand repeated adsorption-desorption cycles.

Surface area and pore characteristics are determined through nitrogen adsorption-desorption experiments at cryogenic temperatures. BET surface area calculations and pore distribution analysis provide essential information correlating structure with adsorption capacity [11].

Gas adsorption experiments are performed using volumetric analyzers to generate adsorption isotherms for CO₂, CH₄, and H₂ at varying pressures and temperatures. These measurements help determine adsorption capacity, working capacity, and selectivity [8].

Selectivity toward gas mixtures is estimated using theoretical models such as Ideal Adsorbed Solution Theory (IAST), which predicts competitive adsorption behavior under realistic conditions.

Functionalization strategies include pre-synthetic linker modification and post-synthetic grafting methods designed to introduce functional groups that increase interaction with targeted gases [4].

Mixed-matrix membrane fabrication involves dispersing activated MOF particles into polymer solutions followed by casting and solvent evaporation to form uniform films [7]. Membrane performance is evaluated in terms of permeability and selectivity.

Stability testing includes exposure to humidity, thermal cycling, and repeated adsorption-desorption experiments. These tests assess long-term operational viability and regeneration efficiency.

Computational modeling through density functional theory and Monte Carlo simulations is widely used in Indian studies to investigate adsorption energy landscapes, diffusion kinetics, and gas-framework interactions [8].

Finally, comparative benchmarking against conventional adsorbents is performed to highlight the advantages of MOFs in terms of capacity, selectivity, and regeneration performance.

III. RESULTS

Indian studies consistently report that functionalized MOFs show significantly enhanced CO₂ adsorption due to stronger electrostatic and chemical interactions between gas molecules and framework functional groups.

Frameworks containing open metal sites demonstrate higher adsorption enthalpy, enabling selective capture of CO₂ even at low partial pressures relevant to industrial exhaust streams.

Moisture-stable zirconium-based frameworks maintain structural integrity after repeated exposure to humidity, representing a major improvement over early-generation MOFs.

Methane storage investigations reveal that optimized pore sizes and high volumetric surface area enhance storage density, making MOFs attractive for natural gas applications.

Hydrogen adsorption studies indicate that lightweight frameworks with high porosity and metal centers improve uptake at cryogenic temperatures, supporting potential use in hydrogen fuel infrastructure.

Mixed-matrix membranes developed by Indian researchers exhibit improved permeability–selectivity balance compared to pure polymer membranes, demonstrating practical separation advantages.

Adsorption–desorption cycling studies confirm that several MOFs retain performance after multiple cycles, indicating efficient regeneration and long-term stability.

Computational predictions correlate well with experimental adsorption data, validating simulation-guided framework design approaches.

Catalytic MOFs demonstrate dual functionality by adsorbing CO₂ and converting it into cyclic carbonates or related chemicals, highlighting the potential for integrated carbon utilization technologies.

Table 1: Representative MOFs in Indian Gas Capture Studies

MOF Type	Target Gas	Structural Feature	Major Outcome
Amine-functionalized MOF	CO ₂	Polar linker groups	High selectivity at low pressure
Zr-based MOF	CO ₂ /N ₂	Strong metal–oxygen bond	Excellent moisture stability
High-porosity MOF	CH ₄	Large pore volume	Enhanced methane storage
Open metal-site MOF	H ₂	Unsaturated metal centers	Increased adsorption affinity

Table 2: Observed Trends Across Indian MOF Studies

Parameter	Observed Effect
Increased surface area	Higher gas uptake capacity
Linker functionalization	Improved CO ₂ binding strength
Metal-site accessibility	Higher selectivity
Composite membranes	Better permeability/selectivity trade-off
Structural stability	Improved recyclability

IV. DISCUSSION AND CONCLUSION

Indian research on MOFs demonstrates strong progress in addressing key scientific challenges associated with selective gas capture and storage. The combination of chemical functionalization and structural engineering has significantly improved adsorption performance and selectivity.

One of the major achievements lies in the development of hydrolytically stable MOFs capable of operating under humid conditions, a prerequisite for industrial carbon capture processes. These materials represent a significant advancement toward practical deployment.

Integration of theoretical modeling with experimental work has accelerated material discovery and provided a deeper understanding of adsorption mechanisms. This approach enables rational framework design rather than trial-based synthesis.

Despite promising laboratory-scale results, challenges remain in scaling MOF synthesis economically. Large-scale production must reduce solvent usage, synthesis time, and cost while maintaining consistent structural quality.

Energy-efficient regeneration is another critical factor. Adsorbents requiring low regeneration energy will be essential for commercial adoption, and ongoing Indian research is beginning to address this issue.

The emergence of multifunctional MOFs capable of simultaneous capture and catalytic conversion represents a transformative direction, potentially enabling closed carbon cycles in industrial processes.

In conclusion, Indian studies clearly demonstrate that MOFs provide a versatile and scientifically robust platform for selective gas capture and storage. Continued interdisciplinary research involving materials chemistry, process engineering, and computational modeling will be essential for transitioning MOFs from laboratory innovation to large-scale environmental and energy solutions.

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