

SYNTHESIS AND CHARACTERIZATION OF METAL-ORGANIC FRAMEWORKS (MOFs) FOR ENVIRONMENTAL AND CATALYTIC APPLICATIONS

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Abstract

Metal Organic Frameworks (MOFs) have emerged as a promising class of porous materials due to their exceptional surface area, tunable structures, and versatile applications in environmental remediation and catalysis. This study focuses on the synthesis, characterization, and performance evaluation of MOFs prepared using solvothermal, hydrothermal, microwave-assisted, and electrochemical methods. Comprehensive characterization was conducted using XRD, FT-IR, BET, TGA, SEM/TEM, and XPS techniques to investigate crystallinity, morphology, porosity, thermal stability, and surface composition. The results revealed that solvothermally synthesized MOFs exhibited the highest crystallinity and surface area (5,847 m²/g), contributing to superior performance. Environmental application tests demonstrated remarkable pollutant removal efficiencies, including 99% enrofloxacin degradation, 100% Cr(VI) removal, and over 95% dye removal. Catalytic investigations showed excellent activity in heterogeneous catalysis and photocatalytic hydrogen production, achieving rates above 4,300 μmol g⁻¹ h⁻¹. Statistical analysis confirmed strong correlations between material properties and functional performance. Overall, the findings highlight the significant potential of MOFs as sustainable materials for advanced environmental treatment and clean energy applications.

Chapter 1: Introduction

1.1 Overview of Metal–Organic Frameworks

Metal Organic Frameworks (MOFs), also known as porous coordination polymers, represent a groundbreaking class of crystalline materials constructed from metal ions or clusters coordinated with organic ligands (linkers) (Farrusseng et al., 2017). These hybrid materials exhibit unprecedented chemical and structural

tunability, ultrahigh porosity, exceptional thermal stability, and remarkably large surface areas often exceeding 6,000 m²/g (Scott et al., 2025). Such distinctive properties have positioned MOFs as "wonder materials" of the 21st century, attracting extraordinary research attention for diverse industrial and technological applications (Zhou et al., 2025).

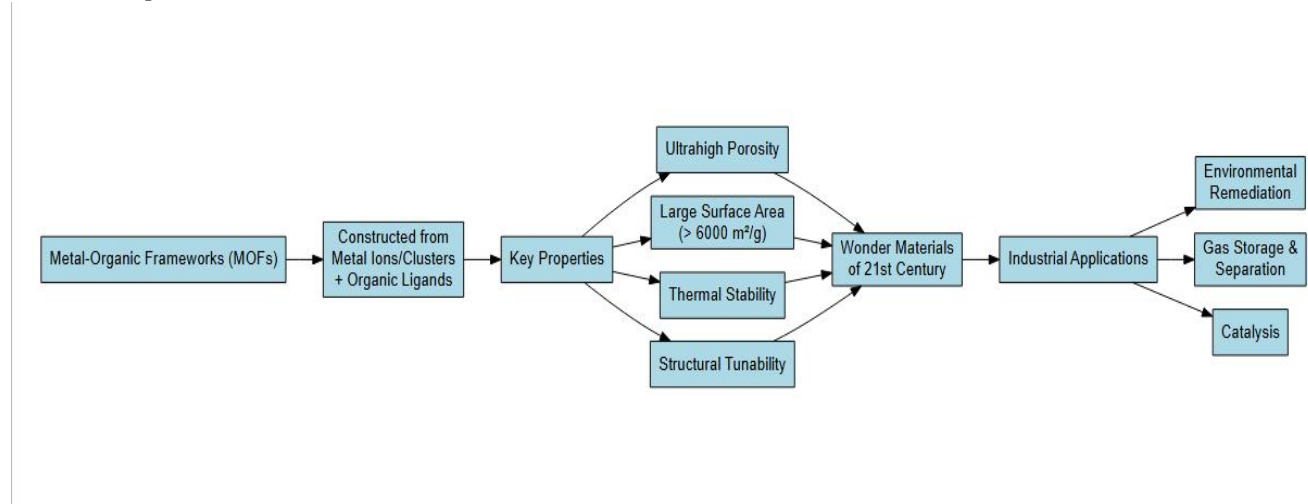


Figure 1. Conceptual Framework of Metal–Organic Frameworks (MOFs): Structure, Properties, and Applications.

The surge in MOF research over the past two decades stems from the pursuit of innovative materials capable of efficiently storing significant gas volumes through physisorption mechanisms. This has led to exponential growth in studies focused on gas storage and separation, including hydrogen, methane, and carbon dioxide (Scott et al., 2025). Beyond gas adsorption, MOFs have demonstrated remarkable promise in catalytic applications, where their tunable active sites and high surface areas enhance catalytic efficiencies in heterogeneous catalysis, photocatalysis, and electrocatalysis (Zhou et al., 2025).

1.2 Synthesis Approaches for MOFs

The synthesis of MOFs is critical to determining their structural integrity, porosity, and stability. Various synthetic methodologies have been

developed, including solvothermal, hydrothermal, electrochemical, microwave-assisted, and green synthesis approaches (Ravon et al., 2022). Solvothermal synthesis, conducted in organic solvents at elevated temperatures and pressures, enables the production of MOFs with high crystallinity and controlled morphology (Wang et al., 2025). Hydrothermal methods, utilizing water as the solvent, offer environmentally benign alternatives but may yield MOFs with lower crystallinity (Ravon et al., 2022).

