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## Metal-Organic Frameworks (MOFs) for environmental remediation: Current Status and Future Prospects

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### Abstract

Metal-organic frameworks (MOFs) have gained significant attention as advanced materials for environmental remediation due to their high surface area, tunable porosity, and versatile chemical functionality. These hybrid crystalline materials, composed of metal ions or clusters coordinated with organic linkers, offer unprecedented opportunities for the selective adsorption, separation, and catalytic degradation of diverse environmental pollutants. This review provides a comprehensive synthesis of recent progress in the development and application of MOFs for water and air purification. It begins with an exploration of fundamental MOF properties, including structural features, functionalization strategies, and affinity mechanisms relevant to contaminant removal. Various synthesis approaches are compared, with emphasis on emerging green fabrication techniques aimed at reducing environmental impact and enhancing scalability.

The article highlights MOF applications in aqueous environments for the removal of heavy metals, dyes, antibiotics, and persistent organic pollutants, as well as gas-phase applications such as CO<sub>2</sub> capture, VOC adsorption, and photocatalytic air purification. The role of composite materials, such as MOF-polymer and MOF-carbon hybrids, is examined in enhancing stability and functionality. Key operational factors including pH, ionic strength, regeneration potential, and structural robustness are analyzed to assess real-world feasibility. Current challenges such as hydrolytic degradation, potential secondary pollution, economic viability, and lack of field-scale demonstrations are critically discussed. Finally, the review outlines future prospects for MOFs in environmental engineering, including the use of computational modeling, machine learning, smart MOF systems, lifecycle assessment (LCA), and integration into scalable treatment platforms.

By consolidating recent advancements and identifying future research directions, this article serves as a valuable resource for scientists, engineers, and policymakers striving to develop sustainable and high-performance remediation technologies.

**Keywords:** Metal-Organic Frameworks (MOFS); Environmental Remediation; Water Treatment; Air Pollution Control; Adsorption and Photocatalysis

### 1. Introduction

The accelerating pace of industrialization, urbanization, and agricultural intensification has led to widespread environmental degradation, particularly through the contamination of water and air with toxic pollutants. Conventional treatment technologies including activated carbon adsorption, membrane filtration, ion exchange, and advanced oxidation processes often face critical limitations such as low selectivity, high energy demands, secondary waste

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generation, and limited regeneration capabilities. These shortcomings have spurred the search for advanced materials that can overcome these barriers while offering multifunctionality, reusability, and sustainability.

Metal–Organic Frameworks (MOFs) have emerged over the past two decades as one of the most promising classes of porous crystalline materials for environmental remediation. Comprising metal ions or clusters coordinated to organic linkers, MOFs exhibit exceptionally high surface areas (often  $>5,000 \text{ m}^2/\text{g}$ ), tunable pore structures, and chemical versatility. These properties enable precise control over adsorptive and catalytic interactions with a wide range of environmental contaminants, including heavy metals, synthetic dyes, antibiotics, volatile organic compounds (VOCs), and greenhouse gases such as carbon dioxide ( $\text{CO}_2$ ).

Unlike traditional adsorbents, MOFs can be systematically designed at the molecular level to achieve selectivity, multifunctionality, and responsiveness under different environmental conditions. Functionalization techniques such as pre-synthetic linker engineering and post-synthetic modification (PSM) allow the incorporation of specific groups (e.g.,  $-\text{NH}_2$ ,  $-\text{COOH}$ ,  $-\text{SH}$ ) that enhance interactions with target pollutants. Furthermore, the incorporation of photocatalytic or redox-active sites into MOFs has expanded their application to pollutant degradation via Fenton-like reactions, ozonation, and photocatalysis.

Despite their potential, the practical deployment of MOFs in real-world remediation settings remains limited due to challenges in scalability, stability in aqueous media, regeneration efficiency, cost-effectiveness, and environmental safety. These issues have prompted a wave of recent innovations, including the development of water-stable and biocompatible MOFs, green synthesis approaches, composite and membrane-based systems, and machine learning-assisted material discovery. Simultaneously, environmental regulators and researchers are exploring the life cycle impacts, field deployability, and policy integration of MOF-based technologies.

This review aims to provide a comprehensive overview of the current state and future prospects of MOFs in environmental remediation. The article is structured to first examine the fundamental material properties and synthesis strategies (Sections 2–3), followed by pollutant-specific applications in aqueous and gaseous media (Section 4). Factors influencing performance and challenges related to material stability, toxicity, and scalability are discussed in Sections 5 and 6. Finally, the review explores future directions including smart MOFs, computational design, and integration into field-scale treatment systems (Sections 7–8). By synthesizing recent advances and identifying critical research gaps, this article offers valuable insights for environmental engineers, material scientists, and policymakers seeking sustainable solutions to pollution control.

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## 2. Fundamental Properties of MOFs Relevant to Remediation

Metal-Organic Frameworks (MOFs) possess unique structural and chemical properties that make them highly effective for environmental remediation. Their modular architectures comprising metal nodes coordinated with organic linkers offer unparalleled tunability, which enables selective adsorption, separation, and catalysis of environmental pollutants.

