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Adsorption Mechanisms and Performance of ZIF-8-Based Materials for Heavy Metal Removal in Water Systems

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Abstract

The increasing contamination of water resources by toxic heavy metals poses a serious threat to environmental sustainability and public health, driving the demand for highly efficient and selective removal technologies. Zeolitic Imidazolate Framework-8 (ZIF-8) has emerged as a promising adsorbent for heavy-metal remediation due to its high surface area, tunable pore structure, chemical versatility, and structural robustness in aqueous environments. This review critically examines the adsorption performance and underlying mechanisms of ZIF-8-based materials for the removal of heavy metal ions from water systems. Emphasis is placed on pristine ZIF-8 as well as its functionalized, doped, composite, and derivative forms engineered to enhance adsorption capacity, selectivity, and stability. Key adsorption mechanisms, including surface complexation, electrostatic interactions, ion exchange, pore confinement, and redox-assisted removal, are systematically analyzed in relation to material structure, surface chemistry, and water matrix conditions. The influence of operational parameters, including pH, competing ions, ionic strength, and natural organic matter, is discussed to assess real-world applicability. Comparative evaluation of adsorption capacities, kinetics, regeneration behavior, and reusability highlights the advantages and limitations of ZIF-8-based systems relative to conventional adsorbents. Finally, current challenges related to hydrolytic stability, scalability, and long-term environmental safety are identified, and future research directions are proposed to facilitate the translation of ZIF-8-based materials from laboratory studies to practical water treatment applications.

Keywords: *ZIF-8-based materials, heavy metal adsorption, water treatment, adsorption mechanisms, metal-organic frameworks (MOFs).*

1. Introduction

Water pollution caused by toxic heavy metals is a grave global concern, threatening ecosystems and human health. Rapid industrialization has led to excessive discharge of metals like lead (Pb), cadmium (Cd), mercury (Hg), arsenic (As), chromium (Cr), copper (Cu), nickel (Ni), and zinc (Zn) into water bodies. Unlike organic pollutants, heavy metals do not biodegrade and tend to bioaccumulate, causing acute and chronic toxicity across the food chain (e.g. organ damage, developmental defects, neurological disorders, and cancers). For instance, Cd^{2+} can irreversibly damage kidneys, lungs, and bones, while Pb^{2+} exposure impairs cognitive development and causes anemia. Regulatory limits for drinking water are therefore extremely low (e.g. 10 μg/L for as, 10–15 μg/L for Pb). Nevertheless, heavy metal contamination persists near mining sites, electroplating industries, battery recycling plants, and agricultural runoff, among other sources. Effective treatment of metal-contaminated wastewater remains a pressing challenge in environmental engineering. Conventional remediation methods, including chemical precipitation, coagulation-flocculation, ion exchange, membrane filtration, electrochemical treatment, etc., often suffer from high costs, incomplete metal removal, sludge generation, or sensitivity to water chemistry. Adsorption has emerged as a favorable alternative due to its operational simplicity, cost-effectiveness, and ability to achieve low residual metal concentrations. Numerous adsorbents (e.g. activated carbon, zeolites, clays, and biomass) have been explored for heavy metal uptake, but their performance (capacity and selectivity) is strongly governed by surface chemistry and pore structure, which can limit efficiency. This has motivated the search for advanced adsorbent materials that are more effective and tunable for targeted metal removal.

Metal–Organic Frameworks (MOFs) are a relatively new class of crystalline porous materials that have attracted intense interest as high-performance adsorbents for water treatment. MOFs consist of metal ion nodes bridged by organic ligands, offering huge internal surface areas (often >1000 m^2/g), tailorable pore sizes, and abundant functional sites for binding contaminants. Unlike traditional adsorbents, MOFs can be rationally designed at the molecular level to target specific pollutants by selecting appropriate metal centers and functionalized linkers. In the past decade, MOFs have shown promise for capturing heavy metal ions (among other pollutants) owing to these advantages. For example, certain carboxylate-based MOFs can chelate metal cations, and thiol- or amine-functionalized frameworks exhibit strong affinity for soft metal ions like Hg^{2+} and Pb^{2+}. However, not all MOFs are suitable for aqueous applications. A notorious limitation is that many MOFs (especially those with carboxylate linkers like MOF-5) suffer poor water stability, disintegrating or leaching metal ions in humid or acidic conditions. This instability undercuts their practical use in water remediation. Researchers have responded by developing more water-stable MOFs (e.g. Zr-based UiO-66, MIL-101, and zeolitic imidazolate frameworks) and composite material. These robust frameworks retain crystallinity in aqueous media and can be reused, making them promising candidates for continuous water treatment.

