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Metal–Organic Frameworks for Adsorptive Remediation of Heavy Metals in Contaminated Water

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Abstract: Heavy-metal contamination of water is a major environmental concern because toxic metals are persistent, non-biodegradable, and can accumulate in aquatic systems and living organisms. Metal–organic frameworks (MOFs) have emerged as promising adsorbents because of their high surface areas, tunable pore structures, diverse metal centres, and functionalizable surfaces. This review examines the application of MOFs for removing Pb(II), Cd(II), Hg(II), Cr(III)/Cr(VI), As(III)/As(V), Cu(II), Ni(II), Zn(II), and other heavy metals from contaminated water. The effects of pH, contact time, adsorbent dosage, initial concentration, temperature, competing ions, and surface chemistry on adsorption performance are discussed, together with mechanisms such as electrostatic attraction, ion exchange, surface complexation, chelation, precipitation, and redox interactions. The review also examines functionalized, magnetic, carbon-based, metal-oxide, and bio-based MOF composites, as well as regeneration, reusability, real wastewater treatment, and continuous-flow applications. Despite their promising performance, challenges related to production cost, scale-up, aqueous stability, leaching, environmental safety, and sustainability remain. Future research should focus on green and scalable synthesis, realistic wastewater testing, life-cycle assessment, techno-economic evaluation, and safe-by-design MOFs. Overall, MOFs provide a versatile platform for developing efficient and sustainable technologies for heavy-metal remediation.

1. Introduction

Heavy-metal contamination of aquatic environments has become a persistent global environmental concern because of the toxicity, non-biodegradability, persistence, and bioaccumulation potential of many metal ions. Metals such as lead (Pb), cadmium (Cd), mercury (Hg), chromium (Cr), arsenic (As), copper (Cu), nickel (Ni), and zinc (Zn) can enter water systems through natural processes and anthropogenic activities, including mining, metal processing, electroplating, industrial discharge, agricultural runoff, and improper waste disposal (Essalmi *et al.,* 2024). Unlike many organic pollutants, heavy metals cannot be degraded into harmless products and may persist in water, sediments, and biological systems for extended periods (Lal *et al.,* 2024). Their environmental behavior and toxicity are strongly influenced by chemical speciation, oxidation state, concentration, and interactions with dissolved and particulate components of aquatic systems (Zhang *et al.,* 2024). Consequently, the

accumulation of toxic metals in aquatic ecosystems represents a significant threat to water quality, ecological stability, and human health.

Several conventional technologies have been employed for the removal of heavy metals from contaminated water, including chemical precipitation, coagulation–flocculation, ion exchange, membrane filtration, electrochemical treatment, and biological processes (Perera *et al.,* 2023). Although these approaches can achieve substantial metal removal, they may involve high operational costs, substantial chemical consumption, generation of secondary sludge, membrane fouling, complex operating requirements, or limited effectiveness at low metal concentrations (Motshekga *et al.,* 2024). Adsorption has therefore attracted considerable attention as an alternative treatment approach because of its operational simplicity, high removal efficiency, flexibility, and potential for adsorbent regeneration and reuse (Husaini, 2026a-e). In this context, metal–organic frameworks (MOFs) have emerged as promising adsorbents for water remediation because their structural and chemical properties can be tailored for specific contaminants (Saini *et al.,* 2024).

Metal–organic frameworks are crystalline porous materials constructed from metal ions or metal clusters coordinated with organic ligands, producing highly ordered structures with tunable pore sizes, large specific surface areas, and chemically adjustable internal surfaces (Essalmi *et al.,* 2024; Husaini, 2026f). These characteristics make MOFs attractive for the selective adsorption of heavy-metal ions from aqueous environments. Their adsorption performance can arise from several mechanisms, including electrostatic attraction, ion exchange, surface complexation, coordination, chelation, pore confinement, precipitation, and redox interactions (Yuan *et al.,* 2025). The incorporation of functional groups containing oxygen, nitrogen, sulfur, phosphorus, or other donor atoms can further increase the affinity of MOFs toward particular metal ions (Zhang *et al.,* 2024). In addition, functionalization and composite formation have been explored to improve aqueous stability, adsorption capacity, selectivity, magnetic separation, and regeneration performance (Akartasse *et al.,* 2022; Hama Aziz *et al.,* 2025).

Despite the substantial progress achieved in MOF-based heavy-metal adsorption, important challenges remain before these materials can be widely implemented in practical water-treatment systems. These challenges include the relatively high synthesis cost of some MOFs, limited stability under strongly acidic or alkaline conditions, possible degradation or metal-ion leaching, difficulties associated with large-scale production, regeneration requirements, and uncertain long-term performance in complex real wastewater matrices (Mubarak *et al.,* 2025; Chaouiki *et al.,* 2026; Husaini *et al.,* 2026). Differences in experimental conditions, including pH, adsorbent dosage, initial metal concentration, contact time, and competing ions, can also make direct comparison of adsorption performance among different studies difficult (Alharthi *et al.,* 2025). Recent research has consequently emphasized the development of stable, low-cost, environmentally sustainable, highly selective, and reusable MOF-based adsorbents for practical water remediation (Yuan *et al.,* 2025). This review critically examines the application of MOFs for the adsorptive remediation of heavy metals in contaminated water, with emphasis on MOF structures and properties, modification strategies, adsorption performance, governing factors, removal mechanisms, kinetic and equilibrium behavior, regeneration and reusability, selectivity, application to real wastewater, sustainability considerations, current limitations, and future research directions.

2. Heavy Metals in Contaminated Water

Heavy metals are persistent contaminants in aquatic environments and pose significant environmental and public-health concerns because of their toxicity, resistance to degradation, and potential for bioaccumulation (Saravanan *et al.,* 2024). Unlike many organic pollutants, metals cannot be

biologically degraded and may remain in water, sediments, and aquatic organisms for long periods. Their distribution and behavior are affected by pH, redox conditions, dissolved organic matter, and interactions with other contaminants (Alaqarbeh *et al.,* 2022; Xu *et al.,* 2024; Husaini, 2025a&b). Understanding their occurrence, toxicity, and mobility is important for developing effective remediation strategies.