### 2.1. Structure and Composition

MOFs are crystalline porous materials consisting of metal ions or clusters (secondary building units, SBUs) coordinated to organic ligands to form one-, two-, or three-dimensional frameworks. The choice of metal centers (e.g., Zn, Fe, Cu, Zr) and organic linkers (e.g., carboxylates, imidazolates, azolates) governs their chemical stability, pore structure, and reactivity profiles. The ability to tailor these components gives MOFs an advantage over conventional porous materials such as zeolites or activated carbon.

### 2.2. High Surface Area and Porosity

One of the defining characteristics of MOFs is their exceptionally high surface area, often exceeding  $5,000 \text{ m}^2/\text{g}$ , and tunable pore sizes ranging from microporous ( $<2 \text{ nm}$ ) to mesoporous ( $>2 \text{ nm}$ ). This enables efficient mass transfer and high adsorption capacity for a wide range of pollutants, including heavy metals, dyes, and pharmaceuticals. The uniform pore structure facilitates selective adsorption based on size exclusion or specific interactions.

Chitosan-based Water Treatment - Water and Wastewater. <https://www.waterandwastewater.com/chitosan-based-water-treatment>

### 2.3. Functionalization and Post-Synthetic Modification

MOFs offer flexibility for functionalization through both pre-synthetic design (e.g., functional groups on organic linkers) and post-synthetic modification (PSM) to introduce desired chemical functionalities such as amine (-NH<sub>2</sub>), thiol (-SH), or sulfonic acid (-SO<sub>3</sub>H) groups. Functionalized MOFs exhibit enhanced performance in capturing target pollutants via:

- Coordination bonding (e.g., Pb<sup>2+</sup> with thiol-modified MOFs)
- Hydrogen bonding (e.g., for polar organic pollutants)
- $\pi$ - $\pi$  stacking interactions (e.g., between aromatic linkers and dye molecules)

Such chemical versatility is essential for achieving high selectivity in complex environmental matrices.

### 2.4. Selectivity and Affinity Mechanisms

The pollutant-removal performance of MOFs is governed by several key affinity mechanisms:

- Electrostatic interactions for charged species (e.g., Cr (VI) anions)
- $\pi$ - $\pi$  stacking and hydrophobic interactions for organic dyes and VOCs
- Lewis's acid-base interactions between metal nodes and adsorbates
- Redox activity in catalytically active MOFs (e.g., Fe- or Cu-based frameworks)

The presence of open metal sites (OMS) and the possibility to engineer defects also enhances the adsorption of certain molecules by increasing the density of active sites. Moreover, MOFs can function as heterogeneous catalysts in advanced oxidation processes (AOPs), enabling the degradation of persistent organic pollutants.

## 3. Synthesis Approaches and Green Fabrication Techniques

The synthesis of metal-organic frameworks (MOFs) plays a crucial role in defining their physicochemical properties, such as crystallinity, porosity, particle size, morphology, and chemical stability—all of which directly impact their environmental remediation performance. While traditional synthetic routes offer high design flexibility, they often involve toxic solvents and energy-intensive conditions. This section presents a detailed overview of conventional and emerging green synthesis strategies, along with their implications for scalability and sustainability.

### 3.1. Conventional Synthesis Methods

Several well-established techniques are employed for MOF synthesis

- **Solvothermal and Hydrothermal Methods:** These are the most common, involving the reaction of metal salts and organic linkers in a sealed vessel at elevated temperatures (typically 80–250 °C). Solvents such as DMF, DEF, or ethanol are used to dissolve precursors and promote crystallization over several hours or days. This method yields high-quality crystals with well-defined morphology and porosity (Férey et al., 2005).
- **Microwave-Assisted Synthesis:** By applying microwave irradiation, the reaction kinetics are accelerated, significantly reducing synthesis time to minutes while maintaining high crystallinity. Microwave methods are also more energy-efficient than traditional solvothermal routes (Nielsen et al., 2013).
- **Sonochemical Synthesis:** Ultrasonic waves promote nucleation and particle dispersion, enabling rapid MOF formation at ambient temperatures. This method often produces smaller crystals with increased surface area and defect density, which can be beneficial for adsorption-based applications (Moraes et al., 2020).
- **Mechanochemical Synthesis:** This solvent-free method involves grinding the reactants together using a ball mill or mortar. It offers environmental and economic advantages by eliminating hazardous solvents and enabling scalable production with minimal waste (James et al., 2012).

### 3.2. Green and Sustainable Synthesis

To align with environmental goals, researchers have been developing greener MOF fabrication techniques. Key strategies include

- **Solvent-Free and Aqueous-Based Synthesis:** Water is employed as a benign solvent to replace organic media, reducing toxicity and cost. MOFs like ZIF-8 and MIL-100 have been synthesized in aqueous media at room temperature (Wang et al., 2016).