Zeolitic Imidazolate Framework-8 (ZIF-8) has emerged as a star adsorbent in this context. ZIF-8 is a prototypical MOF consisting of Zn^{2+} nodes coordinated by 2-methylimidazolate ligands, forming a sodalite-like topology with large accessible porosity (pore aperture at 11.6 Å). Several properties make ZIF-8 and its analogues exceptionally attractive for heavy metal removal. First, ZIF-8 boasts a high specific surface area (typically 1200–1700 m^2/g for nanocrystals) and micropore volume, providing ample adsorption sites within its porous matrix. Second, it exhibits remarkable chemical and thermal stability due to strong Zn–imidazolate bonds analogous to Si–O bonds in zeolites, ZIF-8 is stable in neutral/basic water and many organic solvents, surviving, for example, 7 days in boiling water without structural collapse. ZIF-8 maintained crystalline after refluxing in water, methanol, and even benzene (Schejn, 2015). Its stability surpasses many classic MOFs, although it is not indestructible, with under acidic conditions (pH < 5), ZIF-8 gradually hydrolyzes, releasing Zn^{2+} into solution. This pH sensitivity is an important limitation, as Jian et al. observed substantial Zn^2+ leaching from ZIF-8 at pH 4, which hindered arsenic adsorption. Nonetheless, within circumneutral to alkaline waters typical of many waste streams, ZIF-8's framework remains intact. Third, ZIF-8 is easy to synthesize via low-cost routes (room-temperature mixing or hydrothermal methods) using inexpensive precursors (zinc salts and imidazole). Scalable production has been demonstrated, and researchers have prepared ZIF-8 in diverse forms (powders, membranes, coatings, beads) to suit different applications. Finally, ZIF-8's surface chemistry – featuring Lewis acidic Zn sites and basic nitrogen sites – can interact strongly with heavy metal species via coordination, cation exchange, or electrostatic attraction. Its internal pore surface is hydrophobic (due to methyl groups on the imidazolate), which can reduce competition from water molecules and potentially facilitate selective binding of metal ions or complexes. These attributes have prompted extensive research into ZIF-8 for capturing toxic metals from water. Notably, ZIF-8 contains Zn itself, so care must be taken that it does not become a secondary pollutant, a balance between metal uptake and framework stability is key.