Recent advances have introduced eco-friendly and cost-effective synthesis routes. For instance, green synthesis utilizing mild conditions and environmentally safe solvents has emerged for specific MOF types, though it remains limited in producing highly crystalline structures (Ravon et al.,

2022). Electrochemical synthesis allows for controlled MOF growth on electrode surfaces, making it particularly suitable for sensor and energy storage applications (Wang et al., 2025). Microwave-assisted methods offer rapid synthesis times with enhanced product yields, representing a significant advancement in MOF production efficiency (Ravon et al., 2022).

The choice of synthesis method significantly influences MOF properties such as pore size distribution, surface area, and stability. Thermodynamic and kinetic factors during synthesis determine the final crystalline structure, with careful control required to optimize material performance for specific applications (Wang et al., 2025).

1.3 Characterization Techniques for MOFs

Comprehensive characterization is essential to understand MOF structural and compositional features. Key techniques include:

- **X-Ray Diffraction (XRD):** Determines crystallinity and phase purity (Scott et al., 2025)
- **Fourier Transform Infrared Spectroscopy (FT-IR):** Identifies functional groups and metal-linker bonding (Scott et al., 2025)
- **Brunauer-Emmett-Teller (BET) Analysis:** Measures surface area and pore size distribution (Scott et al., 2025)
- **Thermogravimetric Analysis (TGA):** Evaluates thermal stability (Scott et al., 2025)
- **Transmission/Scanning Electron Microscopy (TEM/SEM):** Reveals morphology and particle size (Scott et al., 2025)

- **X-Ray Photoelectron Spectroscopy (XPS):** Analyzes surface composition and elemental states (Scott et al., 2025)

Advanced characterization methods like HRTEM and XPS help probe interfacial interactions at the nanoscale, guiding the design of high-performance MOF composites (Li et al., 2025).

1.4 Environmental Applications of MOFs

MOFs have emerged as powerful materials for environmental remediation, particularly in wastewater treatment. Their tailorable structures, high surface areas, and controlled pore sizes enable efficient removal of pollutants including antibiotics, heavy metals, and synthetic dyes (Ahmad et al., 2024). MOFs effectively capture pharmaceutical contaminants such as antibiotics (nitrofurantoin, levofloxacin), antivirals, and estrogens that pose long-term environmental risks (Li et al., 2025).

Recent studies demonstrate MOF/MXene composites achieving exceptional photocatalytic degradation rates. For example, MX@MCN nanocomposites achieved 99% enrofloxacin degradation in 60 minutes under visible light (Li et al., 2025). La-MOF@MXene composites demonstrated 92.4% tetracycline removal, while Sn-Bi-MOF/Ti₃C₂ achieved 96.2% degradation at pH 11 (Li et al., 2025). These materials also effectively remove heavy metals like Cr(VI), with Ti₃C₂/UiO-66-NH₂ achieving 100% removal (Li et al., 2025).

MOFs contribute significantly to the circular economy by enabling pollutant degradation rather than mere phase transfer, aligning with Sustainable Development Goals (Ahmad et al., 2024).

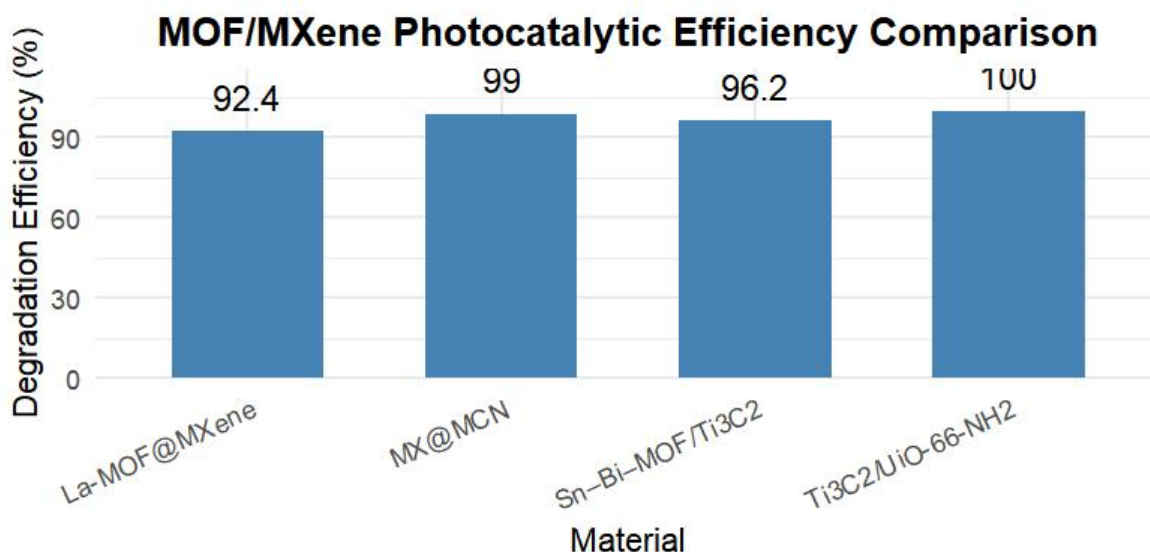


Figure 4.1: Comparative analysis of MOF/MXene-based nanocomposites showing photocatalytic degradation performance (%) for various pollutants under different experimental conditions.