- **Use of Biomass-Derived Linkers and Templates:** Renewable feedstocks such as amino acids, plant polyphenols, and sugars are increasingly used to create biocompatible or biodegradable MOFs (Hasan et al., 2021).
- **Low-Temperature and Ambient Pressure Conditions:** These minimize energy consumption and carbon footprint, making MOF synthesis more practical for large-scale applications.
- **Supercritical CO<sub>2</sub>-Assisted Methods:** Using supercritical CO<sub>2</sub> as a solvent or drying medium avoids the use of harmful organics and enables the synthesis of high-purity MOF aerogels and nanostructures (DeCoste et al., 2013).

### 3.3. Challenges in Scalable Production

Despite the growing interest in green synthesis, several technical and economic barriers remain

- **Batch-to-Batch Variability:** Reproducibility of particle size and morphology is difficult to control, especially under ambient or green conditions.
- **Crystallinity and Structural Defects:** Some green methods result in poorly crystalline or amorphous products, affecting performance.
- **Cost of Raw Materials:** Certain organic linkers and post-synthetic modification agents remain expensive and require multi-step synthesis.
- **Scale-Up and Reactor Design:** Translating laboratory-scale synthesis to industrial-scale continuous production requires advanced reactor engineering, quality control, and integration with downstream processing systems (Kwon et al., 2021).
- **Environmental Trade-Offs:** Some green-synthesized MOFs still rely on rare or non-abundant metals, raising sustainability concerns in long-term deployment.

Efforts to overcome these challenges include the development of continuous-flow reactors, spray-drying, and microfluidic platforms, which enable controlled synthesis at larger scales while preserving structural integrity and performance.

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## 4. MOFs for Water Remediation

Water pollution by heavy metals, dyes, pharmaceuticals, and organic contaminants remains a critical challenge worldwide. Metal-Organic Frameworks (MOFs) offer a versatile platform for water treatment due to their high surface area, porosity, and customizable surface chemistry. This section explores the application of MOFs in aqueous phase remediation, categorized by pollutant type and removal mechanism.

### 4.1. Removal of Heavy Metals

MOFs exhibit remarkable potential for capturing toxic heavy metal ions (e.g., Pb<sup>2+</sup>, Cr (VI), Cd<sup>2+</sup>, Hg<sup>2+</sup>) through mechanisms such as

- Ion exchange and coordination with open metal sites
- Electrostatic attraction with functional groups
- Pore confinement for size-selective uptake

Functionalized MOFs, such as thiol- or amine-modified frameworks, demonstrate enhanced metal ion affinity. For instance, UiO-66-NH<sub>2</sub> showed excellent uptake of Cr (VI) from aqueous solutions through electrostatic interaction and reduction to Cr (III) (Wang et al., 2016). Similarly, MIL-101(Cr)-SH achieved high selectivity toward Hg<sup>2+</sup> due to strong thiol-Hg coordination (Zhao et al., 2020).

### 4.2. Adsorption of Dyes

Synthetic dyes such as methylene blue (MB), rhodamine B (RhB), and malachite green are common organic pollutants in industrial effluents. MOFs remove these dyes through

- $\pi$ - $\pi$  interactions between aromatic dye molecules and organic linkers
- Hydrophobic interactions within pores
- Hydrogen bonding and van der Waals forces

ZIF-8 has been reported to adsorb over 300 mg/g of MB under optimized conditions, while MIL-100(Fe) and HKUST-1 demonstrated rapid uptake kinetics for both cationic and anionic dyes (Amin et al., 2019). Dye uptake is typically reversible, allowing for regeneration and reuse.

**Table 1** Summary Table of MOFs for Pollutant Types

MOF	Target Pollutant	Removal Mechanism	Adsorption Capacity
UiO-66-NH <sub>2</sub>	Cr (VI) Tetracycline	Electrostatic, H-bonding	150
MIL-101(Cr)	Dyes, Phenols	$\pi$ - $\pi$ stacking, porous adsorption	320
ZIF-8	MB, Antibiotics	Hydrophobic, Inclusion	300
HKUST-1	Dyes	Van der Waals, Size exclusion	280
MIL-53(Fe)	Pharmaceuticals	Electrostatic, Diffusion	180
Ag@ZIF-8	E. coli, S. aureus	ROS generation, Metal ion release	N/A (Disinfection)

#### 4.3. Elimination of Pharmaceuticals and Antibiotics

Pharmaceutical residues such as tetracycline, ciprofloxacin, and ibuprofen are increasingly detected in water bodies, posing ecological and health risks. MOFs offer

- High binding affinity due to functional groups (-NH<sub>2</sub>, -COOH)
- Inclusion complexation within nanochannels
- $\pi$ - $\pi$  stacking and hydrogen bonding