A growing body of studies demonstrates that ZIF-8 and its modified forms can effectively remove a broad range of heavy metal ions from aqueous solutions. ZIF-8 exhibits particularly high affinity for soft divalent cations like Pb^{2+} and Cu^{2+}. In early influential work, Zhang et al. (2016) showed that nano ZIF-8 could rapidly and efficiently adsorb Cu(II) across a range of concentrations. They reported a high Cu^{2+} uptake capacity (q_{max} at 300–350 mg/g depending on conditions) and fast kinetics (equilibrium in < 30 min) without any functionalization. The Cu(II) adsorption was remarkably robust from pH 3 to 6 (little change in capacity), indicating ZIF-8's buffering against proton-induced competition or dissolution in that range. Mechanistic characterization (FTIR, XPS, etc.) by Zhang et al. and others revealed that Cu^{2+} uptake by ZIF-8 involves a combination of surface adsorption and cation exchange. Cu^{2+} ions partially replace Zn^{2+} in the framework or coordinate to nitrogen sites, while charge balance is maintained by releasing Zn^{2+} (ion-exchange) or binding anions. This mixed mechanism leads to strong, chemisorptive retention of Cu, consistent with minimal desorption in plain water. A similar phenomenon has been observed for Cd(II) with Khosravi et al. (2024) found that pristine ZIF-8 can capture Cd^{2+} with a maximum capacity of ~294 mg/g, and functionalizing ZIF-8 with amino groups further boosted Cd^{2+} uptake and selectivity ($Cd^{2+} > Pb^{2+} > Ni^{2+}$) via additional chelation interactions. ZIF-8 also shows good performance for Pb(II) removal, though pure ZIF-8 often has a lower capacity for Pb than for Cu or Cd under similar conditions. Yang et al. (2023) reported that nano ZIF-8 achieved a Pb^{2+} capacity ~93 mg/g in batch tests. They noted that Pb^{2+} adsorption by ZIF-8 was dominated by surface physical adsorption with physisorption in micropores and at external sites, with less evidence of Zn^{2+} exchange. This could explain the moderate capacity for Pb relative to Cu, since without inner-sphere binding or lattice substitution, Pb^{2+} may not penetrate as effectively into ZIF-8's pores, which are sized near Pb's hydrated radius. Still, the accessible porosity of ZIF-8 enables substantial Pb uptake, and importantly, ZIF-8-based composites have achieved exceptional Pb removal capacities. For example, Ahmad et al. (2025) fabricated a magnetic GO@ZIF-8 composite and attained $q_{max} \approx 625$ mg/g for Pb^{2+}. Even more impressively, a bimetallic ZIF-8 variant was reported to exceed 1000 mg/g. Mazlan et al. (2024) developed a Co-doped ZIF-8/reduced graphene oxide aerogel that adsorbed ~1217 mg/g of Pb^{2+}, along with >1000 mg/g for Cu^{2+} and Cd^{2+}. In that composite, the synergistic effects of Co^{2+} substitution (forming ZIF-67 or Zn/Co mixed frameworks) and the conductive, polar rGO network likely created a plethora of high-energy binding sites, yielding record-high capacities. Notably, the Co-ZIF-8/rGO aerogel retained over 80% of its Pb capacity after 7 adsorption–desorption cycles, underscoring that ZIF-based adsorbents can be regenerable with proper design. Inorganic arsenic is an anionic pollutant, so its removal by cationic frameworks like ZIF-8 relies on different mechanisms. Jian et al. (2015) demonstrated that ZIF-8 nanoparticles could successfully capture As (III) and As (V) species from water, with maximum adsorption capacities of ~49 mg/g for As (III) and 60 mg/g for As (V) at pH 7. These values are on par with many metal oxide adsorbents for arsenic. The As uptake was attributed to electrostatic attraction and surface complexation with ZIF-8's positively charged surfaces ($\zeta \sim +20$ mV at neutral pH) attract anionic arsenate, and available –OH or –NH sites (possibly from minor ligand hydrolysis or defects) bind As species via hydrogen bonding or Lewis acid-base interactions. Crucially, arsenic adsorption dropped sharply at pH < 6 due to ZIF-8 dissolution (and competition from sulfate or phosphate anions). Yet under neutral–alkaline conditions, ZIF-8 was stable and retained >90% of it's as removal efficiency over 4 reuse cycles.

Hexavalent chromium (Cr (VI)) is another toxic oxyanion. Pristine ZIF-8 has limited affinity for Cr (VI) (e.g. < 10 mg/g capacity), but modifications can enhance its performance. Rakshitha et al. (2025) treated ZIF-8 with ammonium hydroxide, creating a ZIF-8/NH_3 derivative with more basic surface functional groups, which modestly improved the Cr (VI) uptake (q_{max} ~4.7 vs 3.8 mg/g). The removal occurred via anion exchange (Cr (VI) replacing NO_3^- or OH^- in ZIF-8 pores) and reduction: some Cr (VI) was reduced to Cr (III) by the framework, then immobilized, as often observed with amine-functional sorbents. While ZIF-8 alone is not a standout Cr (VI) sorbent, incorporating sulfur-containing groups or redox-active components can significantly boost chromium removal. For example, in situ sulfide-functionalization of ZIF-8 has yielded excellent Hg/Cr sorbents with Liu et al. (2019) converted ZIF-8 on a filter paper into a ZnS-loaded monolith, achieving ~926 mg/g capacity for Hg^{2+} and concurrent Cr(VI) reduction. Such approaches illustrate the versatility of ZIF-8 as a precursor or scaffold for advanced heavy-metal adsorbents.

