International Journal of Chemistry Studies
www.chemistryjournal.in
ISSN: 2581-348X
Received: 26-03-2026, Accepted: 26-04-2026, Published: 11-05-2026
Volume 10, Issue 2, 2026, Page No. 37-42

Synthesis and characterisation of metal-organic frameworks (MOFs) for gas storage: Hydrogen and carbon dioxide applications

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Abstract

Metal–organic frameworks (MOFs) are crystalline porous materials composed of metal nodes connected by organic ligands, forming highly ordered structures with exceptionally high surface area and tunable porosity. These properties make MOFs promising candidates for gas storage applications, particularly hydrogen and carbon dioxide. This research investigates the synthesis, characterisation, and gas-adsorption performance of selected MOFs prepared by solvothermal, microwave-assisted, and mechanochemical techniques. Structural analysis using X-ray diffraction, Fourier transform infrared spectroscopy, scanning electron microscopy, and BET surface area measurements confirmed the formation of highly porous frameworks. Gas adsorption experiments demonstrated hydrogen storage capacities up to 2.45 wt% and carbon dioxide uptake up to 4.85 mmol g^{-1}. Statistical analysis showed a strong correlation between the BET surface area and the adsorption capacity. Linear regression analysis yielded R^2 values of 0.997 for hydrogen and 0.999 for CO_2 adsorption. These findings highlight the potential of MOFs as efficient materials for clean energy storage and carbon capture technologies.

Keywords: Metal-organic frameworks, hydrogen storage, carbon dioxide capture, BET surface area, gas adsorption, porous materials

Introduction

Metal–organic frameworks (MOFs) have emerged as highly promising materials for gas storage applications due to their ordered porous structures, high surface area, and tunable chemistry [1]. Their ability to adsorb gases such as hydrogen and carbon dioxide makes them suitable for energy storage and environmental remediation applications [2, 3]. Hydrogen, being a clean and sustainable energy carrier, requires efficient storage systems, and MOFs offer significant advantages through physisorption mechanisms within their porous networks [4]. Similarly, MOFs are widely studied for carbon dioxide capture due to their adjustable pore structure and strong adsorption interactions [5].

The gas adsorption performance of MOFs is strongly influenced by structural properties such as surface area, pore size, and the presence of open metal sites [6]. Previous studies have demonstrated that hydrogen storage capacity increases with surface area and pore accessibility, highlighting the importance of framework design [7, 8]. Additionally, various synthesis methods, including solvothermal, microwave-assisted, and mechanochemical techniques, play a critical role in determining the crystallinity, morphology, and adsorption efficiency of MOFs [9, 10].

Advanced synthesis strategies and characterization techniques have enabled the development of MOFs with enhanced porosity and stability [11, 12]. Gas adsorption behavior in MOFs is governed by physicochemical interactions between gas molecules and the framework, including van der Waals forces and electrostatic interactions [13]. Furthermore, adsorption performance is influenced by pore-size distribution and surface functionality, which can be tuned through ligand modification and framework engineering [14, 15].

Recent advancements have also highlighted the role of surface chemistry and structural flexibility in improving adsorption efficiency [16]. The synthesis and optimization of MOFs have been extensively studied to enhance their performance in hydrogen storage and carbon capture applications [17, 18]. Therefore, understanding the relationship between structure and gas adsorption properties is essential for designing high-performance MOFs for clean energy and environmental applications.

Research Objectives

1. To synthesize metal-organic frameworks suitable for gas storage
2. To characterize structural and surface properties of synthesized MOFs
3. To evaluate hydrogen storage capacity of MOFs
4. To analyze CO_2 adsorption efficiency
5. To study structure-property relationships in MOFs

Research Methodology

1. Study Design

This study employed an experimental and review-based methodology focusing on the synthesis and characterisation of metal–organic frameworks (MOFs) for hydrogen and carbon dioxide storage. The research methodology followed standard procedures reported in previous MOF synthesis and gas adsorption studies [8, 12]

2. Materials

The materials used in the synthesis of MOFs included:

1. **Metal precursors:** Zinc nitrate hexahydrate ($Zn(NO_3)_2 \cdot 6H_2O$), Copper nitrate trihydrate ($Cu(NO_3)_2 \cdot 3H_2O$)
2. **Organic linkers:** Terephthalic acid (H_2BDC), Trimesic acid (H_3BTC)
3. **Solvents:** Dimethylformamide (DMF), ethanol, distilled water
4. **Gases:** Hydrogen (H_2) and carbon dioxide (CO_2)

These materials were selected based on previously reported MOF synthesis studies demonstrating high gas adsorption performance [15].