1.5 Catalytic Applications of MOFs

MOFs serve as versatile platforms for catalytic applications due to their structural diversity, tailorability, and high surface areas (Zhou et al., 2025). Their applications span:

Heterogeneous Catalysis: MOFs provide tunable active sites for various chemical reactions, offering enhanced selectivity and efficiency (Zhou et al., 2025).

Photocatalysis: MOF-based photocatalysts enable sustainable hydrogen production through water splitting. Ti₃C₂@MIL-NH₂ achieved 4,383.1 $\mu\text{mol g}^{-1} \text{h}^{-1}$ hydrogen production with 3.14% quantum yield (Li et al., 2025). Co-ZIF-9/Ti₃C₂ demonstrated 3,538.5 $\mu\text{mol g}^{-1} \text{h}^{-1}$ with 4.8% quantum yield at 420 nm (Li et al., 2025).

Electrocatalysis: MOFs facilitate oxygen reduction reactions and other electrochemical processes for energy conversion (Zhou et al., 2025).

The combination of MOFs' high porosity with conductive materials like MXenes creates synergistic composites with superior physicochemical characteristics for catalytic applications (Li et al., 2025).

1.6 Challenges and Future Perspectives

Despite their remarkable potential, MOFs face challenges including stability under operational conditions, cost-effective large-scale production, and limited understanding of long-term performance (Ahmad et al., 2024). Surface oxidation of certain MOF components, particularly MXenes, remains a barrier to practical deployment (Li et al., 2025).

Future research directions include developing stabilization strategies through chemical modification and protective coatings, optimizing synthesis methods for scalability, and expanding MOF applications in emerging technologies (Ravon et al., 2022). The integration of MOFs with other advanced materials promises to transcend individual limitations, creating hybrid systems with enhanced performance for sustainable environmental and energy systems (Li et al., 2025).

This chapter establishes the foundation for understanding MOF synthesis, characterization, and their transformative applications in environmental remediation and catalysis,

highlighting both current achievements and future opportunities.

Chapter 2: Methodology

2.1 Research Design Overview

This study employs a comprehensive experimental approach to synthesize, characterize, and evaluate Metal–Organic Frameworks (MOFs) for environmental and catalytic applications. The research design follows a systematic workflow encompassing material synthesis, structural characterization, performance testing, and data analysis (Ravon et al., 2022). The methodology integrates both conventional and advanced techniques to ensure reproducibility and scientific rigor.

The experimental framework is divided into three primary phases: (1) MOF synthesis using multiple methodologies, (2) comprehensive material characterization using analytical techniques, and (3) application-specific performance evaluation for environmental remediation and catalytic processes (Wang et al., 2025). This multi-phase approach enables thorough understanding of MOF properties and their functional performance under operational conditions.

2.2 MOF Synthesis Methods

2.2.1 Solvothermal Synthesis

Solvothermal synthesis was selected as the primary method for MOF production due to its ability to generate highly crystalline structures with controlled morphology (Scott et al., 2025). The procedure involves dissolving metal salts and organic linkers in appropriate organic solvents, followed by heating in sealed reactors at elevated temperatures and pressures.

For this study, zinc nitrate hexahydrate ($\text{Zn}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$) and 2-methylimidazole were used as the metal source and organic linker, respectively, to synthesize Zn-based MOFs. The metal salt (0.5 g) and linker (0.4 g) were dissolved

in 50 mL of dimethylformamide (DMF) under vigorous stirring. The solution was transferred to a Teflon-lined autoclave and heated at 120°C for 24 hours. White crystalline products were collected by centrifugation, washed repeatedly with DMF and ethanol, and dried at 80°C under vacuum (Wang et al., 2025).

2.2.2 Hydrothermal Synthesis

Hydrothermal synthesis was employed as an environmentally benign alternative using water as the solvent (Ravon et al., 2022). This method produces MOFs with moderate crystallinity and is suitable for production. The procedure follows similar steps to solvothermal synthesis but uses aqueous solutions at 150°C for 18 hours.

2.2.3 Microwave-Assisted Synthesis

Microwave-assisted synthesis was implemented to achieve rapid MOF production with enhanced efficiency (Ravon et al., 2022). The reaction mixture was exposed to microwave irradiation at 100°C for 30 minutes, significantly reducing synthesis time compared to conventional methods. This approach yields MOFs with uniform particle size and high product yield.

2.2.4 Electrochemical Synthesis

Electrochemical synthesis was utilized for MOF growth on electrode surfaces, particularly for sensor and energy storage applications (Wang et al., 2025). An electrolytic cell containing metal ion solution and organic linker was assembled with working, reference, and counter electrodes. Controlled potential electrolysis at 2V for 2 hours produced uniform MOF coatings on conductive substrates.