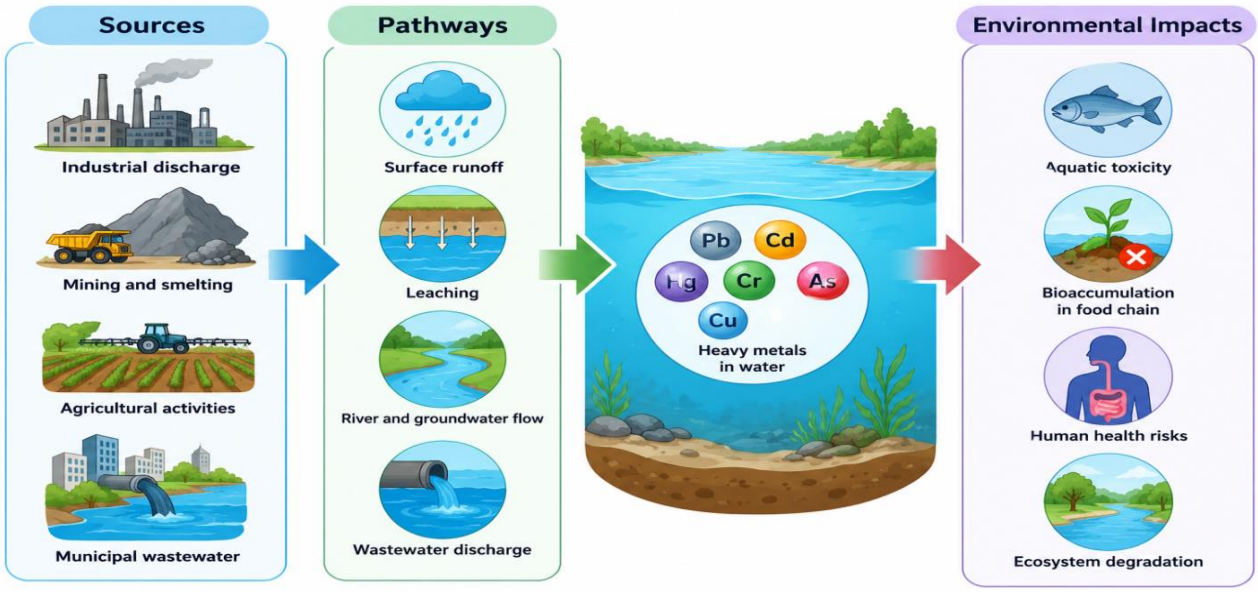


Figure 1: Sources, pathways and environmental impacts of heavy-metal contamination in water.

2.1. Major Heavy Metals of Concern

Important heavy metals and potentially toxic elements found in contaminated water include lead (Pb), cadmium (Cd), mercury (Hg), chromium (Cr), arsenic (As), copper (Cu), nickel (Ni), and zinc (Zn) (Razzouki *et al.,* 2015; Akartasse *et al.,* 2017; Sanusi *et al.,* 2025). Their risks depend on concentration, chemical form, exposure duration, and bioavailability. Lead and cadmium can cause neurological and renal effects, while mercury is particularly concerning because some forms can accumulate and biomagnify through aquatic food chains (El Hammari *et al.,* 2023; Jomova *et al.,* 2025). Chromium and arsenic also exhibit different toxicity and mobility depending on their oxidation states. For example, Cr(VI) is generally more soluble and toxic than Cr(III), while As(III) and As(V) display different environmental behaviors (Xu *et al.,* 2024). Copper, nickel, and zinc are essential at low concentrations but may become toxic at elevated levels (Zhu, 2025).

2.2. Sources and Occurrence

Heavy metals enter aquatic systems through natural processes such as rock weathering, erosion, volcanic activity, and mineral dissolution, as well as anthropogenic activities including mining, metallurgy, electroplating, battery manufacture, industrial discharge, agriculture, and waste disposal (Ondrasek *et al.,* 2025). Agricultural inputs may arise from fertilizers, pesticides, manure, and contaminated irrigation water (Udongwo, 2025). Following their release, metals may remain dissolved or become associated with suspended particles, organic matter, and sediments. Sediments can therefore act as reservoirs and secondary sources when environmental conditions change. Their distribution and transport are strongly influenced by water chemistry, sediment properties, and human activities (Kanwel *et al.,* 2025).

2.3. Toxicity and Environmental Effects

The toxicity of heavy metals depends on their concentration, chemical form, exposure duration, and bioavailability. Lead can impair neurological development, cadmium can affect renal and skeletal functions, and mercury can damage the nervous system (Jomova *et al.,* 2025). Arsenic and Cr(VI) are also associated with serious health risks. In aquatic ecosystems, excessive metal concentrations can disrupt microbial activity, growth, reproduction, respiration, and other biological processes. Metals may accumulate in aquatic organisms and transfer through food chains, increasing exposure at higher trophic levels (Saidon *et al.,* 2024). Fish can accumulate metals from water and food, resulting in oxidative stress and tissue damage (Zahran *et al.,* 2025).

2.4. Speciation and Mobility of Heavy Metals

Heavy-metal speciation describes the distribution of an element among its different chemical forms, which can differ in toxicity, solubility, mobility, and bioavailability. Chromium commonly occurs as Cr(III) and Cr(VI), while arsenic occurs mainly as As(III) and As(V), with their distribution influenced by pH and redox conditions (Xu *et al.,* 2024). Metal mobility is also controlled by interactions with sediments, minerals, organic matter, and inorganic ligands. Dissolved metal species are generally more mobile than those strongly bound to particles or sediments, although environmental changes can promote their release (Ondrasek *et al.,* 2025). Speciation is therefore important in adsorption because the charge and coordination properties of metal species influence their interaction with adsorbent surfaces (Sharma *et al.,* 2024).

3. Metal–Organic Frameworks as Adsorbents

Metal–organic frameworks (MOFs) are porous crystalline materials constructed by coordinating metal ions or metal-containing clusters with organic ligands. Their structural diversity, high surface areas, and tunable pore systems have made them attractive materials for environmental applications, particularly water treatment (Motshekga *et al.,* 2024; Lal *et al.,* 2024). The combination of adjustable pore dimensions and chemically active sites enables MOFs to interact with dissolved pollutants through mechanisms such as ion exchange, electrostatic attraction, surface complexation, and coordination (Xie *et al.,* 2024). These characteristics make MOFs promising adsorbents for the remediation of heavy-metal-contaminated water.

3.1. Structure and Properties of MOFs

The basic structure of a MOF consists of metal ions or secondary building units (SBUs) connected by multitopic organic linkers to form extended networks. The nature, coordination geometry, and connectivity of the metal centres and organic ligands determine the framework topology and pore characteristics (Mosupi *et al.,* 2025; Zhao *et al.,* 2025). Depending on the components employed, MOFs can contain ordered channels, cages, and interconnected cavities that provide accessible sites for pollutant capture. Their chemical functionality can also be adjusted through linker selection and post-synthetic modification, allowing the adsorption properties of MOFs to be tailored toward particular contaminants (Wang *et al.,* 2024).

3.2. Common MOF Families

Several MOF families have been widely investigated because of their structural diversity and chemical stability. Important examples include zeolitic imidazolate frameworks (ZIFs), University of Oslo

frameworks (UiOs), Materials of Institute Lavoisier (MILs), and HKUST-type frameworks. ZIFs commonly contain Zn or Co centres coordinated with imidazolate linkers, while UiO frameworks, particularly Zr-based materials, are recognized for their high structural stability. MIL-type frameworks offer diverse pore structures and tunable surface chemistry, whereas HKUST-type materials contain accessible Cu-based sites that can contribute to adsorption. These differences allow MOF families to be selected according to the target contaminant and treatment conditions (Motshekga *et al.,* 2024; Lal *et al.,* 2024).