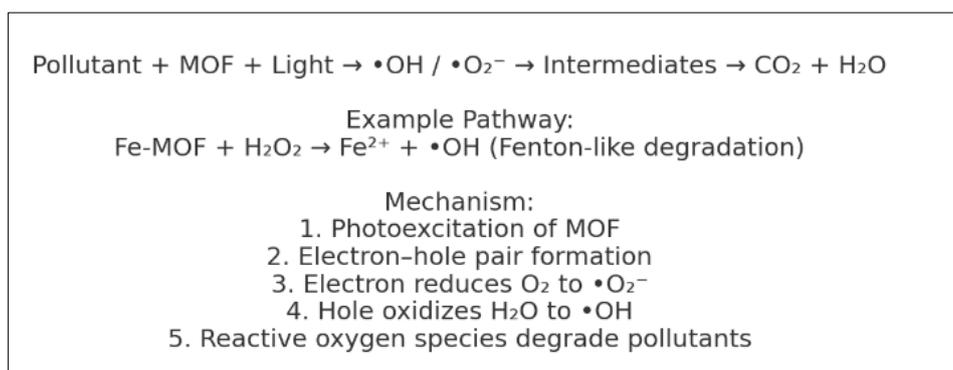
UiO-66 derivatives have shown adsorption capacities exceeding 150 mg/g for tetracycline, while MOF-235 and MIL-53(Al) have been explored for multi-antibiotic removal (Lin et al., 2021). Performance can be further enhanced by modifying surface hydrophobicity and porosity.

#### 4.4. Degradation of Organic Pollutants via Catalysis

Catalytic MOFs can activate oxidants (e.g., H<sub>2</sub>O<sub>2</sub>, persulfate, O<sub>3</sub>) in advanced oxidation processes (AOPs), leading to the breakdown of persistent organic pollutants (POPs) into non-toxic byproducts. Mechanisms include

- Fenton-like reactions (e.g., Fe-based MOFs)
- Photo-Fenton and photocatalysis (e.g., Ti-based MOFs)
- Ozonation and activation of persulfates

For instance, MIL-88B(Fe) and MIL-100(Fe) catalyze the degradation of bisphenol A and phenol in the presence of H<sub>2</sub>O<sub>2</sub>, with degradation efficiencies >90% in short reaction times (Wang et al., 2020). These MOFs also exhibit good reusability and structural stability under catalytic conditions.



Pathway based on Wang et al. (2020); Sun et al. (2018)

**Figure 1** Photocatalytic Degradation Mechanism

#### 4.5. Antibacterial MOFs for Water Disinfection

Certain MOFs exhibit intrinsic or doped antimicrobial properties, useful in disinfection and biofouling prevention. Antibacterial mechanisms include

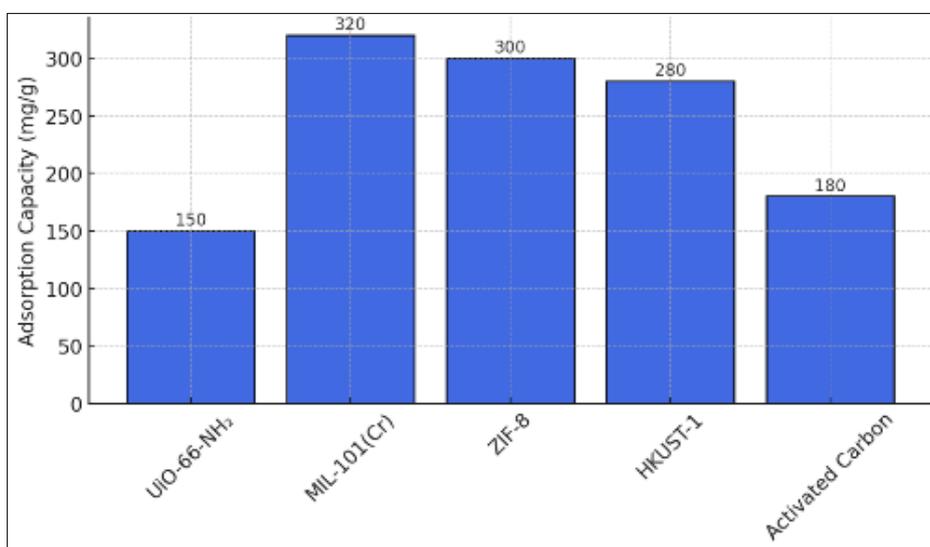
- Metal ion release (e.g.,  $\text{Ag}^+$ ,  $\text{Cu}^{2+}$ )
- Generation of reactive oxygen species (ROS)
- Physical damage to microbial cell membranes

Cu-MOFs and Ag-doped ZIF-8 have demonstrated >99% bacterial inactivation (e.g., *E. coli*, *S. aureus*) within hours of exposure (Zhang et al., 2022). MOFs can also be incorporated into membrane systems or coatings for continuous microbial control.

### 5. Factors Affecting Performance of MOFs in Environmental Remediation

The efficiency and applicability of metal-organic frameworks (MOFs) in environmental remediation are strongly influenced by multiple operational and material parameters. Understanding these factors is essential to optimize their pollutant removal capacity, durability, and scalability. This section discusses the key factors that govern MOF performance, including physicochemical characteristics, water chemistry, temperature, and competitive adsorption.