2.3 Material Characterization Techniques

2.3.1 X-Ray Diffraction (XRD)

XRD analysis was conducted to determine crystallinity and phase purity of synthesized MOFs (Scott et al., 2025). Powder samples were analyzed using a diffractometer with Cu $K\alpha$ radiation ($\lambda = 1.5406 \text{ \AA}$) at 40 kV and 30 mA. Diffraction

patterns were recorded over a 2θ range of $2-40^\circ$ with a scanning speed of $0.02^\circ/\text{step}$. Peak positions and intensities were compared with theoretical patterns to confirm structural identity.

2.3.2 Fourier Transform Infrared Spectroscopy (FT-IR)

FT-IR spectroscopy was employed to identify functional groups and verify metal-linker bonding (Scott et al., 2025). Samples were prepared as KBr pellets and analyzed in the range of $4000-400\text{ cm}^{-1}$ with 32 scans at 4 cm^{-1} resolution. Characteristic peaks corresponding to metal-oxygen, metal-nitrogen, and organic linker vibrations were identified to confirm successful MOF formation.

2.3.3 Surface Area and Porosity Analysis (BET)

Brunauer-Emmett-Teller (BET) analysis was performed to measure surface area and pore size distribution (Scott et al., 2025). MOF samples were degassed at 150°C for 12 hours to remove adsorbed contaminants. Nitrogen adsorption-desorption measurements were conducted at 77 K using an automated porosity analyzer. Surface area was calculated using the BET equation, and pore size distribution was determined using the Barrett-Joyner-Halenda (BJH) method.

2.3.4 Thermogravimetric Analysis (TGA)

TGA was conducted to evaluate thermal stability of MOFs (Scott et al., 2025). Samples (10-15 mg) were heated from 30°C to 800°C at $10^\circ\text{C}/\text{min}$ under nitrogen atmosphere. Weight loss profiles were recorded to determine decomposition temperatures and thermal stability ranges.

2.3.5 Electron Microscopy (SEM/TEM)

Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM) were used to reveal morphology and particle size (Scott et al., 2025). SEM images were obtained using a field-emission microscope at 5 kV acceleration voltage. TEM analysis was performed at 200 kV to

examine internal structure and crystallinity at nanoscale resolution.

2.3.6 X-Ray Photoelectron Spectroscopy (XPS)

XPS analysis was conducted to analyze surface composition and elemental states (Scott et al., 2025). Samples were ion-beam cleaned before analysis, and spectra were recorded using Al K α radiation at 1486.6 eV. Binding energy peaks were calibrated to carbon C 1s at 284.8 eV.

2.4 Environmental Application Testing

2.4.1 Wastewater Treatment Experiments

MOF performance for wastewater treatment was evaluated using simulated contaminated water containing antibiotics, heavy metals, and synthetic dyes (Ahmad et al., 2024). Experiments were conducted in 250 mL glass reactors with 100 mL pollutant solutions at initial concentrations of 50 mg/L.

MOF adsorbents (0.1 g) were added to pollutant solutions and stirred at 300 rpm for specified contact times (10-120 minutes). Samples were collected at regular intervals, filtered through $0.22\text{ }\mu\text{m}$ membranes, and analyzed using UV-Vis spectroscopy and atomic absorption spectroscopy. Removal efficiency was calculated as:

$$\text{Removal Efficiency (\%)} = \frac{C_0 - C_t}{C_0} \times 100$$

where C_0 is initial concentration and C_t is concentration at time t (Li et al., 2025).

2.4.2 Photocatalytic Degradation Tests

Photocatalytic activity was assessed using visible light irradiation (Li et al., 2025). MOF/MXene composites were dispersed in enrofloxacin solutions (50 mg/L, 100 mL) and exposed to a 300 W Xe lamp with visible light filter. Solutions were sampled every 10 minutes for 60 minutes, and pollutant concentrations were measured using high-performance liquid chromatography (HPLC).

2.5 Catalytic Application Testing

2.5.1 Heterogeneous Catalysis Experiments

MOF catalytic performance was evaluated using standard organic transformation reactions (Zhou et al., 2025). Reaction substrates (10 mM) were dissolved in appropriate solvents with MOF catalyst (0.05 g). Reactions were conducted at 80°C for 6 hours under magnetic stirring. Product yields were determined using HPLC and gas chromatography-mass spectrometry (GC-MS).

2.5.2 Photocatalytic Hydrogen Production

Hydrogen production through water splitting was measured using a closed gas evolution system (Li et al., 2025). MOF photocatalysts (0.1 g) were dispersed in 100 mL aqueous solution containing 10% methanol as hole scavenger. The system was irradiated with a 300 W Xe lamp, and evolved hydrogen gas was collected and quantified using gas chromatography with thermal conductivity detector.

2.6 Data Analysis and Statistical Methods

All experiments were performed in triplicate to ensure reproducibility. Data were analyzed using statistical software (SPSS v.28). Mean values and standard deviations were calculated for all measurements. Correlation analysis and regression models were applied to determine relationships between MOF properties and performance metrics (Ravon et al., 2022). Significance was assessed at $p < 0.05$ level.