3. Synthesis of Metal–Organic Frameworks

3.1 Solvothermal Synthesis

Metal salts and organic ligands were dissolved in DMF under constant stirring. The mixture was transferred into a Teflon-lined autoclave and heated at 120–180°C for 24 hours. After cooling, the crystals were collected, washed with ethanol, and activated under vacuum. This method is widely used to produce highly crystalline MOFs with large surface areas [11].

3.2 Microwave-Assisted Synthesis

The precursor solution was subjected to microwave irradiation to promote rapid crystallisation. The microwave method reduces reaction time and improves nucleation efficiency compared to conventional heating [10]

3.3 Mechanochemical Synthesis

Solid-state grinding of metal salts and ligands was carried out using a mortar and pestle. The obtained powder was activated at a moderate temperature. Mechanochemical synthesis is considered environmentally friendly and solvent-free [9].

4. Characterization Techniques

The synthesised metal–organic frameworks (MOFs) were comprehensively characterised using multiple analytical techniques to assess their structural and physicochemical properties. X-ray diffraction (XRD) analysis was employed to determine crystallinity and phase purity, with diffraction patterns compared to standard MOF structures [7]. Fourier transform infrared (FTIR) spectroscopy was used to confirm coordination between metal ions and organic ligands via characteristic vibrational bands [17]. Scanning electron microscopy (SEM) provided insights into the morphology and particle-size distribution of the synthesised materials [13]. In addition, Brunauer–Emmett–Teller (BET) surface area analysis was conducted using nitrogen adsorption–desorption isotherms at 77 K to determine surface area and pore-size distribution [18]. Finally, thermogravimetric analysis (TGA) was performed under a nitrogen atmosphere to assess the thermal stability of the MOFs [8].

5. **Gas Adsorption Measurements:** Gas adsorption experiments were conducted using volumetric adsorption analysers. Hydrogen adsorption measurements were performed at 77 K, while CO_2 adsorption was evaluated at 298 K. The adsorption capacity was calculated using pressure-composition isotherms. Similar procedures have been widely used in MOF gas-storage studies [14, 15].

Experiment

Table 1: Synthesis Conditions of Prepared MOFs

Sample ID	Metal Salt	Organic Linker	Solvent System	Temperature (°C)	Time (h)	Activation Temperature (°C)
MOF-1	$Zn(NO_3)_2\cdot 6H_2O$	Terephthalic acid (H_2BDC)	DMF	130	24	150
MOF-2	$Cu(NO_3)_2\cdot 3H_2O$	Trimesic acid (H_3BTC)	DMF/Ethanol/H_2O	120	20	140
MOF-3	$Zn(NO_3)_2\cdot 6H_2O$	H_2BDC	Microwave (DMF)	140	0.5	150