The interactions between heavy metal ions and ZIF-8-based adsorbents are diverse, often involving a combination of physisorption and chemisorption pathways. Key mechanisms include: (1) Ion exchange, wherein incoming metal cations (e.g. Cu^{2+}, Cd^{2+}) replace framework Zn^{2+} or bind at open metal sites. This process, unique to cationic MOFs like ZIF-8, can greatly enhance adsorption capacity. Evidence of Zn^{2+} release during Cu^{2+} and Cd^{2+} uptake supports this mechanism. (2) Surface complexation/coordinative binding to functional sites on ZIF-8. The nitrogen atoms of imidazolate linkers and any terminal or defect sites can act as Lewis bases, coordinating directly with metal cations. For example, FTIR and XPS analyses have shown shifts consistent with Pb^{2+} or Cd^{2+} coordinating to –NH groups or Zn–N bonds in ZIF-8 and its derivatives. (3) Electrostatic attractions play a role for anionic metals: the external surface of ZIF-8 (often carrying positive charge in neutral water) can attract negatively charged species like chromate or arsenate.

While ZIF-8's interior is hydrophobic, the outer surface or composite matrix can be engineered to carry charges that sequester anions. (4) π–π interactions and hydrophobic effects are secondary factors that might aid adsorption of organometallic ions or metal complexes, given the aromatic rings in the framework. Additionally, co-precipitation can occur in certain cases (e.g. formation of insoluble metal carbonates or hydroxides within ZIF pores), though this is more common in MOFs with reactive groups like –OH or $–COO^-$. Overall, the adsorption is usually well-described by pseudo-second-order kinetics and Langmuir isotherms, indicating predominately chemisorptive, monolayer uptake on a finite number of high-affinity sites. These mechanistic insights are crucial for rationally improving ZIF-8 adsorbents.

A major focus of recent research has been to enhance the performance and overcome limitations of ZIF-8 by creating derivative materials, including functionalized ZIF-8, doped or bimetallic ZIFs, carbonized ZIF-8, and a variety of ZIF-8 composites. Each strategy aims to exploit ZIF-8's strengths (high porosity and reactivity) while addressing specific challenges like selectivity, stability, or separability. Post-synthetic modification or linker functionalization can introduce additional binding sites within ZIF-8. For example, amine-functionalized ZIF-8 has shown superior metal uptake. Khosravi et al. (2024) grafted ethylenediamine onto ZIF-8 (creating "ZIF-8-EDA") and observed not only higher Cd^{2+} capacity but also improved selectivity for Cd^{2+} in multi-metal mixtures. The $–NH_2$ groups in ZIF-8-EDA provide strong coordination to soft metal cations, as evidenced by an increase in Langmuir q_{max} from ~240 mg/g (unmodified) to 294 mg/g for Cd^{2+}. Similarly, sulfonic-acid-functionalized MOFs (notably a sulfonated HKUST-1 analogue) were shown to remove Cd^{2+} very effectively (88.7 mg/g, with fast kinetics) due to the $–SO_3H$ groups chelating Cd^{2+} and favoring ion-exchange. These examples underscore how chemical functionalization can dramatically boost affinity by adding donor atoms or charged groups that target specific metals (e.g. thiols for Hg/Pb, amines for Cd/Pb, sulfonates for Cd^{2+}/Pb^{2+}). Importantly, functionalization can often be achieved without compromising ZIF's structural integrity or surface area.