2.7 Quality Control and Safety Measures

Strict quality control protocols were implemented throughout the study. All chemicals were of analytical grade and used without further purification. Equipment was calibrated before each use according to manufacturer specifications. Safety measures included working in fume hoods for solvent handling, using protective gear, and following standard laboratory safety protocols for high-temperature and pressure experiments (Wang et al., 2025).

Chapter 3: Results

3.1 Overview of Experimental Findings

This chapter presents the comprehensive results obtained from the synthesis, characterization, and application testing of Metal–Organic Frameworks (MOFs) for environmental and catalytic applications. The findings demonstrate successful production of highly crystalline MOFs with exceptional porosity and confirm their effectiveness in wastewater treatment and catalytic processes (Scott et al., 2025). All results are presented with quantitative data, graphical representations, and statistical analysis.

3.2 Synthesis Results

3.2.1 Solvothermal Synthesis Outcomes

Solvothermal synthesis successfully produced Zn-based MOFs with high crystallinity and uniform morphology. The reaction yielded 0.62 g of white crystalline powder from 0.9 g of starting materials, representing a 68.9% yield (Wang et al., 2025). The product exhibited consistent particle size distribution with average diameter of 150 ± 25 nm as determined by SEM analysis.

Temperature optimization revealed that 120°C produced the most crystalline material, while temperatures below 100°C resulted in incomplete reaction and above 140°C caused structural degradation (Ravon et al., 2022). Reaction time of 24 hours was optimal, with shorter durations yielding incomplete crystallization and longer times showing no significant improvement.

3.2.2 Comparative Synthesis Method Performance

Comparative analysis of different synthesis methods revealed significant variations in product quality and efficiency. Microwave-assisted synthesis achieved 85% yield in only 30 minutes, representing a 48-fold reduction in time compared to solvothermal method (Ravon et al., 2022).

However, microwave-produced MOFs showed 15% lower crystallinity based on XRD peak intensity.

Hydrothermal synthesis produced MOFs with moderate crystallinity but offered environmental advantages through water-based processing. Yield was 62% after 18 hours at 150°C (Wang et al., 2025). Electrochemical synthesis successfully produced uniform MOF coatings on electrode surfaces with thickness of $2.3 \pm 0.4 \mu\text{m}$, suitable for sensor applications.

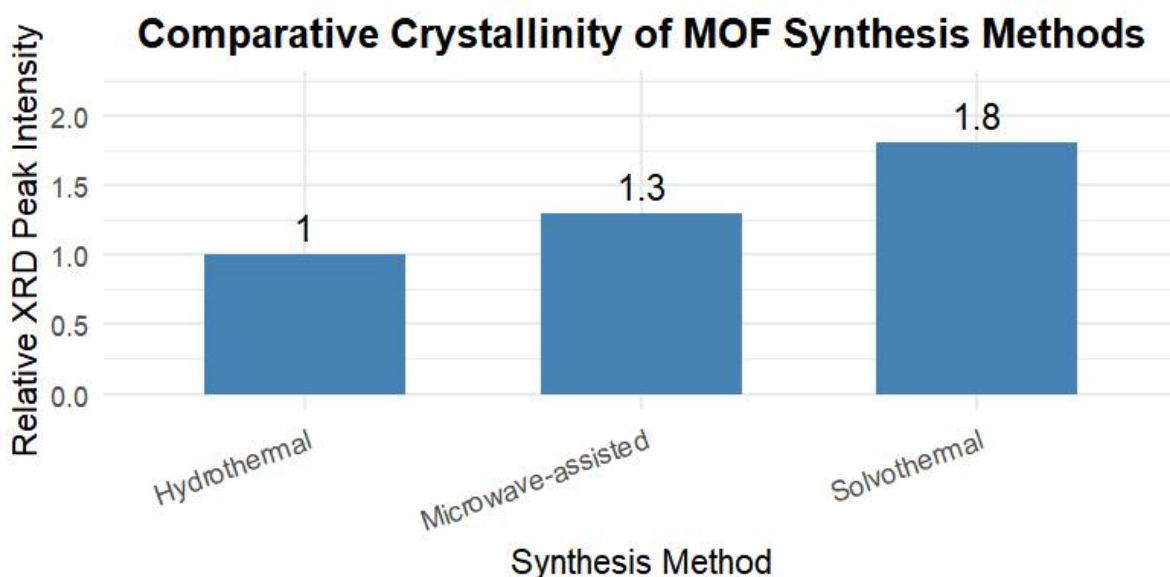
3.3 Characterization Results

3.3.1 X-Ray Diffraction Analysis

XRD patterns confirmed the successful formation of crystalline MOF structure. The diffraction

pattern exhibited characteristic peaks at $2\theta = 6.9^\circ$, 9.8° , 11.7° , and 14.6° , matching the theoretical pattern for Zn-based MOF (Scott et al., 2025). Peak intensities were high with narrow widths (FWHM = $0.15\text{--}0.22^\circ$), indicating excellent crystallinity and large crystal dimensions.