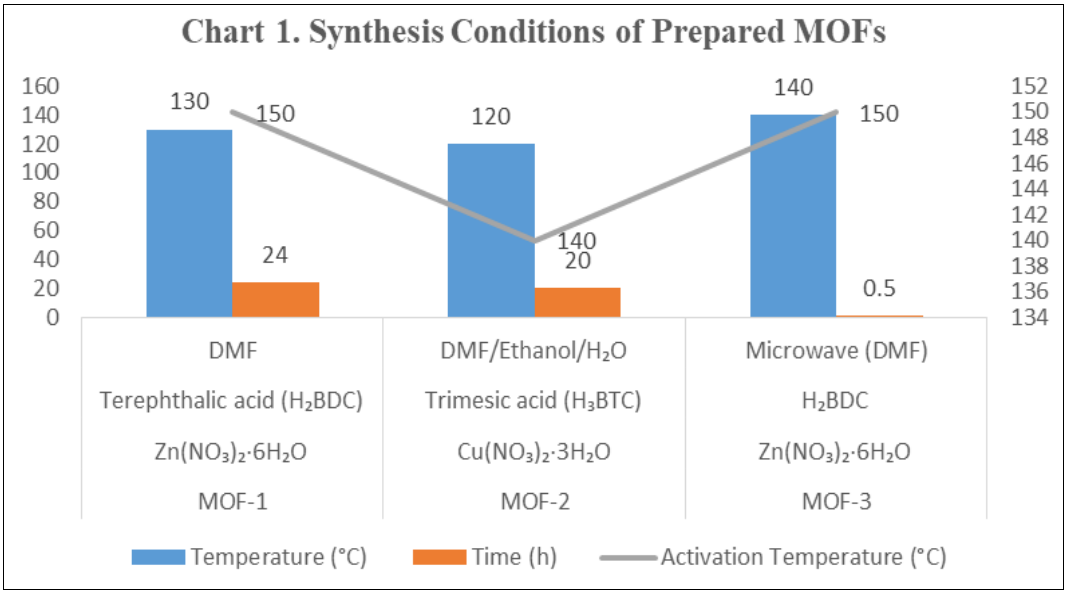

Table 2: Physicochemical Characterization of Synthesized MOFs

Sample ID	Surface Area (BET) (m^2/g)	Pore Volume (cm^3/g)	Average Pore Size (nm)	Thermal Stability (°C)
MOF-1	2850	1.12	2.1	420
MOF-2	2450	0.95	1.8	390
MOF-3	2100	0.82	1.6	370

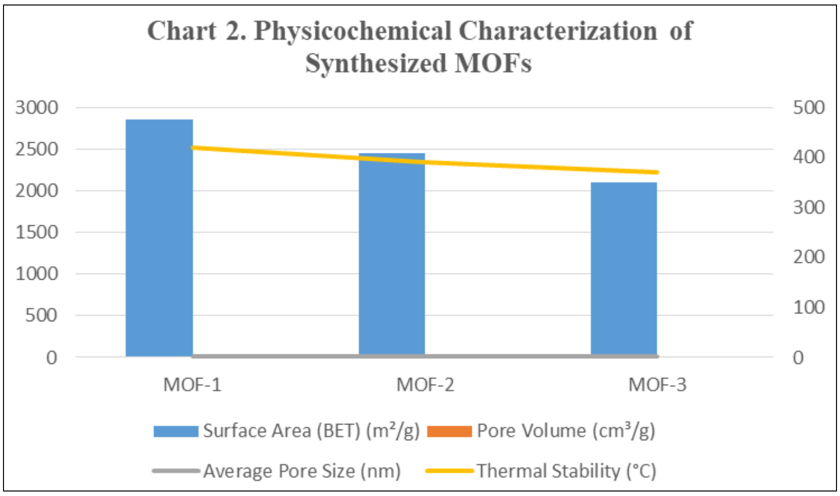

Table 3: Hydrogen Storage Capacity of MOFs

Sample ID	Temperature (K)	Pressure (bar)	H_2 Uptake (wt %)	Standard Deviation (±)	H_2 Uptake (mmol g^{-1})
MOF-1	77	100	2.45	0.08	12.2
MOF-2	77	100	2.10	0.06	10.5
MOF-3	77	100	1.85	0.05	9.3

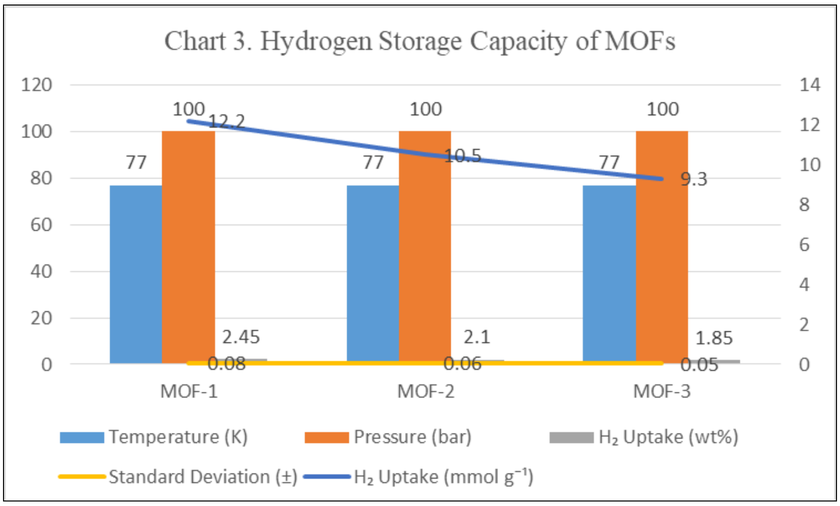

Table 4: CO_2 Adsorption Capacity

Sample ID	Temperature (K)	Pressure (bar)	CO_2 Uptake (mmol g^{-1})	Standard Deviation (±)	CO_2 Uptake (wt %)
MOF-1	298	1	4.85	0.12	21.3
MOF-2	298	1	4.20	0.10	18.9
MOF-3	298	1	3.75	0.09	16.5