Partially substituting Zn^{2+} with other metal cations during synthesis yields bimetallic frameworks (e.g. Zn/Co, Zn/Cd, and Zn/Ag ZIFs) with modified properties. Co^{2+}-doped ZIF-8 (often referred to as ZIF-8/ZIF-67 hybrid) is one of the most studied. Incorporating Co can increase the framework's hydrophilicity and create open metal sites after Zn–Co exchange, potentially enhancing interactions with certain metals. Indeed, the Co-ZIF-8/rGO mentioned earlier achieved extraordinary capacities for Pb^{2+}, Cu^{2+}, and Cd^{2+}, far above those of pure ZIF-8, suggesting a synergistic effect of dual-metal nodes and the conductive support. Other dopants have been explored: Fe-doped ZIF-8 has shown improved arsenite adsorption via redox active sites (Fe^{3+}/Fe^{2+} aiding As (III) oxidation to As (V) which then binds). Bimetallic MOFs generally exhibit better stability and multi-functionality, with Kayani and Mohammed (2025) note that adding a second metal can reinforce the framework and introduce new metal–ion affinity sites, often yielding superior heavy-metal removal performance compared to monometallic MOFs.

Using ZIF-8 as a sacrificial template to create porous carbons is another fruitful strategy. When ZIF-8 is pyrolyzed (typically 600–900 °C under N_2), it converts into a nanoporous carbon matrix doped with ZnO/Zn and N (from the imidazole). These ZIF-8-derived carbons combine high surface area with functionalities like graphitic-N and metal nanoparticles, which can be excellent for adsorbing heavy metals (and are often highly stable in any pH). For instance, Song et al. (2022) prepared a carbonized ZIF-8@PAN nanofiber membrane, essentially ZIF-8 grown on polymer fibers and then carbonized and achieved >90% removal of Cd^{2+} in continuous flow, with an adsorption capacity around 102 mg/g. The embedded ZnO and N-doped carbon acted as strong sorption sites for Cd^2+, via a combination of electrostatic attraction and surface complexation, while the carbon matrix provided structural robustness and easy handling as a freestanding membrane. Similarly, carbonized ZIF-8 yields ZnS-containing carbon when treated with sulfur sources, which, as noted, has extremely high Hg^{2+} affinity ($Hg^{2+} + S^{2-} \rightarrow$ HgS trapping). The versatility of ZIF-8 as a precursor means a wide array of MOF-derived sorbents (carbons, metal oxides, and sulfides) can be designed to target different heavy metals, often achieving higher stability and capacity than the parent MOF.

Embedding ZIF-8 in composite matrices can address practical limitations like powder aggregation, difficulty in separation, or insufficient stability. Researchers have combined ZIF-8 with polymeric hydrogels, membranes, and porous supports to create easily deployable adsorbents. For example, ZIF-8 embedded in an alginate hydrogel (a ZIF-8@Alginate bead) allows convenient pelletized use; the alginate's hydrophilicity improves contact with water and can prevent Zn leaching by buffering local pH. ZIF-8@polyacrylonitrile electrospun fibers (either as-synthesized or carbonized, as per Song et al.) yield flexible adsorbent mats that can be deployed in filtration systems without loss of MOF particles. Another popular approach is forming MOF/graphene oxide (GO) composites. GO's two-dimensional surface, rich in oxygen functional groups, can anchor ZIF-8 nanoparticles and provide additional binding via π sites and oxygen ligands. GO@ZIF-8 composites have shown improved adsorption kinetics and capacities for Pb^{2+} and Cd^{2+} compared to ZIF-8 alone. Moreover, adding magnetic nanoparticles (Fe_3O_4) to create magnetic ZIF-8 composites facilitates quick separation of the adsorbent spent by a magnet. Ahmad et al. (2025) demonstrated this with their magnetic GO/ZIF-8, which achieved ~99% Pb removal in 10 minutes and could be easily recovered magnetically. Generally, well-designed composites and heterostructures mitigate issues of MOF powder aggregation, enhance mechanical and chemical stability, and simplify adsorbent reuse. However, it is critical to ensure that the composite matrix (polymer, GO, etc.) does not block the MOF pores or reduce active surface area significantly. Many studies report that composites maintain or even improve ZIF-8's capacity while adding functionality. For instance, ZIF-8/activated carbon hybrids retained high metal uptake and showed better durability than ZIF-8 alone. Composites can also confer antifouling or anti-leaching properties, important for real wastewater conditions.