3.3. Synthesis and Characterization

MOFs can be prepared through solvothermal, hydrothermal, microwave-assisted, sonochemical, mechanochemical, electrochemical, and other synthesis routes (Motshekga *et al.,* 2024; Wang *et al.,* 2024). Conventional solvothermal synthesis involves reacting a metal precursor with an organic linker in a suitable solvent under controlled conditions, whereas alternative approaches may reduce reaction time, energy consumption, or solvent use. Characterization is essential for establishing the structural, morphological, chemical, and textural properties of the synthesized material. Common techniques include powder X-ray diffraction (PXRD) for phase and crystallinity, Fourier-transform infrared spectroscopy (FTIR) for functional-group identification, scanning electron microscopy (SEM) for morphology, energy-dispersive X-ray spectroscopy (EDX) for elemental composition, thermogravimetric analysis (TGA) for thermal stability, and nitrogen adsorption–desorption analysis for surface area and pore characteristics (Payam *et al.,* 2024).

3.4. Porosity, Surface Area and Functional Groups

The adsorption performance of MOFs is strongly influenced by their pore architecture, surface area, pore-size distribution, and surface chemistry. Their interconnected pores facilitate the movement of heavy-metal ions into the framework, while a large accessible surface provides more potential adsorption sites (Lal *et al.,* 2024; Xie *et al.,* 2024). However, adsorption capacity is not determined by surface area alone because the nature and accessibility of functional groups are also important. Groups containing oxygen, nitrogen, sulfur, and other donor atoms can interact with metal ions through electrostatic attraction, ion exchange, coordination, and surface complexation. Modification of these functional groups can consequently improve the affinity and selectivity of MOFs toward specific heavy metals (Al-Anazi *et al.,* 2025; He *et al.,* 2025).

3.5. Stability in Aqueous Media

Aqueous stability is a critical consideration for MOFs intended for water treatment because exposure to water can cause hydrolysis, structural degradation, or metal–ligand bond disruption. The stability of a framework depends on factors such as metal–ligand bond strength, metal valence, linker chemistry, framework topology, pH, and the composition of the aqueous medium (Xiao *et al.,* 2024; Lal *et al.,* 2024). Zr-, Al-, and some Fe-based frameworks generally exhibit greater resistance to aqueous degradation because of their strong coordination bonds. Water stability can also be improved through hydrophobic modification, pore engineering, and appropriate selection of metal centres and organic linkers (Rastin *et al.,* 2025; Payam *et al.,* 2024). Therefore, evaluating structural integrity before and after adsorption is essential when assessing the practical suitability and recyclability of MOFs for contaminated-water treatment.

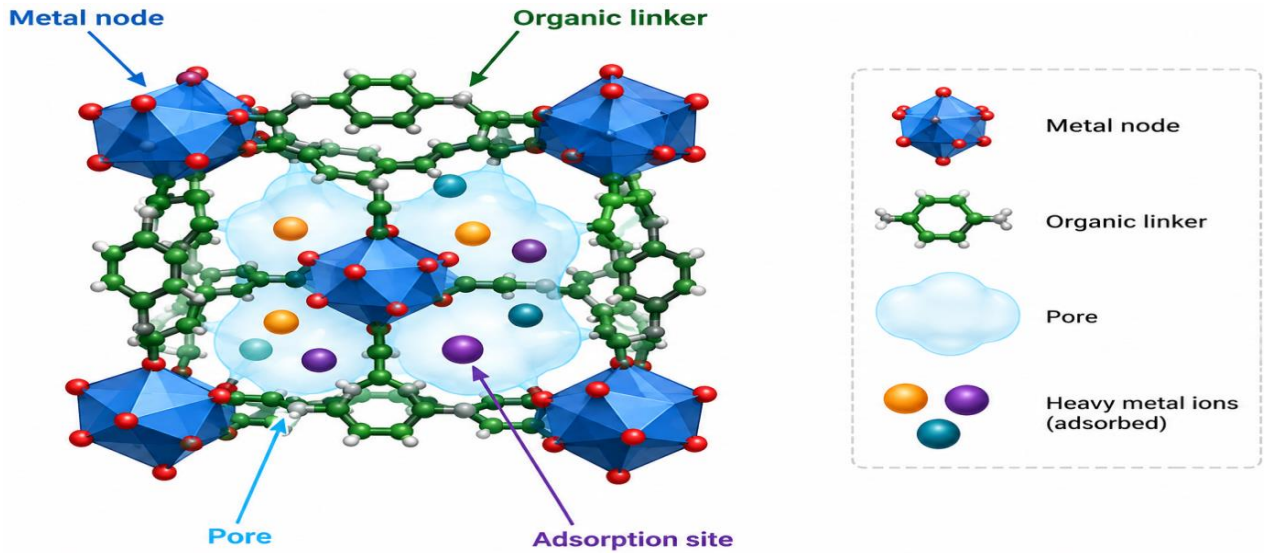


Figure 2: Basic structure of a MOF showing metal nodes, organic linkers, pores and active adsorption sites.

4. Adsorptive Removal of Heavy Metals Using MOFs

Metal–organic frameworks (MOFs) have attracted considerable attention for heavy-metal removal because their pore structures and surface chemistry can be tailored to interact with specific metal ions. Adsorption onto MOFs may involve electrostatic attraction, ion exchange, coordination, surface complexation, pore filling, and interactions with functional groups containing oxygen, nitrogen, sulfur, or other donor atoms (Yuan *et al.,* 2025; Ghumman *et al.,* 2025). The efficiency of the process is influenced by solution pH, initial metal concentration, adsorbent dosage, contact time, temperature, competing ions, and the physicochemical characteristics of the MOF (Mubarak *et al.,* 2025). Functionalization and incorporation of different metal centres or ligands can further improve adsorption affinity and selectivity, making MOFs promising materials for treating water containing multiple heavy metals (Hama Aziz *et al.,* 2025).

4.1. Pb(II)

Lead is one of the most frequently investigated toxic metals because of its persistence and adverse effects on human health and aquatic ecosystems. MOFs can capture Pb(II) through coordination with oxygen-, nitrogen-, or sulfur-containing functional groups, together with electrostatic interactions and ion-exchange processes (Yuan *et al.,* 2025). Functionalization of MOF surfaces can increase the number and accessibility of active sites, thereby improving Pb(II) uptake. Recent studies have also demonstrated the potential of bimetallic MOFs for heavy-metal sequestration because the incorporation of different metal centres can modify surface chemistry and adsorption selectivity (Kayani and Mohammed, 2025). However, competing ions present in real wastewater may occupy adsorption sites and reduce Pb(II) removal efficiency (Ghumman *et al.,* 2025).