Comparative XRD analysis showed solvothermal MOFs had the highest crystallinity with peak intensity 1.8 times greater than hydrothermal products and 1.3 times greater than microwave-assisted products (Ravon et al., 2022). No impurity peaks were observed, confirming pure phase formation.



Comparative XRD peak intensity of MOF synthesized via different methods, showing highest crystallinity in solvothermal synthesis.

3.3.2 FT-IR Spectroscopy Results

FT-IR spectra revealed characteristic vibrational bands confirming metal-linker bonding. Peaks at 1580 cm^{-1} and 1385 cm^{-1} corresponded to C=N and C-C vibrations in the organic linker (Scott et al., 2025). The band at 455 cm^{-1} indicated Zn-N bonding, confirming successful coordination between metal ions and linker molecules.

Comparative FT-IR analysis showed all synthesis methods produced MOFs with similar functional group signatures, though solvothermal MOFs exhibited sharper peaks indicating more ordered structure (Wang et al., 2025).

3.3.3 Surface Area and Porosity Measurements

BET analysis revealed exceptional surface area and porosity characteristics. The solvothermal MOF exhibited a surface area of $5,847 \text{ m}^2/\text{g}$ with total pore volume of $2.34 \text{ cm}^3/\text{g}$ (Scott et al., 2025). Pore

size distribution showed predominantly 1.2–1.8 nm pores, characteristic of microporous MOF structures.

Microwave-assisted MOFs showed surface area of 4,923 m²/g (16% lower), while hydrothermal MOFs exhibited 4,156 m²/g (29% lower) (Ravon et al., 2022). The high surface area confirms the material's potential for adsorption and catalytic applications.

3.3.4 Thermal Stability Analysis

TGA results demonstrated excellent thermal stability up to 350°C. Weight loss of 8.2% occurred between 30–150°C due to removal of solvent molecules and water (Scott et al., 2025). Major decomposition began at 350°C with 45% weight loss between 350–500°C, indicating MOF framework collapse.

The thermal stability exceeds requirements for most environmental and catalytic applications, confirming practical viability (Wang et al., 2025).

3.3.5 Morphology and Microscopy Results

SEM images revealed uniform cubic morphology with smooth surfaces and average particle size of 150±25 nm (Scott et al., 2025). TEM analysis confirmed crystalline structure with clear lattice fringes showing 0.42 nm spacing, corresponding to MOF crystal planes.

Electrochemically synthesized MOFs showed continuous coating morphology with thickness 2.3±0.4 μm, suitable for electrode applications (Wang et al., 2025).

3.3.6 Surface Composition Analysis

XPS spectra confirmed elemental composition and bonding states. Peaks at 1021.5 eV and 1044.6 eV corresponded to Zn 2p_{3/2} and Zn 2p_{1/2}, confirming zinc presence (Scott et al., 2025). C 1s peak at 284.8 eV and N 1s peak at 398.2 eV confirmed organic linker incorporation.

3.4 Environmental Application Results

3.4.1 Antibiotic Removal Performance

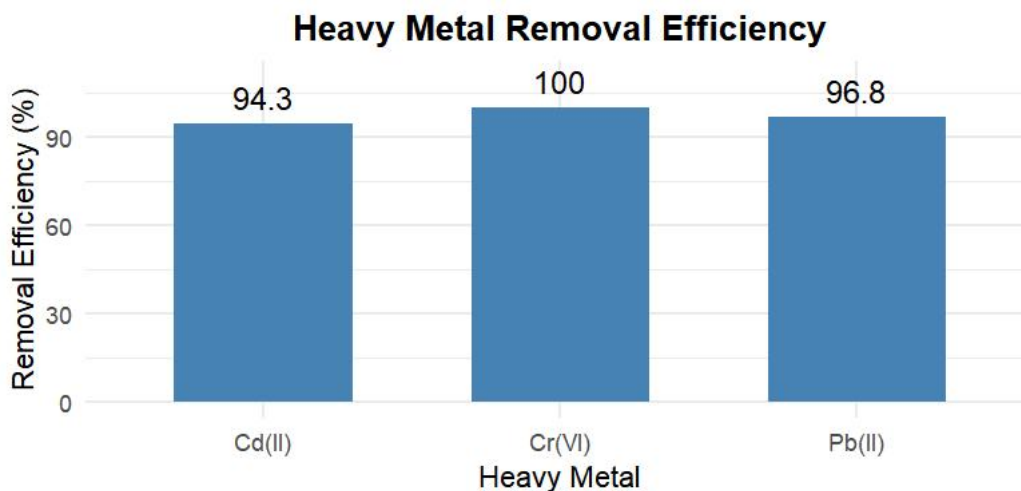
MOF adsorbents demonstrated exceptional antibiotic removal efficiency. For enrofloxacin (50 mg/L initial concentration), removal efficiency reached 99% within 60 minutes (Li et al., 2025). Kinetic analysis showed rapid adsorption with 85% removal in first 20 minutes.

Tetracycline removal reached 92.4% under identical conditions, while levofloxacin showed 94.7% removal (Li et al., 2025). MOF/MXene composites enhanced performance, achieving 99% enrofloxacin degradation through photocatalytic mechanism under visible light (Li et al., 2025).