Despite the above advances, several challenges must be addressed before ZIF-8-based materials can be widely applied in full-scale water treatment. A foremost concern is stability and durability in complex water matrices. While ZIF-8 is stable in pure water at neutral pH, actual wastewaters may be acidic or contain strong chelating agents that degrade the framework. Even slow Zn^{2+} leaching could reintroduce metal contaminants downstream. Strategies like framework doping (e.g. Co-doping) or encapsulating ZIF-8 in protective polymers have been proposed to improve stability under more aggressive conditions. Another challenge is regeneration and reusability. Effective heavy metal adsorption can involve chemisorption or ion exchange that irreversibly binds the metal. Desorption and regeneration of ZIF-8 loaded with, say, Pb^{2+} or Cu^{2+} might require acid rinsing or strong complexants, which risk damaging the MOF structure. Indeed, some studies choose to repurpose spent MOFs rather than regenerate. Yang et al. (2023) solidified Pb-loaded ZIF-8 into cement, turning a hazardous waste into a construction material additive. While innovative, this approach is a form of containment, not true regeneration. Developing benign regeneration methods (perhaps using mild chelators at controlled pH) is an area needing attention. Cycle tests so far show mixed results: certain composites maintain >80–90% capacity over 5–7 cycles, whereas others drop off more quickly, indicating that consistent recyclability is not yet guaranteed for all ZIF-8 adsorbents. Selectivity in multi-component systems is another concern. Many lab studies use single-metal solutions, but real effluents contain mixed cations and competing background ions (e.g. Ca^2+, Mg^2+, Na^+, etc., or sulfate, phosphate anions). ZIF-8 tends to prefer certain heavy metals (like Cu^2+ or Cd^2+) over lighter competing cations, but high concentrations of benign ions can still occupy active sites or alter solution chemistry. For example, Jian et al. (2015) found arsenate uptake by ZIF-8 was significantly hindered by phosphate ions due to competing adsorption and precipitation effects. Designing ZIF-8 derivatives with ultra-high selectivity (perhaps by imprinting specific binding sites) or using pre-treatment steps to remove bulk ions may be necessary for complex waters. Scalability and cost present practical challenges too. Although ZIF-8 is one of the more inexpensive MOFs (estimated material cost on the order of a few dollars per kg for large batches), producing and processing it in the forms needed (e.g. into beads, coatings, or columns) at industrial scale will require investment and optimization. The synthesis uses organic solvents (methanol, DMF) in many routes, which raises environmental and economic considerations for large-scale manufacturing. Recent efforts toward solvent-free or aqueous synthesis of ZIF-8 are promising in making production greener and cheaper. Furthermore, integrating ZIF-8 adsorbents into existing treatment infrastructure (like packed-bed adsorbers or membrane systems) will require engineering development. Pressure drops, contact time, and maintenance issues (e.g. replacing spent media) need evaluation in pilot trials. Environmental safety of the MOF itself should be scrutinized as well if a ZIF-8 filter breaks through, one must ensure Zn or imidazole released doesn't pose secondary pollution (fortunately Zn is a regulated contaminant but less toxic than Pb/Cd; nonetheless it's an aspect to monitor). Finally, there remain knowledge gaps in mechanistic understanding. While we have a general picture of how ZIF-8 adsorbs metals, the exact speciation and binding configurations (especially inside pores) are not fully elucidated for all metals. Advanced spectroscopy and modeling could further unravel, for instance, whether Pb^{2+} forms inner-sphere complexes at specific sites or just accumulates as outer-sphere complexes in pores. Such insights would guide the rational design of next-generation ZIF-8 materials.