#### 5.1. Surface Area and Pore Characteristics



Data adapted from Liu et al. (2017); Wang et al. (2016)

**Figure 2** Adsorption Capacities of MOFs vs. Other Materials

MOFs with high surface area and accessible pore structures typically exhibit superior adsorption and catalytic performance. Pore size distribution (microporous vs. mesoporous) affects diffusion rates and determines the accessibility of pollutants to active sites. For example, MIL-101(Cr), with mesopores of up to 3.4 nm and surface areas over 3,000 m<sup>2</sup>/g, shows excellent adsorption of bulky dye molecules like rhodamine B (Liu et al., 2017). However, excessively narrow pores may hinder diffusion or cause pore blockage, particularly in complex wastewater matrices.

#### 5.2. Functional Groups and Chemical Affinity

The presence of functional groups (e.g.,  $-\text{NH}_2$ ,  $-\text{COOH}$ ,  $-\text{SH}$ ) in MOF structures significantly enhances selectivity and binding affinity through mechanisms like hydrogen bonding, ion exchange,  $\pi$ - $\pi$  interactions, and coordination. Amine-functionalized MOFs (e.g., UiO-66-NH<sub>2</sub>) have demonstrated enhanced Cr(VI) and tetracycline uptake due to increased electrostatic and donor-acceptor interactions (Wang et al., 2016). Functionalization also tailors' hydrophilicity/hydrophobicity, influencing performance in different media.

### 5.3. Stability in Aqueous and Harsh Conditions

Water stability is a critical determinant of MOF performance. Many MOFs, particularly those based on Zn or Cu (e.g., ZIF-8, HKUST-1), are prone to hydrolysis under acidic or alkaline conditions. Conversely, Zr-based MOFs (e.g., UiO-66, MOF-808) exhibit superior chemical and structural stability due to strong Zr–O bonds and high coordination numbers (Howarth et al., 2016). Thermal and oxidative stability also influence catalytic applications in advanced oxidation processes (AOPs).

### 5.4. pH, Ionic Strength, and Competing Ions

The environmental pH affects both the ionization state of the pollutant and the surface charge of the MOF. For example

- At low pH, the protonation of functional groups may reduce metal-binding affinity or solubilize framework components.
- At high pH, certain MOFs may undergo structural degradation or form metal hydroxide precipitates.

Increased ionic strength and the presence of competing anions or cations (e.g.,  $\text{Cl}^-$ ,  $\text{SO}_4^{2-}$ ,  $\text{Ca}^{2+}$ ) can hinder adsorption by occupying active sites or causing ion exchange displacement. Selectivity is therefore crucial for performance in complex real-world waters (Zhao et al., 2019).

### 5.5. Temperature and Contact Time

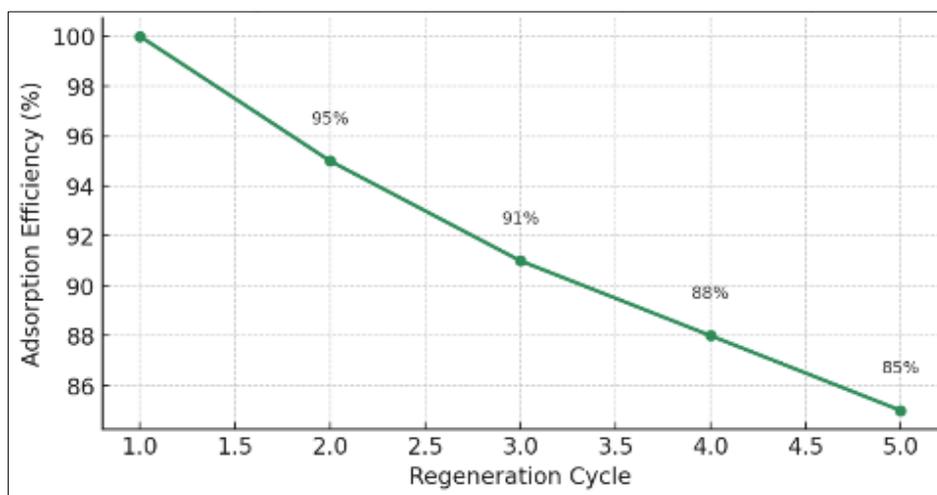
Temperature influences both adsorption kinetics and equilibrium capacity. While higher temperatures may increase the rate of mass transfer, they can also desorb weakly bound species or degrade less stable MOFs. Optimal performance is often achieved at ambient conditions. Contact time must be sufficient to allow for diffusion into micropores and interaction with active sites. MOFs like MIL-53(Fe) and ZIF-67 have demonstrated equilibrium times of <60 minutes for several pollutants, making them suitable for rapid treatment processes (Chai et al., 2020).