4.2. Cd(II)

Cadmium contamination is associated with industrial activities such as electroplating, battery manufacture, mining, and metal processing. MOFs provide several pathways for Cd(II) capture, including electrostatic attraction, ion exchange, surface complexation, and coordination with functional groups within the framework (Mubarak *et al.,* 2025). Nitrogen- and oxygen-containing groups are particularly useful because they provide electron-donor sites capable of interacting with Cd(II).

Modification of MOF surfaces can increase the density and accessibility of these sites and consequently improve adsorption efficiency (Hama Aziz *et al.,* 2025). The adsorption of Cd(II), however, may be affected by pH and the presence of other dissolved metal ions, making competitive adsorption studies important for evaluating performance under realistic water conditions (Ghumman *et al.,* 2025).

4.3. Hg(II)

Mercury is highly toxic and can persist in aquatic environments in different chemical forms. The strong affinity of sulfur-containing donor groups for Hg(II) has encouraged the development of functionalized MOFs for selective mercury removal. Thiol, thioether, sulfide, and related sulfur-containing groups can form strong interactions with Hg(II), while the porous framework provides access to numerous active sites (Yuan *et al.,* 2025). A recent study demonstrated the potential of a MOF grown on nickel foam as an adsorptive medium for mercury-contaminated water, highlighting the possibility of integrating MOFs into practical treatment configurations (Yosef *et al.,* 2025). Nevertheless, framework stability, metal or linker leaching, and regeneration remain important considerations for repeated application (Ghumman *et al.,* 2025).

4.4. Cr(III)/Cr(VI)

Chromium occurs mainly as Cr(III) and Cr(VI), and their different chemical characteristics strongly influence adsorption behavior. Cr(VI) generally exists as negatively charged chromate species in aqueous solution, whereas Cr(III) commonly occurs as positively charged or hydrolyzed species depending on pH. Consequently, positively charged or amine-functionalized MOFs can promote Cr(VI) removal through electrostatic attraction, hydrogen bonding, and anion exchange (Yuan *et al.,* 2025). Recent research has also demonstrated the application of MOFs specifically designed for Cr(VI) adsorption, including UiO-based materials, with adsorption performance influenced by surface functionality and framework chemistry (Lin *et al.,* 2024). Some MOF systems may additionally facilitate the reduction of Cr(VI) to the less toxic Cr(III), followed by adsorption or immobilization. Therefore, chromium remediation requires careful consideration of oxidation state, solution pH, competing ions, and MOF surface chemistry (Ghumman *et al.,* 2025).

4.5. As(III)/As(V)

Arsenic contamination presents a major challenge because As(III) and As(V) differ substantially in their chemical forms and adsorption behavior. As(V) commonly occurs as negatively charged oxyanions, whereas As(III) can predominantly exist as a neutral species under mildly acidic to neutral conditions. MOFs containing positively charged centres or metal sites with strong affinity for oxyanions can therefore be effective for As(V) adsorption (Yuan *et al.,* 2025). A Fe–Ti heterometallic MOF with defect sites demonstrated particularly high As(V) removal, with Fe incorporation and oxygen vacancies contributing to arsenic adsorption (Shang *et al.,* 2024). Fe-, Ti-, and other metal-based frameworks are therefore promising for arsenic remediation because their metal centres can form strong interactions with arsenic species. The presence of competing anions such as phosphate and sulfate, however, may influence adsorption efficiency and should be considered when evaluating practical applications (Ghumman *et al.,* 2025).

4.6. Cu(II), Ni(II), Zn(II) and Other Heavy Metals

MOFs have also been investigated for the removal of Cu(II), Ni(II), Zn(II), and other potentially toxic metal ions from aqueous systems. These metals can interact with MOF surfaces through ion exchange,

electrostatic attraction, and coordination with functional groups containing O, N, or S donor atoms (Mubarak *et al.,* 2025). Recent research has demonstrated the application of Co-based MOFs for Ni(II) adsorption, indicating that the nature of the metal centre and framework chemistry can strongly influence adsorption performance (Hernández-Martínez *et al.,* 2024). Co-derived MOFs have also shown potential for the simultaneous removal of different heavy metals, demonstrating the importance of synergistic interactions between framework components and metal ions (Peña-Rodríguez *et al.,* 2024). In multicomponent wastewater, competition among metal ions may substantially alter adsorption compared with single-metal solutions (Bi *et al.,* 2024). Consequently, future MOF-based systems should emphasize selective removal, regeneration, resistance to competing ions, and performance in real wastewater rather than relying solely on high adsorption capacities obtained under ideal laboratory conditions (Kayani and Mohammed, 2025).

5. Factors and Mechanisms Governing Adsorption

The efficiency of heavy-metal adsorption by MOFs depends on solution conditions, adsorbent properties, and the chemical nature of the metal. Important factors include pH, contact time, adsorbent dosage, initial concentration, temperature, competing ions, and surface chemistry. These variables influence the availability of adsorption sites and the interactions between metal ions and the framework (Zhang *et al.,* 2024). Understanding their effects is important for optimizing MOF-based water treatment.

5.1. Effect of pH, Contact Time and Adsorbent Dosage

pH strongly affects heavy-metal adsorption by changing metal speciation and the charge of MOF functional groups. At low pH, H^+ ions may compete with metal cations for active sites, whereas increasing pH can promote deprotonation and improve metal binding (Essalmi *et al.,* 2024). Contact time determines the rate of adsorption, with rapid uptake commonly occurring initially and becoming slower as adsorption sites are occupied. Increasing adsorbent dosage generally improves percentage removal by providing more active sites, although excessive dosage may reduce the adsorption capacity per unit mass. These effects were also demonstrated in MOF-based Pb(II) adsorption studies (Nurhasni *et al.,* 2024).

5.2. Initial Metal Concentration and Temperature

Initial metal concentration influences adsorption by controlling the concentration gradient between the solution and MOF surface. Higher concentrations can increase adsorption capacity by providing a stronger driving force for mass transfer, but excessive concentrations may eventually saturate the available sites. Temperature affects adsorption through changes in diffusion, molecular mobility, and adsorption equilibrium. Depending on the nature of the interaction, increasing temperature may either enhance or reduce metal uptake (Khamis *et al.,* 2024). Studies of MOF-based heavy-metal adsorption have therefore used concentration and temperature variations to evaluate adsorption capacity and energetic behaviour (Nurhasni *et al.,* 2024).

5.3. Competing Ions and Coexisting Contaminants

The presence of other ions can reduce heavy-metal adsorption because different species may compete for the same active sites. Common ions such as Ca^{2+} and Mg^{2+}, as well as other heavy metals, can interfere with target-metal uptake. Anions such as phosphate and sulfate may similarly compete with

oxyanionic contaminants for positively charged or metal-centred sites (Essalmi *et al.,* 2024). Natural organic matter can also block pores or interact with dissolved metals. Recent research therefore emphasizes testing MOFs in multicomponent solutions and real wastewater rather than relying exclusively on single-metal systems (Peng *et al.,* 2025).