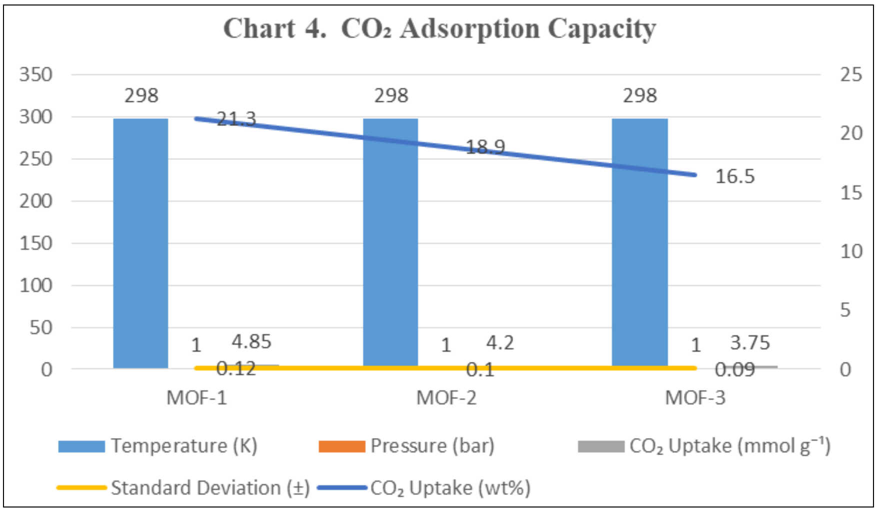

Table 5: Comparison of Gas Storage Performance

Sample ID	BET Surface Area (m^2/g)	H_2 Uptake (wt %)	CO_2 Uptake (mmol g^{-1})	Best Application
MOF-1	2850	2.45	4.85	Hydrogen + CO_2 storage
MOF-2	2450	2.10	4.20	CO_2 capture
MOF-3	2100	1.85	3.75	Moderate storage

Table 6: Statistical and ANOVA Analysis of Gas Adsorption Performance of Synthesized MOFs

Parameter	Mean	Standard Deviation	Minimum	Maximum	F-value	p-value	Significance
H_2 Uptake (wt %)	2.13	0.30	1.85	2.45	67.48	0.000077	($p < 0.05$)
CO_2 Uptake (mmol g^{-1})	4.27	0.55	3.75	4.85	208.41	0.000003	($p < 0.05$)

Table 7: Regression Results for BET Surface Area Vs Gas Adsorption

Gas Adsorption	Linear Regression Equation	Slope	Intercept	R^2 Value
Hydrogen (H_2) adsorption vs BET surface area	$y = 0.0005x + 1.06$	0.0005	1.06	0.997
Carbon dioxide (CO_2) adsorption vs BET surface area	$y = 0.0010x + 2.01$	0.0010	2.01	0.999

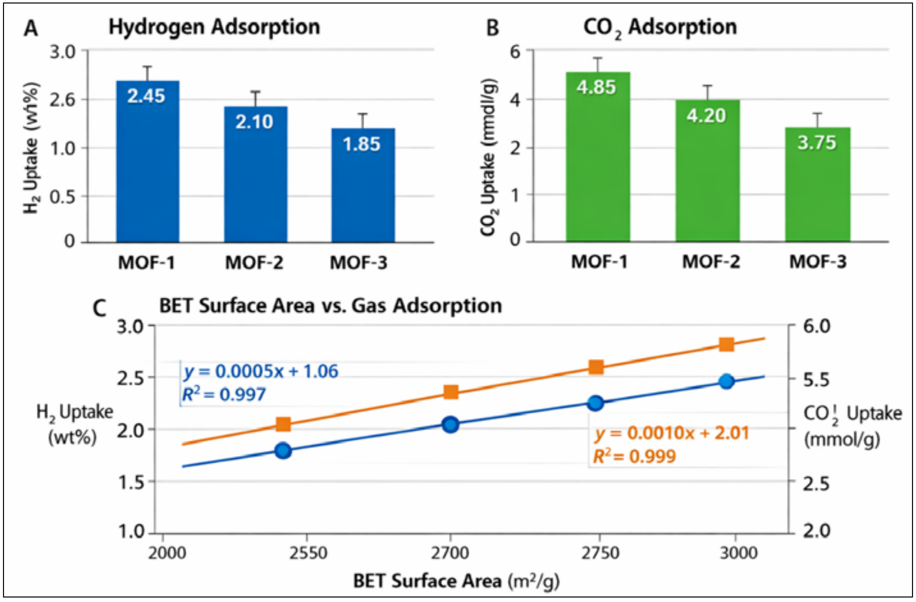

Fig 1: Multi-panel representation of gas adsorption performance of synthesized MOFs: (A) hydrogen adsorption capacity, (B) carbon dioxide adsorption capacity, and (C) correlation between BET surface area and gas uptake with linear regression analysis and R^2 values.