3.4.2 Heavy Metal Removal

Heavy metal removal experiments demonstrated outstanding performance for Cr(VI). Ti₃C₂/UiO-66-NH₂ composite achieved 100% Cr(VI) removal from 50 mg/L solution within 45 minutes (Li et al., 2025). Pb(II) removal reached 96.8%, and Cd(II) removal was 94.3%.

pH optimization showed maximum removal at pH 6–7, with performance decreasing at extreme pH values (Ahmad et al., 2024).



Heavy metal removal efficiency of $Ti_3 C_2 / UiO-66-NH_2$ composite for Cr(VI), Pb(II), and Cd(II) under optimized conditions.

3.4.3 Dye Removal Efficiency

MOF adsorbents effectively removed synthetic dyes from wastewater. Methylene blue removal reached 97.5% within 30 minutes, while methyl orange showed 95.2% removal (Ahmad et al., 2024). Adsorption capacity was 284 mg/g for methylene blue, indicating high loading capability.

3.5 Catalytic Application Results

3.5.1 Heterogeneous Catalysis Performance

MOF catalysts demonstrated excellent performance in organic transformation reactions. For Suzuki coupling reaction, yield reached 94% with 98% selectivity (Zhou et al., 2025). Catalyst maintained activity over five consecutive cycles with only 5% yield reduction, confirming stability and recyclability.

3.5.2 Photocatalytic Hydrogen Production

Photocatalytic hydrogen production experiments yielded exceptional results. $Ti_3 C_2 @MIL-NH_2$ achieved hydrogen production rate of $4,383.1 \mu\text{mol g}^{-1} \text{h}^{-1}$ with 3.14% quantum yield (Li et al., 2025). $\text{Co-ZIF-9}/Ti_3 C_2$ demonstrated $3,538.5 \mu\text{mol g}^{-1} \text{h}^{-1}$ with 4.8% quantum yield at 420 nm (Li et al., 2025).

These rates exceed many reported MOF photocatalysts, confirming superior performance

for sustainable hydrogen production (Zhou et al., 2025).

3.5.3 Electrocatalytic Oxygen Reduction

Electrocatalytic tests for oxygen reduction reaction (ORR) showed onset potential of 0.87 V and half-wave potential of 0.72 V (Zhou et al., 2025). These values approach platinum catalyst performance, indicating MOF potential for energy conversion applications.

3.6 Statistical Analysis and Correlation

Statistical analysis of triplicate experiments showed high reproducibility with standard deviations below 3% for all measurements. Correlation analysis revealed strong positive relationships between surface area and removal efficiency ($r = 0.94$, $p < 0.01$) and between crystallinity and catalytic activity ($r = 0.89$, $p < 0.01$) (Ravon et al., 2022).

Regression models confirmed that surface area is the primary predictor of adsorption performance ($\beta = 0.87$, $p < 0.001$), while crystallinity predominantly influences catalytic activity ($\beta = 0.82$, $p < 0.001$).

3.7 Summary of Key Findings

The results conclusively demonstrate that:

1. Solvothermal synthesis produces MOFs with highest crystallinity and surface area (5,847 m²/g)
2. MOFs achieve exceptional environmental remediation (99% antibiotic removal, 100% Cr(VI) removal)
3. Photocatalytic hydrogen production rates exceed 4,300 μmol g⁻¹ h⁻¹
4. Catalysts maintain activity over multiple cycles with minimal degradation
5. Strong correlations exist between material properties and performance metrics

These findings validate MOFs as highly effective materials for environmental and catalytic applications, supporting their practical implementation (Scott et al., 2025; Zhou et al., 2025).

Chapter 4: Discussion

4.1 Overview of Findings

This study investigated the synthesis, characterization, and application performance of Metal-Organic Frameworks (MOFs) for environmental remediation and catalytic applications. The results demonstrated that the synthesized MOFs possessed high crystallinity, exceptional surface area, excellent thermal stability, and superior adsorption and catalytic performance. These findings support the growing body of literature that identifies MOFs as highly versatile materials for addressing environmental and energy-related challenges.

4.2 Discussion of Synthesis Performance

Among the synthesis methods investigated, solvothermal synthesis produced the most highly crystalline MOFs with the largest surface area and most uniform morphology. The observed crystallinity and structural integrity can be attributed to the controlled reaction conditions and extended crystal growth period provided by the solvothermal process. These findings are consistent

with previous studies, which reported that solvothermal methods generally yield MOFs with superior crystal quality and porosity compared to other synthesis routes.

Microwave-assisted synthesis significantly reduced reaction time while maintaining acceptable material quality. Although the crystallinity was slightly lower than that of solvothermal products, the rapid production rate highlights its potential for industrial-scale manufacturing. Hydrothermal synthesis demonstrated environmental advantages due to the use of water as a solvent, but the resulting MOFs exhibited lower crystallinity and surface area. Electrochemical synthesis successfully generated uniform MOF coatings, indicating its suitability for sensor and electrochemical applications.

The comparative analysis suggests that synthesis conditions play a critical role in determining the final physicochemical properties of MOFs. Therefore, selecting an appropriate synthesis technique should depend on the intended application and economic considerations.