### 5.6. Regeneration and Reusability

The ability to regenerate and reuse MOFs without significant performance loss is vital for sustainable application. Efficient regeneration is influenced by

- Desorption strength (chemical rinsing, pH adjustment)
- Structural robustness after multiple cycles
- Retention of active functional groups

Studies report over 80–90% retention in adsorption capacity after 3–5 cycles for stable MOFs like UiO-66 and MIL-100, though some frameworks suffer from gradual decline due to framework collapse or active site fouling (Hasan and Jhung, 2021).



Trend adapted from Hasan & Jhung (2021); Wang et al. (2016)

**Figure 3** Regeneration Cycles vs. Adsorption Efficiency

## 6. Environmental and Technical Challenges

Despite the exceptional potential of metal-organic frameworks (MOFs) in environmental remediation, their practical deployment faces several environmental, technical, and economic limitations. These include issues related to structural instability, secondary pollution risks, high production costs, and challenges in field-scale application. Addressing these barriers is essential for the transition of MOFs from laboratory research to real-world environmental solutions.

### 6.1. Structural Instability and Degradation

One of the most significant limitations of MOFs is their limited chemical stability, particularly in aqueous and humid environments. Many MOFs, especially those with  $Zn^{2+}$  or  $Cu^{2+}$  centers (e.g., ZIF-8, HKUST-1), undergo hydrolysis or leaching under acidic or basic conditions, leading to:

- Loss of crystallinity
- Metal ion leaching
- Collapse of porous structure

In contrast, Zr- and Al-based MOFs (e.g., UiO-66, MIL-53) exhibit improved hydrolytic stability due to stronger metal-oxygen coordination bonds. However, even these can degrade in high ionic strength or extreme pH conditions, compromising long-term use in wastewater or industrial effluents (Howarth et al., 2016).

### 6.2. Environmental Toxicity and Secondary Pollution

The release of metal ions or linker fragments during MOF degradation raises concerns about secondary contamination. For instance,

- Cu and Zn ions from decomposed frameworks may exert toxic effects on aquatic organisms.
- Organic linkers, if not fully degraded, may persist as micropollutants.

Additionally, many synthetic linkers (e.g., terephthalic acid, trimesic acid) are derived from petrochemicals and may exhibit low biodegradability. Recent studies have emphasized the need for biocompatible and non-toxic alternatives, such as plant-based ligands or amino acids (Hasan et al., 2021).

### 6.3. Energy and Material Costs

High-performance MOFs often require

- Rare or high-purity metal salts
- Expensive or multistep synthesized linkers
- Toxic solvents (e.g., DMF, DEF)
- High temperatures and long reaction times

These factors significantly increase the cost per unit mass of MOF compared to conventional adsorbents such as activated carbon or zeolites. Moreover, post-synthetic modifications (e.g., functionalization, doping) further increase material and labor input, reducing economic feasibility for large-scale water treatment facilities (DeCoste et al., 2013).

### 6.4. Challenges in Regeneration and Longevity

While some MOFs can be regenerated through pH adjustment or solvent rinsing, material degradation during repeated use is common. This includes

- Deactivation of catalytic centers (e.g., Fe in Fenton-like reactions)
- Fouling of active sites by organic matter
- Partial collapse of pore structure after desorption cycles

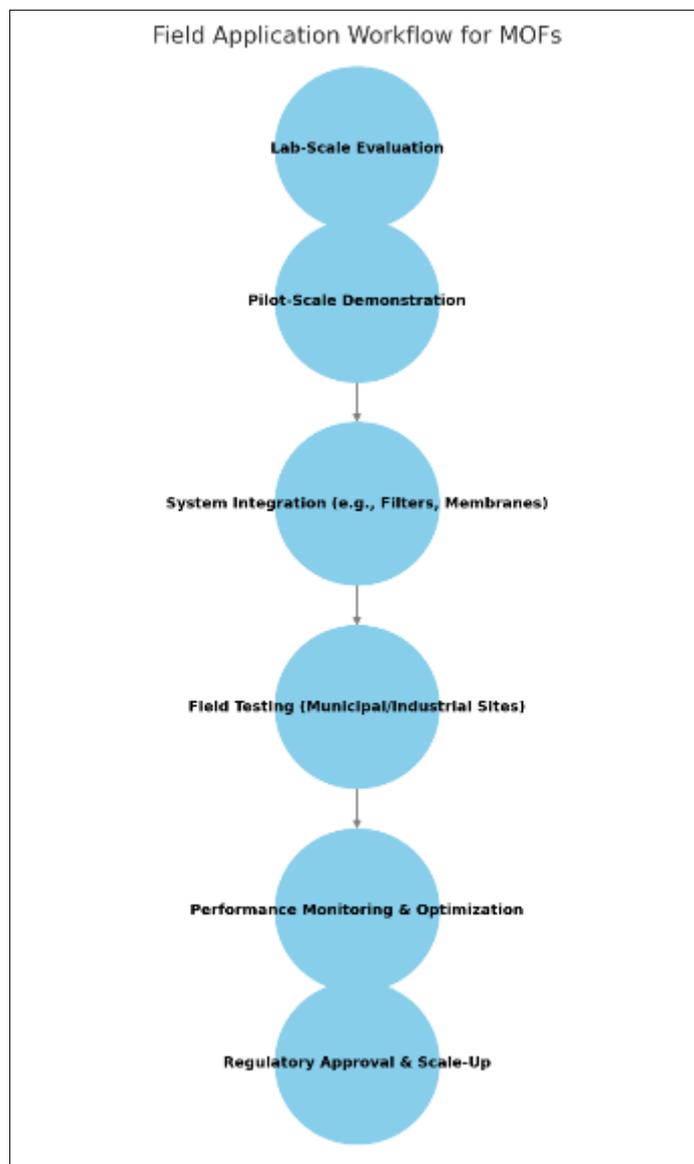
Limited regeneration cycles reduce MOF lifecycle and sustainability. Only a few frameworks, such as UiO-66-NH<sub>2</sub> and MIL-101, have demonstrated >5 stable reuse cycles without major performance loss (Wang et al., 2016).