5.4. Electrostatic Attraction

Electrostatic attraction occurs when oppositely charged MOF surfaces and dissolved contaminants interact. Negatively charged MOF surfaces can favour the adsorption of cationic metals such as Pb^{2+}, Cd^{2+}, Cu^{2+}, and Ni^{2+}, while positively charged surfaces can promote uptake of oxyanions such as arsenate and chromate (Zhang *et al.,* 2024). Surface charge is strongly influenced by pH, making pH an important factor in this mechanism. However, increasing ionic strength can weaken electrostatic interactions through charge screening. Electrostatic attraction therefore commonly operates together with ion exchange and chemical complexation rather than acting alone (Li *et al.,* 2024).

5.5. Ion Exchange

Ion exchange involves the replacement of ions associated with the MOF by dissolved heavy-metal ions. Metal ions may replace H^+, Na^+, or other exchangeable species located on charged framework sites. The extent of exchange depends on the number of available sites and the chemical properties of the competing ions. Evidence for this mechanism can be obtained by detecting the release of displaced ions into solution after adsorption. Co-derived MOFs, for example, have demonstrated combined ion-exchange and surface-binding contributions during heavy-metal removal (Peña-Rodríguez *et al.,* 2024).

5.6. Surface Complexation and Chelation

Surface complexation occurs when heavy-metal ions form chemical bonds with donor atoms present on MOF surfaces. Functional groups containing O, N, and S, such as carboxylate, hydroxyl, amino, and thiol groups, can provide suitable coordination sites (Essalmi *et al.,* 2024). Chelation is particularly important when several donor atoms from the same ligand bind a metal ion simultaneously, producing stable metal–ligand complexes. Functionalization of MOFs can therefore improve both adsorption capacity and selectivity. Spectroscopic changes observed after adsorption can provide evidence for the involvement of these functional groups (Li *et al.,* 2024).

5.7. Precipitation and Redox Interactions

Heavy-metal removal may also involve precipitation and redox reactions in addition to surface adsorption. Precipitation can occur when metal ions form poorly soluble hydroxides, carbonates, phosphates, or sulfides, particularly under favourable pH conditions. Redox reactions can change the oxidation state, charge, solubility, and adsorption affinity of contaminants such as chromium and arsenic. MOF-based materials have been investigated for coupling arsenic oxidation with subsequent capture, demonstrating that transformation and adsorption can occur together (G-Saiz *et al.,* 2024). Therefore, changes in metal speciation should be considered when determining the dominant removal mechanism.

5.8. Adsorption Kinetics, Isotherms and Thermodynamics

Kinetic, isotherm, and thermodynamic models are widely used to evaluate heavy-metal adsorption by MOFs. Pseudo-first-order, pseudo-second-order, and intraparticle-diffusion models provide

information about adsorption rate and possible mass-transfer limitations. Equilibrium data are commonly analysed using Langmuir and Freundlich models to describe adsorption capacity and surface heterogeneity (Zhang *et al.,* 2024). Thermodynamic parameters, including ΔG°, ΔH°, and ΔS°, provide information about spontaneity, heat effects, and changes at the adsorbent–solution interface. These models should be interpreted alongside experimental and spectroscopic evidence because mathematical fitting alone cannot conclusively establish the adsorption mechanism (Khamis *et al.,* 2024).

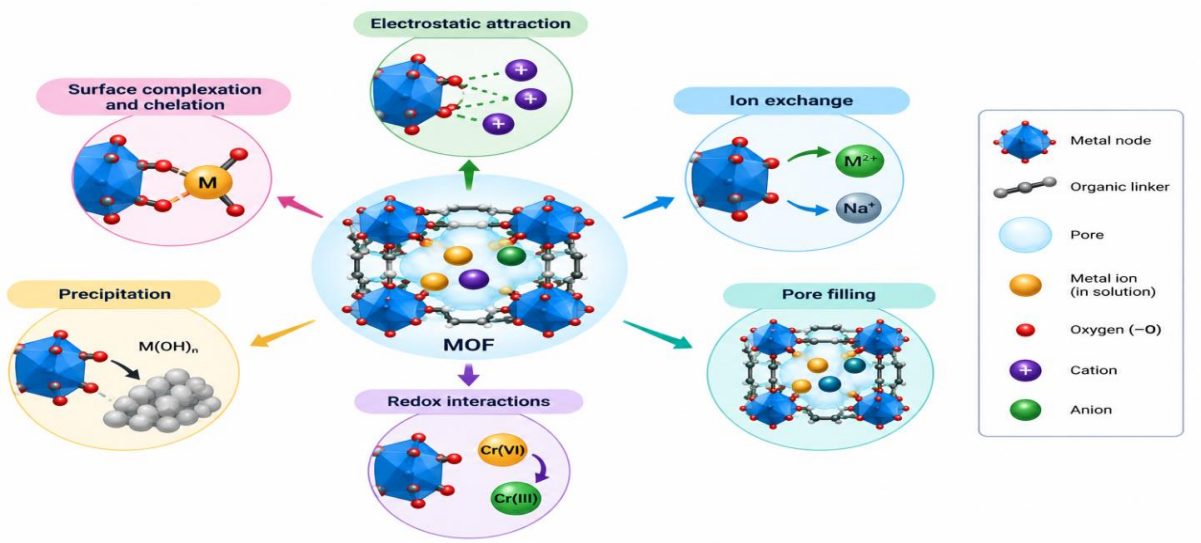


Figure 3: Proposed mechanisms for heavy-metal adsorption onto MOFs.

6. Modified and Composite MOFs

Modification and composite formation are important strategies for improving the performance of metal–organic frameworks (MOFs) for heavy-metal removal from contaminated water. Although pristine MOFs possess high surface areas, tunable pore structures, and chemically active sites, their practical application can be limited by particle aggregation, difficult recovery, insufficient stability, or inadequate selectivity. Structural modification and integration with other materials can introduce additional adsorption sites, improve mechanical properties, facilitate separation, and enhance interactions with target contaminants. The development of MOF macrostructures and hybrid materials has therefore received increasing attention for improving the practical application of MOFs in water treatment (Yang *et al.,* 2025; Singh *et al.,* 2024).

6.1. Functionalized MOFs

Functionalized MOFs are obtained by introducing specific chemical groups into the framework or onto its surface to increase the affinity of the material for target metal ions. Groups such as amino ($–NH_2$), hydroxyl (–OH), carboxyl (–COOH), and other oxygen-, nitrogen-, or sulfur-containing functionalities can provide additional coordination and binding sites. Amine functionalization is particularly useful because nitrogen donor atoms can interact strongly with several dissolved metal ions and can modify the surface properties of the framework. The incorporation of functional groups may also improve adsorption selectivity by creating binding environments that favour particular contaminants. Consequently, rational functionalization is an important approach for controlling the adsorption behaviour of MOFs and improving their performance in aqueous treatment systems (Magida *et al.,*

2025). Structural and mechanistic studies further indicate that the nature and distribution of functional groups can influence the interaction between MOFs and dissolved metal species (Mishra *et al.,* 2024).