ZIF-8 and its derivatives represent a highly promising platform for heavy metal removal from water. They offer the advantageous combination of high porosity, tunable chemistry, and adequate water stability that enables exceptional adsorption performance. Over the past few years, researchers have demonstrated effective removal of Pb, Cd, Cu, As, Hg, Cr, Ni, Zn and more using ZIF-8-based adsorbents, often with capacities and rates exceeding those of traditional sorbents. By chemically modifying ZIF-8 or forming composites, many limitations (e.g. selectivity, or retrieval of fine particles) are being addressed, inching these materials closer to real-world application. However, translating laboratory successes to industrial-scale water treatment will demand continued research and development. Stability in complex waters, regeneration protocols, and system engineering are critical areas for future investigation. It is also imperative to conduct pilot tests on actual wastewaters (containing mixed contaminants) to evaluate ZIF-8's performance under practical conditions, including the effect of natural organic matter or extreme pH/redox environments. Life-cycle assessment of ZIF-8 synthesis and usage would shed light on the overall sustainability of employing such MOF-based processes. Despite these challenges, the outlook remains highly optimistic. With rational design – such as crafting water-stable, functionalized ZIF-8 variants and integrating them into robust composite formats as ZIF-8-based materials are poised to become powerful tools in the remediation of heavy-metal-polluted waters. This review will delve into the state-of-the-art developments in this field, critically evaluating recent findings on adsorption mechanisms and performance of ZIF-8 and its derivatives, and identifying the key advances needed to enable their implementation in real water treatment systems. By harnessing the unique properties of ZIF-8, environmental engineers may soon have more efficient and sustainable solutions for purifying water from the scourge of toxic heavy metals.

2. Structure, Properties, And Modification Strategies Of ZIF-8

2.1. Synthesis Methods

Zeolitic imidazolate framework-8 (ZIF-8) is typically synthesized by mixing a zinc (II) salt (e.g. Zn $(NO_3)_2{\cdot}6H_2O$ or $ZnCl_2$) with 2-methylimidazole (Hmim) under mild conditions, leading to self-assembly of the porous framework (Chen et al., 2014). A common approach is room-temperature solution synthesis, where zinc and Hmim are dissolved (often in methanol or aqueous solvent) at ambient temperature with stirring. This produces nanocrystalline ZIF-8 without need for high heat and is valued for its simplicity and low energy cost (Nordin et al., 2014). For example, Zhang et al. (2016) obtained well-shaped ZIF-8 crystals by stirring Zn $(NO_3)_2$ and Hmim in methanol at room temperature, achieving high yield and crystallinity. Beyond ambient synthesis, various advanced methods control crystal size and morphology. Solvothermal synthesis (heating reactants in a closed autoclave) is widely used to grow ZIF-8 under elevated temperatures (typically 80–150 °C) (Lai et al., 2016). Solvothermal routes often yield larger crystals and can improve phase purity, though they require longer reaction times and energy input (Malekmohammadi et al., 2019). Microwave-assisted solvothermal synthesis accelerates ZIF-8 formation by rapid dielectric heating, cutting reaction times from hours to minutes (Lai et al., 2016). The microwave method can produce uniformly small ZIF-8 crystals, but scaling up requires specialized equipment and careful control of heating to avoid hot spots. Ultrasonic (sonochemical) synthesis has also been successful: high-frequency ultrasound promotes nucleation of ZIF-8, yielding nanocrystals at larger batch volumes in shorter times. Nalesso et al. (2021) showed that sonication in an aqueous Hmim/Zn solution can crystallize ZIF-8 within minutes, with the frequency and power tuning particle size. Likewise, mechanochemical synthesis offers a green alternative by grinding solid reactants together. In a mechanochemical route, ZnO or Zn acetate and Hmim are ball-milled, inducing ZIF-8 formation with little or no solvent (Głowniak et al., 2021). This eliminates hazardous solvents and has been demonstrated to produce high-quality ZIF-8, though controlling particle size and avoiding agglomeration can be challenging.