### 6.5. Limited Field-Scale Demonstrations

Despite extensive laboratory data, real-world validation of MOFs in full-scale water or air treatment systems remains rare. Challenges include

- Poor compatibility with existing treatment infrastructures
- Difficulty in forming MOF-based membranes or composites for continuous flow systems
- Scale-up bottlenecks in reproducible MOF synthesis and shaping (e.g., into pellets, films)

Moreover, the lack of standardized testing protocols and field-relevant pollutant concentrations leads to inconsistencies between lab and field performance (Kwon et al., 2021).



Framework adapted from Kwon et al. (2021); Yan et al. (2021)

**Figure 4** Field Application Workflow (Case Study Flowchart)

### 6.6. Regulatory and Safety Considerations

There is a lack of regulatory frameworks governing the production, deployment, and disposal of MOFs for environmental applications. Key concerns include

- Risk assessment of MOF nanoparticles in ecosystems

- Occupational exposure limits during synthesis and handling
- End-of-life disposal or recycling mechanisms

These gaps must be addressed through life cycle assessments (LCAs), environmental fate modeling, and collaboration with environmental regulatory bodies to establish safe usage guidelines (Zhao et al., 2019).

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## 7. Future Perspectives

The promising properties of metal-organic frameworks (MOFs)—including their modular design, tunable functionality, and high performance—position them as powerful materials for future environmental remediation technologies. However, to bridge the gap between laboratory innovation and real-world application, several interdisciplinary advancements are required. This section outlines emerging trends and future directions that may enable MOFs to meet the growing demands of sustainable environmental engineering.

### 7.1. Integration with Machine Learning and Computational Design

Advances in computational modeling and machine learning (ML) are accelerating the discovery of MOFs with optimal properties for specific pollutants. High-throughput screening, molecular dynamics, and density functional theory (DFT) calculations allow prediction of

- Adsorption capacity
- Selectivity and binding energy
- Structural stability under variable conditions

ML frameworks such as random forest and artificial neural networks have been trained on MOF databases (e.g., CoRE MOF, CSD MOF) to guide linker/metal selection and design of multifunctional frameworks (Cheng et al., 2022). These digital tools reduce trial-and-error synthesis and help customize MOFs for targeted applications.

### 7.2. Modular Design for Multi-Pollutant Remediation

Next-generation MOFs are being designed with dual or multi-functionality, enabling simultaneous removal of:

- Heavy metals and organic dyes
- Antibiotics and pathogens
- CO<sub>2</sub> and VOCs

Multivariate MOFs (MTV-MOFs) containing multiple linkers or metal nodes show enhanced versatility and synergistic effects in adsorption and catalysis. For example, bimetallic MOFs like Fe–Cu-BTC can catalyze advanced oxidation while adsorbing pollutants (Kang et al., 2020). These materials are suited for complex environmental matrices such as industrial or hospital effluents.

### 7.3. Membrane and Filter Integration

To move beyond batch adsorption, MOFs are being embedded into membrane systems, monoliths, or composite filters to facilitate

- Continuous-flow water treatment
- Gas-phase pollutant filtration
- Antibacterial and antifouling coatings

Recent work on MOF-based thin-film composite membranes (e.g., MOF@PES, MOF@PVDF) has shown increased permeability, selectivity, and fouling resistance. ZIF-8 and UiO-66 have been successfully integrated into polymeric matrices without compromising structural integrity (Zhang et al., 2021). These hybrid systems open pathways for scalable modular deployment in decentralized water treatment.

### 7.4. Smart and Stimuli-Responsive MOFs

The development of stimuli-responsive MOFs capable of changing their behavior in response to pH, temperature, light, or redox conditions offers potential for

- Controlled release of disinfectants or nutrients
- On-demand adsorption and desorption
- Real-time pollutant sensing and feedback

Photo-responsive MOFs based on azobenzene or spiropyran linkers have been studied for light-triggered pollutant degradation and self-cleaning applications (Sun et al., 2018). Integration with optical or electronic sensors may allow deployment in intelligent remediation platforms.