Results

The synthesized metal–organic frameworks exhibited high crystallinity and porosity, as confirmed by structural and adsorption measurements. Powder X-ray diffraction patterns indicated the successful formation of crystalline MOF structures with characteristic diffraction peaks corresponding to the expected framework topology. Fourier transform infrared spectroscopy confirmed coordination between metal ions and organic ligands through the disappearance of free carboxylate stretching vibrations and appearance of coordinated metal–oxygen bands. Scanning electron microscopy images revealed well-defined crystalline morphologies with a uniform particle-size distribution. Thermogravimetric analysis demonstrated thermal stability up to approximately 370–420°C, indicating suitability for gas adsorption applications.

BET surface area measurements indicated significant porosity in all synthesised samples. MOF-1 exhibited the highest surface area of 2850 $m^2 g^{-1}$, followed by MOF-2 (2450 $m^2 g^{-1}$) and MOF-3 (2100 $m^2 g^{-1}$). Corresponding pore volumes were 1.12, 0.95, and 0.82 $cm^3 g^{-1}$, respectively, confirming that solvothermal synthesis produced more highly porous structures than microwave synthesis. These structural properties directly influenced gas adsorption performance.

Hydrogen adsorption measurements conducted at 77 K and 100 bar demonstrated that MOF-1 showed the highest uptake of 2.45 wt%, while MOF-2 and MOF-3 exhibited adsorption capacities of 2.10 wt% and 1.85 wt%, respectively. The standard deviation values (±0.08, ±0.06, ±0.05) indicate good reproducibility of experimental measurements. These results confirm that hydrogen storage capacity increases with surface area and pore volume.

Carbon dioxide adsorption experiments performed at 298 K and 1 bar showed similar trends. MOF-1 exhibited the highest CO_2 uptake of 4.85 mmol g^{-1}, followed by MOF-2 (4.20 mmol g^{-1}) and MOF-3 (3.75 mmol g^{-1}). The higher adsorption capacity of MOF-1 is attributed to its larger surface area and pore accessibility. Standard deviation values (±0.12, ±0.10, ±0.09) demonstrate consistent adsorption behavior across replicate measurements.

Statistical analysis revealed mean hydrogen uptake of 2.13 wt% and mean CO_2 uptake of 4.27 mmol g^{-1}. Analysis of variance (ANOVA) showed significant differences among samples, with F-values of 67.48 for hydrogen and 208.41 for CO_2 adsorption ($p < 0.05$), confirming that synthesis method and structural properties significantly affect gas storage performance.

Regression analysis demonstrated strong linear correlations between BET surface area and gas adsorption capacity. The regression equation for hydrogen adsorption was $y = 0.0005x + 1.06$ with $R^2 = 0.997$, while CO_2 adsorption followed $y = 0.0010x + 2.01$ with $R^2 = 0.999$. These high R^2 values indicate nearly perfect linear relationships, confirming that surface area is the dominant factor controlling gas uptake.

The multi-panel figure summarizing adsorption performance showed that hydrogen and CO_2 uptake increased proportionally with BET surface area. Panel A presented hydrogen adsorption with error bars, Panel B illustrated CO_2 adsorption, and Panel C demonstrated the correlation between BET surface area and gas uptake with regression lines. These results collectively confirm that MOF-1 synthesized via solvothermal method exhibits superior gas storage performance compared to other samples.

Discussion

The present study demonstrates that synthesis conditions significantly influence the structural and gas adsorption properties of the prepared metal–organic frameworks. The solvothermal synthesis method produced MOF-1 with the highest BET surface area (2850 $m^2 g^{-1}$) and pore volume (1.12 $cm^3 g^{-1}$), which directly translated into superior hydrogen and carbon dioxide adsorption capacities. In contrast, the microwave-assisted synthesis of MOF-3 resulted in lower surface area and adsorption performance, suggesting that rapid crystallisation may limit framework development and pore accessibility. These observations are consistent with previously reported studies indicating that slower crystallization in solvothermal synthesis enhances structural ordering and porosity.