6.2. Magnetic MOFs

Magnetic MOFs are developed by incorporating magnetic components into MOF structures or by combining MOFs with magnetic nanoparticles. Their major advantage is the possibility of recovering the adsorbent rapidly from treated water using an external magnetic field. This property can reduce separation requirements and improve the practicality of repeated adsorption–regeneration cycles. Magnetic incorporation may also introduce additional surface sites and alter the textural properties of the material. Recent studies have explored the controlled assembly of magnetic MOF composites to obtain improved adsorption performance while retaining magnetic separability (Liu *et al.,* 2025). More broadly, magnetic composites have attracted attention for water decontamination because their magnetic response facilitates the recovery of adsorbent materials after treatment (Niculescu *et al.,* 2024). However, excessive magnetic loading may occupy pores or reduce the accessible surface area, making optimization of the MOF-to-magnetic-component ratio necessary.

6.3. MOF–Carbon and Graphene-Based Composites

MOF–carbon composites combine the porous structure and tunable chemistry of MOFs with the surface properties of carbonaceous materials. Activated carbon, biochar, graphene, graphene oxide, and related carbon materials can provide additional adsorption sites and improve the dispersion of MOF particles. Graphene oxide is particularly attractive because its oxygen-containing functional groups can interact with metal ions and provide anchoring sites for MOF growth. The resulting composites may exhibit improved surface accessibility, structural stability, and adsorption performance compared with individual components (Naser *et al.,* 2023). Biochar-based MOF composites also provide an opportunity to combine the adsorption properties of biomass-derived carbon with the highly tunable porosity of MOFs. For example, MOF–walnut-shell biochar composites have been investigated for the removal of Pb(II) and Cr(VI) from aqueous environments, demonstrating the potential of carbon-supported MOFs for heavy-metal remediation (Pochampally *et al.,* 2024).

6.4. MOF–Metal Oxide Composites

MOF–metal oxide composites integrate MOFs with inorganic oxides to combine high porosity with the surface reactivity and stability of metal oxides. Metal oxides can provide additional adsorption sites, modify surface charge, and contribute to interactions such as surface complexation, electrostatic attraction, ion exchange, and redox processes. Depending on the oxide selected, the composite may also exhibit photocatalytic or other functional properties that extend its application beyond conventional adsorption. Immobilization of MOF materials into structured systems is another approach for improving their practical use because it can reduce particle loss and facilitate recovery after treatment. Recent research on immobilized Fe-MOFs demonstrates the growing interest in structured MOF materials for water purification and resource recovery (Yang *et al.,* 2024/2025). The development of MOF-based macrostructures similarly provides opportunities to improve material handling and separation while retaining useful adsorption characteristics (Yang *et al.,* 2025).

6.5. Bio-Based MOF Composites

Bio-based MOF composites combine MOFs with renewable materials such as cellulose, chitosan, lignin, agricultural residues, biochar, and other biomass-derived substances. These materials are attractive because they are generally abundant and can contain hydroxyl, carboxyl, amino, and phenolic

groups capable of interacting with dissolved metal ions. Incorporating biomass-derived materials into MOFs can introduce additional binding sites while potentially reducing material cost and improving the sustainability of the adsorbent. For example, walnut-shell biochar has been combined with MOFs to produce composites capable of removing Pb(II) and Cr(VI) from water, illustrating how agricultural biomass can be incorporated into advanced adsorbent systems (Pochampally *et al.,* 2024). MOF growth on renewable or polymeric supports can also improve material handling and create multifunctional structures for simultaneous removal of different contaminants (Peng *et al.,* 2025). Such approaches support the development of more sustainable MOF-based treatment technologies, although stability, regeneration, possible leaching, and consistency of biomass-derived components must be considered before large-scale implementation (Singh *et al.,* 2024).

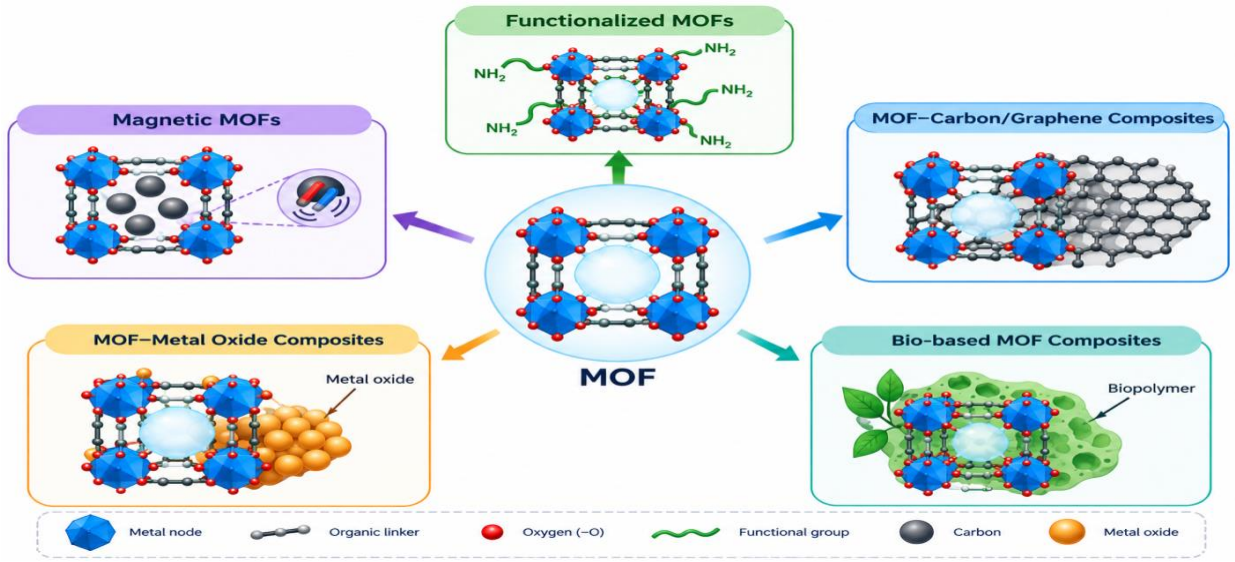


Figure 4: Strategies for functionalization and composite formation of MOFs for enhanced heavy-metal adsorption.

7. Regeneration, Selectivity and Practical Applications

The practical application of MOFs for heavy-metal removal depends not only on their adsorption capacity but also on their ability to be regenerated, reused, and operated effectively under realistic water-treatment conditions. Factors such as selective uptake, resistance to competing ions, stability in complex wastewater, ease of recovery, and compatibility with batch or continuous-flow systems are important for determining whether MOFs can move from laboratory studies to practical treatment technologies. Recent studies have increasingly emphasized the development of MOFs with improved recyclability, selective binding, rapid adsorption, and better compatibility with practical treatment systems (Vasudhevan *et al.,* 2025; Mubarak *et al.,* 2025).