### 7.5. Sustainable and Green Chemistry Approaches

Sustainable synthesis will remain a priority. Future research should focus on:

- Waste valorization (e.g., using agricultural residues as ligands)
- Low-carbon fabrication (e.g., mechanochemistry, water-based synthesis)
- Biodegradable frameworks (e.g., amino acid- or peptide-based MOFs)

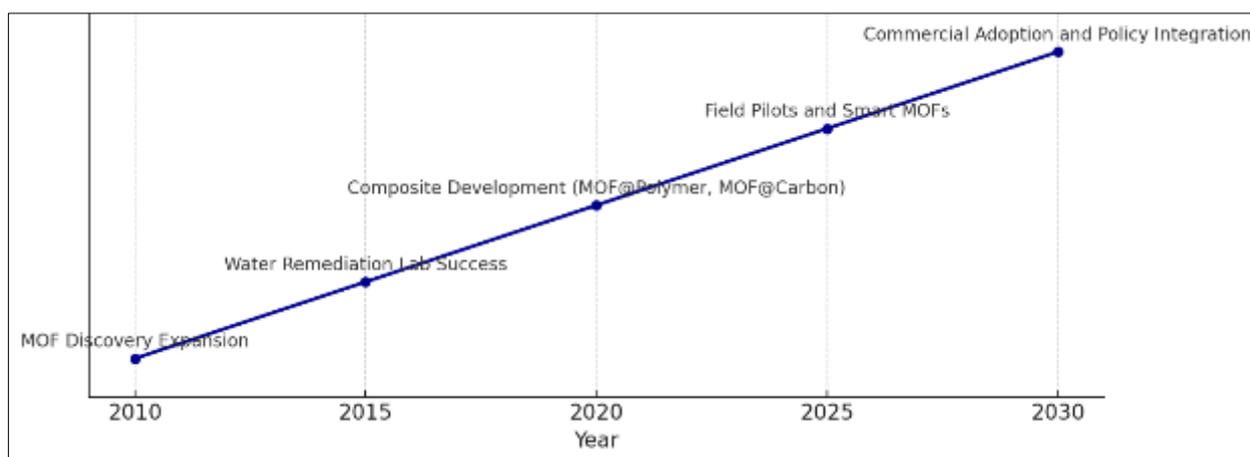
Biopolymer–MOF hybrids such as chitosan@MOFs are already under investigation for biodegradable adsorbents with high performance (Hasan and Jhung, 2021). Emphasizing circular material design and lifecycle compatibility will enhance environmental acceptance and regulatory compliance.

### 7.6. Policy, Regulation, and Lifecycle Assessment (LCA)

For MOFs to be broadly implemented, policy development and regulatory frameworks are needed to

- Standardize performance and safety evaluations
- Monitor environmental release and degradation products
- Guide end-of-life management and reuse/recycling

Lifecycle assessments (LCAs) are still rare but crucial for benchmarking MOFs against conventional materials. Comprehensive LCA studies incorporating synthesis inputs, operational stability, regeneration, and disposal will inform sustainable deployment strategies (Yan et al., 2021).



Roadmap inspired by Cheng et al. (2022); Kang et al. (2020)

**Figure 5** Timeline and Roadmap for MOF Development (2010–2030)

## 8. Conclusion

Metal–organic frameworks (MOFs) represent a transformative class of porous materials offering unique advantages for environmental remediation. Their high surface areas, tunable porosity, and modifiable functional groups enable highly selective and efficient removal of diverse pollutants including heavy metals, dyes, pharmaceuticals, and volatile organic compounds from water and air. Moreover, their catalytic capabilities allow for the degradation of persistent organic pollutants via advanced oxidation processes.

In water treatment, MOFs such as UiO-66, MIL-101, ZIF-8, and their functionalized derivatives have demonstrated superior adsorption capacities, fast kinetics, and potential for regeneration. In the gas phase, MOFs show promise for CO<sub>2</sub> capture, VOC sequestration, and photocatalytic degradation. However, translating these laboratory successes into scalable, field-deployable technologies remains a critical challenge.

Key technical barriers include instability in aqueous or harsh conditions, complex and costly synthesis routes, potential for secondary pollution, and limited integration with existing treatment infrastructure. Environmentally, concerns about toxicity of degradation products, lack of regulatory frameworks, and unknown long-term impacts must be addressed through comprehensive life cycle assessments (LCAs) and policy-driven innovation.

### Future Research

Looking forward, future research must prioritize

- Green and scalable synthesis using benign solvents and renewable precursors
- Multifunctional MOFs capable of simultaneous pollutant removal and catalysis
- Integration into modular systems such as membranes, filters, and smart sensors
- Computational and AI-guided design for precision-engineered MOFs
- Sustainable end-of-life strategies to ensure environmental safety

By combining advances in materials science, chemical engineering, and environmental policy, MOFs can evolve from promising laboratory materials to mainstream tools for sustainable environmental remediation.

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