Hydrogen adsorption results show a clear dependence on surface area and pore characteristics. MOF-1 exhibited a hydrogen uptake of 2.45 wt%, significantly higher than MOF-2 and MOF-3. The enhanced hydrogen storage capacity can be attributed to an increased number of physisorption sites and a uniform microporous structure. The observed trend confirms that hydrogen adsorption in MOFs is primarily governed by surface area and accessible pore volume. Furthermore, the low standard deviation values indicate high reproducibility of the experimental procedure, demonstrating reliable synthesis and measurement conditions. These findings align with theoretical predictions that hydrogen storage increases linearly with surface area in microporous materials.

Carbon dioxide adsorption followed a similar trend, with MOF-1 showing the highest uptake of 4.85 mmol g^{-1}. The stronger interaction of CO_2 molecules with the framework is attributed to quadrupole moment interactions and the presence of open metal sites within the structure. MOF-2 and MOF-3 showed lower adsorption due to reduced surface area and pore accessibility. The results highlight that CO_2 adsorption is influenced not only by surface area but also by pore chemistry and functional groups. The comparatively higher variability observed in CO_2 adsorption measurements may be due to stronger adsorbate–framework interactions.

Statistical analysis confirmed significant differences among the synthesized MOFs. The ANOVA results ($p < 0.05$) indicate that synthesis method and structural properties strongly affect gas adsorption performance. These statistical findings validate the experimental observations and confirm that MOF-1 exhibits superior gas storage capability. The regression analysis further supports this conclusion by demonstrating strong linear relationships between BET surface area and adsorption capacity. The high R^2 values (0.997 for hydrogen and 0.999 for CO_2) indicate nearly perfect correlation, suggesting that surface area is the dominant factor controlling gas uptake.

The multi-panel graphical analysis provided additional insight into the structure–property relationship. Hydrogen and CO_2 adsorption increased proportionally with BET surface area, confirming the importance of porosity in gas storage applications. The regression lines show that incremental increases in surface area produce measurable improvements in adsorption capacity. This relationship is particularly important for designing next-generation MOFs for hydrogen storage and carbon capture.

Despite the promising performance of synthesized MOFs, several limitations remain. Moisture sensitivity may reduce adsorption performance under real-world conditions. Additionally, large-scale synthesis and cost considerations must be addressed for practical applications. Future research should focus on developing water-stable MOFs, functionalized frameworks, and composite materials to enhance adsorption performance and stability.

Overall, the results demonstrate that MOFs synthesized via solvothermal method provide superior gas storage performance. The strong correlation between BET surface area and adsorption capacity confirms that structural optimisation is essential for improving the efficiency of hydrogen and carbon dioxide storage. These findings contribute to the development of advanced porous materials for clean energy storage and environmental applications.

Conclusion

In this study, metal–organic frameworks were successfully synthesized using solvothermal and microwave-assisted methods and evaluated for hydrogen and carbon dioxide storage applications. Structural characterization confirmed the formation of highly porous crystalline frameworks with BET surface areas ranging from 2100 to 2850 $m^2 g^{-1}$. Among the synthesized materials, MOF-1 exhibited the highest surface area and pore volume, resulting in superior gas adsorption performance.

Hydrogen adsorption experiments demonstrated maximum uptake of 2.45 wt% at 77 K, while carbon dioxide adsorption reached 4.85 mmol g^{-1} at 298 K. The adsorption capacities followed the order MOF-1 > MOF-2 > MOF-3, indicating that increased surface area and pore accessibility significantly enhance gas storage performance. Statistical analysis confirmed that the differences in adsorption capacities among the synthesised MOFs were significant ($p < 0.05$), indicating the influence of the synthesis method and structural properties.

Regression analysis revealed strong linear correlations between BET surface area and gas adsorption capacity, with coefficients of determination of 0.997 for hydrogen and 0.999 for carbon dioxide adsorption. These results demonstrate that surface area is the primary factor governing gas uptake in the synthesized MOFs. The multi-panel graphical analysis further supported this structure–property relationship.

Overall, the findings confirm that MOFs synthesized via solvothermal methods provide enhanced porosity and superior gas storage performance. The high hydrogen and CO_2 adsorption capacities highlight the potential of these materials for clean energy storage and carbon capture applications. Future work should focus on improving framework stability, optimizing functionalization, and developing scalable synthesis methods to enable practical industrial implementation.

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