7.1. Regeneration and Reusability

Regeneration involves removing adsorbed metal ions from the MOF surface so that the material can be used again. Common regeneration approaches include washing with acidic or alkaline solutions, salt solutions, chelating agents, or other suitable eluents. The choice of regenerating agent should provide effective desorption without causing significant degradation of the framework or loss of active functional groups. A useful MOF adsorbent should retain a substantial proportion of its original adsorption capacity after several adsorption–desorption cycles. Recent research on functionalized

MOFs has demonstrated that strong and reversible metal binding can be achieved, providing opportunities for repeated adsorption and regeneration (Felder *et al.,* 2026). Reusability can reduce adsorbent consumption and improve process economics, although repeated regeneration may cause structural changes, loss of functional groups, or metal and linker leaching.

7.2. Selectivity and Competitive Adsorption

Selectivity refers to the ability of an MOF to preferentially capture a particular heavy-metal ion when several contaminants are present simultaneously. This property is influenced by pore dimensions, surface charge, functional groups, coordination chemistry, and the size and hydration characteristics of the target metal. Functionalization can improve selectivity by creating binding environments with high affinity for specific metal ions. For example, selective Pb(II) adsorption has been achieved using functionalized MOF-based composites, demonstrating the importance of tailored surface chemistry in discriminating between competing metal ions (Fouad *et al.,* 2025). In real water, target metals also compete with ions such as Ca^{2+}, Mg^{2+}, Na^{+}, and K^{+}, as well as other heavy metals. The presence of these species can reduce adsorption by occupying active sites or altering metal speciation. Consequently, competitive adsorption experiments are essential for evaluating the selectivity of MOFs under realistic conditions (Ning *et al.,* 2025).

7.3. Treatment of Real Wastewater

Most laboratory investigations of MOFs are initially performed using prepared solutions containing known concentrations of individual heavy metals. Although such experiments are useful for determining adsorption capacity and investigating adsorption mechanisms, they may not adequately represent actual wastewater, which can contain several metals, inorganic ions, organic substances, suspended particles, and natural organic matter. Testing MOFs with real or highly complex water matrices provides a more reliable assessment of practical performance. Recent investigations have emphasized the development of MOF-based systems capable of rapidly removing multiple contaminants from complex aqueous environments (Ning *et al.,* 2025). The use of functionalized and composite MOFs can also improve performance when several contaminants are present simultaneously (Vasudhevan *et al.,* 2025).

7.4. Batch and Continuous-Flow Applications

Batch adsorption is widely used in laboratory studies because it allows important variables such as pH, adsorbent dosage, contact time, temperature, and initial metal concentration to be systematically investigated. However, batch systems do not fully reproduce the operating conditions of many industrial water-treatment processes. Their performance is influenced by flow rate, bed height, influent concentration, particle size, and breakthrough behaviour. Recent research has demonstrated the use of fixed-bed systems for continuous removal of contaminants from water, highlighting the importance of column operation in practical adsorption treatment (Wang *et al.,* 2024). MOF immobilization and macrostructure formation can further improve handling, reduce fine-particle loss, and facilitate the integration of MOFs into continuous treatment units (Yang *et al.,* 2025).

7.5. Comparison with Conventional Adsorbents

MOFs have several potential advantages over conventional adsorbents such as activated carbon, zeolites, clay minerals, and agricultural-waste-derived adsorbents. Their major advantages include high

surface area, tunable pore structures, adjustable surface chemistry, and the possibility of introducing specific functional groups for selective heavy-metal capture. The relatively high cost of some MOF precursors, synthesis requirements, framework stability, regeneration, and recovery can limit their widespread application (Zhang *et al.,* 2024; Dehmani *et al.,* 2026). Consequently, comparison between MOFs and conventional adsorbents should consider more than maximum adsorption capacity. Parameters such as adsorption rate, selectivity, regeneration efficiency, stability, material cost, environmental impact, scalability, and performance in real wastewater should be evaluated together (Vasudhevan *et al.,* 2025).

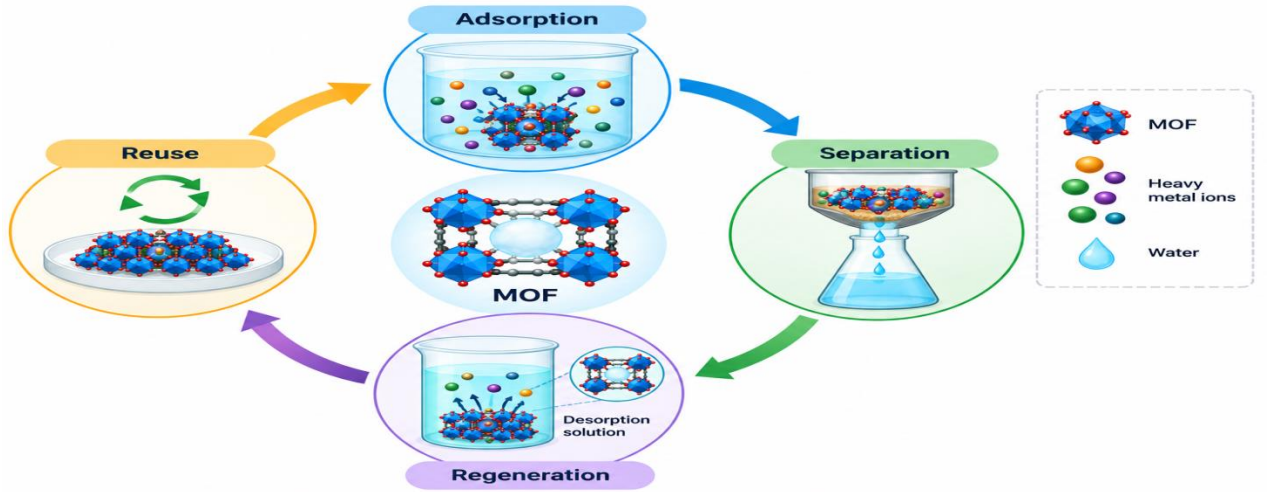


Figure 5: MOF-based water-treatment cycle showing adsorption, separation, regeneration and reuse

8. Sustainability, Challenges and Future Perspectives

Metal–organic frameworks (MOFs) have shown considerable potential for heavy-metal removal from contaminated water, but high adsorption capacity alone does not guarantee practical sustainability. Their wider application depends on synthesis cost, production scale, water stability, resistance to metal or linker leaching, environmental safety, regeneration, and the overall environmental footprint of their production and disposal (Singh *et al.,* 2026; Nassar *et al.,* 2026; Dutta *et al.,* 2026).