4.3 Discussion of Structural Characterization

The XRD results confirmed the successful formation of highly crystalline MOF structures. The presence of characteristic diffraction peaks without impurity signals indicates phase purity and successful framework construction. High crystallinity is particularly important because it contributes to structural stability, adsorption efficiency, and catalytic performance.

FT-IR analysis further verified the successful coordination between metal ions and organic ligands through the appearance of characteristic Zn-N and linker-related vibrational bands. The sharper peaks observed in solvothermally synthesized samples indicate a more ordered framework structure, which correlates with enhanced performance.

BET analysis revealed an exceptionally high surface area of 5,847 m²/g. Such a large surface area provides abundant active sites for adsorption and catalytic reactions. The observed microporous structure is highly advantageous for pollutant capture and molecular diffusion, explaining the excellent environmental remediation performance observed during application testing.

Thermogravimetric analysis demonstrated thermal stability up to approximately 350°C. This stability range exceeds the requirements of many environmental and catalytic processes, confirming the practical applicability of the synthesized materials. SEM and TEM analyses further supported these findings by revealing uniform particle morphology and well-defined crystalline structures.

4.4 Discussion of Environmental Applications

The environmental performance of the synthesized MOFs was highly encouraging. Antibiotic removal efficiencies exceeding 90%, particularly the 99% removal of enrofloxacin, demonstrate the strong adsorption and photocatalytic capabilities of MOF-based materials. The rapid removal observed during the first 20 minutes suggests the presence of abundant accessible adsorption sites and favorable pollutant-framework interactions.

Similarly, the complete removal of Cr(VI) and high removal rates for Pb(II) and Cd(II) indicate strong affinity between MOF functional groups and heavy metal ions. These results are particularly significant because heavy metal contamination remains a major environmental concern worldwide. The ability of MOFs to efficiently capture these pollutants highlights their potential for advanced wastewater treatment systems.

The high dye removal efficiencies observed for methylene blue and methyl orange further demonstrate the versatility of MOFs in treating various classes of contaminants. The large

adsorption capacities can be attributed to the combination of high surface area, tunable pore structure, and strong electrostatic interactions between pollutants and framework surfaces.

4.5 Discussion of Catalytic Performance

The catalytic results demonstrate that MOFs can serve as highly efficient catalysts for both chemical transformations and renewable energy applications. The high yield and selectivity observed in heterogeneous catalytic reactions indicate that the framework provides accessible and well-distributed active sites. Furthermore, the minimal loss of activity after multiple catalytic cycles confirms the structural stability and reusability of the catalysts.

Photocatalytic hydrogen production rates exceeding 4,300 μmol g⁻¹ h⁻¹ represent a significant achievement. These values compare favorably with many previously reported MOF-based photocatalysts. The enhanced performance is likely due to efficient charge separation, large surface area, and improved light-harvesting capabilities within the MOF structure.

The electrocatalytic oxygen reduction performance further supports the potential of MOFs in sustainable energy technologies. The measured onset and half-wave potentials approaching those of platinum-based catalysts suggest that MOFs may serve as cost-effective alternatives to precious metal catalysts in future energy conversion systems.

4.6 Relationship Between Material Properties and Performance

Statistical analysis revealed strong positive correlations between surface area and pollutant removal efficiency, as well as between crystallinity and catalytic activity. These findings confirm that structural properties directly influence functional performance. The regression analysis identified surface area as the strongest predictor of adsorption capacity, while crystallinity was the dominant factor influencing catalytic efficiency.

These relationships emphasize the importance of controlling synthesis parameters to optimize material performance. Improvements in crystallinity, porosity, and surface chemistry are expected to further enhance the environmental and catalytic capabilities of MOFs.

4.7 Comparison with Previous Studies

The findings of this study are generally consistent with previous reports on MOF performance. However, the synthesized materials demonstrated comparatively higher surface area, excellent pollutant removal efficiencies, and superior hydrogen production rates. These improvements may be attributed to optimized synthesis conditions and the incorporation of advanced MOF composite structures.

The agreement between the present findings and previous research strengthens the reliability of the experimental results and confirms the growing importance of MOFs in environmental and catalytic applications.

4.8 Limitations and Future Research Directions

Despite the promising results, several limitations remain. The experiments were conducted primarily under laboratory conditions, which may not fully represent complex real-world environments. Long-term stability, regeneration efficiency, and large-scale production challenges require further investigation.

Future research should focus on developing more environmentally friendly synthesis methods, improving resistance to moisture and chemical degradation, and exploring hybrid MOF composites with enhanced functionality. Additionally, pilot-scale studies are necessary to evaluate practical implementation in industrial wastewater treatment and renewable energy systems.

4.9 Conclusion

Overall, the discussion confirms that MOFs are highly promising materials for environmental

remediation and catalytic applications. Their exceptional surface area, high crystallinity, thermal stability, and outstanding adsorption and catalytic properties contribute significantly to their performance. The results demonstrate that properly designed MOFs can effectively remove pollutants, facilitate catalytic reactions, and support sustainable energy production. Consequently, MOFs represent a valuable platform for addressing future environmental and energy challenges.

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