8.1. Cost and large-scale production

The cost and complexity of MOF production remain important barriers to large-scale water-treatment applications. Conventional synthesis may require expensive precursors, organic solvents, high temperatures, long reaction times, and extensive purification, increasing both material and energy costs (Singh *et al.,* 2026; Li *et al.,* 2026). Scale-up may also affect particle size, crystallinity, porosity, and surface functionality. Continuous and aqueous synthesis methods, including ultrasound-assisted approaches, offer opportunities for improving production efficiency and reducing environmental impacts (Sun *et al.,* 2025). The development of pellets, beads, membranes, and other stable MOF structures can further facilitate recovery and practical use (Iroegbu *et al.,* 2025). Techno-economic evaluation should therefore accompany adsorption studies to determine the actual cost of treating contaminated water (Li *et al.,* 2026).

8.2. Water stability and metal/linker leaching

Aqueous stability is essential for MOFs used in water remediation. Some frameworks may undergo hydrolysis, linker displacement, pore collapse, or structural degradation, particularly under extreme pH

conditions, resulting in reduced adsorption performance and possible release of framework components (Nassar *et al.,* 2026). Metal and linker leaching are particularly important because the adsorbent should not introduce secondary contaminants. Improved metal–ligand bonding, appropriate framework selection, surface modification, defect control, and composite formation can enhance stability. Long-term testing should include different pH values, ionic strengths, competing ions, natural organic matter, and repeated adsorption–desorption cycles (Chakraborty *et al.,* 2025; Lata and Ansari, 2026).

8.3. Environmental safety and toxicity

Environmental safety must be considered alongside adsorption efficiency. Framework degradation or abrasion may release metal ions, organic linkers, nanoparticles, or other transformation products into treated water. Their environmental effects depend on chemical form, concentration, persistence, and bioavailability (Chakraborty *et al.,* 2025; Husaini, 2026g). Consequently, MOF evaluation should include leaching and, where appropriate, ecotoxicological studies. Recent research has emphasized the need to consider toxicity, recyclability, and disposal when assessing MOFs for wastewater treatment (Lata and Ansari, 2026). A suitable adsorbent should therefore provide effective contaminant removal while minimizing secondary pollution and allowing safe recovery or disposal (Nassar *et al.,* 2026).

8.4. Green synthesis and sustainability

Green synthesis can reduce the environmental footprint of MOF production through safer solvents, water-based preparation, lower-energy processes, ultrasound or microwave assistance, mechanochemical methods, and renewable feedstocks (Agrawal *et al.,* 2025; Sun *et al.,* 2025). Renewable and bio-derived precursors can also reduce dependence on non-renewable resources and support more sustainable MOF production (Omrani *et al.,* 2025). However, sustainability should be evaluated beyond the choice of precursor by considering energy consumption, solvent use, waste generation, regeneration, material lifetime, and end-of-life management (Singh *et al.,* 2026; Dutta *et al.,* 2026).

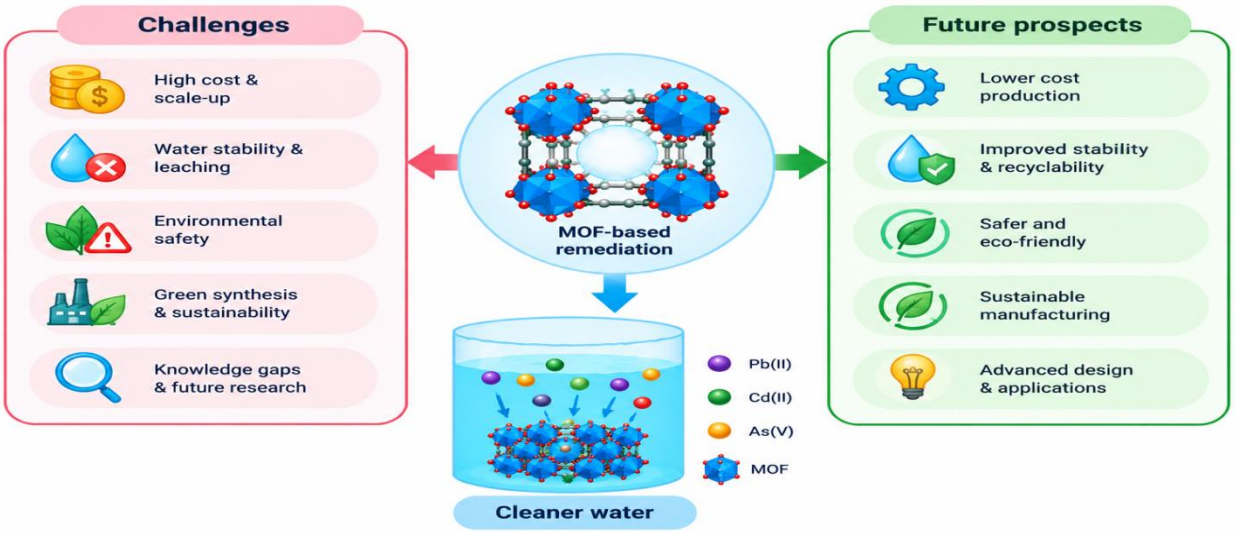


Figure 6 Challenges and future prospects for MOF-based remediation of heavy-metal-contaminated water.

8.5. Research gaps and future directions

Important challenges remain before MOFs can be widely implemented for heavy-metal remediation. Many studies still use single-metal laboratory solutions that do not adequately represent real

wastewater containing multiple contaminants, salts, organic matter, and suspended solids. Greater emphasis should therefore be placed on real wastewater, long-term operation, continuous-flow systems, selectivity, regeneration, stability, low-cost synthesis, and minimal leaching (Iroegbu *et al.,* 2025; Yi *et al.,* 2026). Scalable MOF architectures and improved processing methods may facilitate recovery and integration into treatment systems (Nandi *et al.,* 2026; Li *et al.,* 2026). Future studies should also combine adsorption performance with techno-economic analysis, life-cycle assessment, ecotoxicity evaluation, and realistic operating conditions (Singh *et al.,* 2026; Dutta *et al.,* 2026). Such an integrated approach will support the development of safer, economical, and environmentally sustainable MOF technologies for heavy-metal removal.

Conclusion

Metal–organic frameworks have considerable potential for the adsorptive remediation of heavy-metal-contaminated water because their high surface areas, tunable pore structures, and modifiable chemical functionalities enable effective interactions with diverse metal ions. Their performance is influenced by pH, contact time, adsorbent dosage, concentration, temperature, competing ions, and framework chemistry, with electrostatic attraction, ion exchange, complexation, chelation, precipitation, and redox interactions contributing to metal uptake. Functionalized and composite MOFs can further improve adsorption capacity, selectivity, stability, and recovery. However, high production costs, scale-up difficulties, aqueous instability, possible leaching, regeneration challenges, and environmental safety concerns remain important limitations. Future studies should prioritize green and scalable synthesis, selective and reusable materials, real wastewater testing, continuous-flow applications, techno-economic analysis, life-cycle assessment, and ecotoxicological evaluation. Addressing these challenges will be essential for translating MOFs from promising laboratory adsorbents into safe, cost-effective, and sustainable technologies for heavy-metal removal.

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Compliance with Ethical Standards: This article does not contain any studies involving human or animal subjects.

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