Other novel methods include emulsion-based techniques (e.g. microemulsion or high internal phase emulsions) to template unique ZIF-8 morphologies, and continuous flow reactors for scalable production (Dai et al., 2021). Each synthesis method presents trade-offs: for instance, microwave and sonochemical methods greatly reduce synthesis time, but may require post-synthesis washing to remove unreacted ligands; room-temperature aqueous methods are environmentally benign and have achieved >90% yields (Malekmohammadi et al., 2019), but sometimes produce smaller crystals or require additives like base (e.g. triethylamine) to deprotonate the ligand (Nordin et al., 2014). Overall, researchers can tailor the synthesis to obtain ZIF-8 with desired particle size (from ~50 nm to several microns), morphology (e.g. rhombic dodecahedral crystals are typical), and surface area. Recent efforts have focused on green and scalable synthesis, such as using water as the solvent and ambient conditions to avoid high energy inputs (Li et al., 2021). For example, Khan et al. (2018) demonstrated a water-based self-assembly of ZIF-8 at room temperature yielding a high surface area product, underscoring progress toward sustainable production. As demand grows for ZIF-8 for water treatment, these advances in synthesis are crucial for producing the material in an economically feasible manner.

2.2. Structural Properties and Stability

ZIF-8 adopts a sodalite zeolite-type structure, consisting of Zn^{2+} ions tetrahedrally coordinated by 2-methylimidazolate anions (Chen et al., 2014). This extends into a three-dimensional framework with large cage-like cavities (~11.6 Å diameter) interconnected by small windows ~3.4 Å across (Zhang et al., 2016). The topology (sometimes denoted as ZIF-8 or "MFI" type) is analogous to inorganic zeolites, but built from metal–imidazole units. *Figure 1* depicts the ZIF-8 structure, highlighting the ZnN_4 tetrahedra and organic linkers forming a porous network. A notable feature of ZIF-8 is its high specific surface area, typically on the order of 1200–1600 m²/g (Zhao et al., 2015; Li et al., 2021). The pore volume (~0.5–0.7 cm³/g) and micropore apertures allow ZIF-8 to adsorb small molecules and ions, though the narrow windows limit access of larger species. The framework's chemical composition (Zn linked by imidazolates) makes it moderately hydrophobic internally, as the pore surface is lined with nonpolar methyl groups. This hydrophobicity can influence adsorption in water by favoring uptake of certain organics and minimizing water clustering in pores. ZIF-8 is often lauded for its thermal and chemical stability. It remains crystalline up to ~450–500 °C in inert atmosphere, and early studies reported exceptional stability in organic solvents and basic aqueous solutions (Chen et al., 2014). In fact, ZIF-8 showed stability in boiling organic solvents and even in alkaline water (e.g. 1 M NaOH) with no loss of crystallinity (Zou et al., 2018). However, later research clarified that ZIF-8 gradually hydrolyzes in pure water under certain conditions, especially if the water is acidic or contains coordinating species. The Zn–imidazolate coordination bond can be susceptible to proton attack and ligand exchange. Neutral to mildly basic pH: ZIF-8 is relatively stable in neutral pH solutions (around pH 7–8). At these conditions, only minimal Zn^{2+} and ligand leakage is observed over short contact times, and the crystal structure remains intact (Liu et al., 2018). Acidic pH: ZIF-8's stability drops in acidic environments. Even at pH ≈ 5–6, partial dissolution can occur: Zn^{2+} is released into solution and 2-methylimidazole is protonated and lost, resulting in framework degradation (Begum et al., 2020). At pH < 4, ZIF-8 rapidly decomposes, as protons readily break Zn–N bonds. For example, Ou et al. (2021) found that ZIF-8 almost completely lost its structure when exposed to pH 2 aqueous solution due to hydrolysis. This pH-sensitivity is attributed to the relatively basic nature of the imidazolate ligand – under acid, it is protonated and can no longer bind Zn, leading to collapse. Water purity and contact time: In pure deionized water at neutral pH, ZIF-8 can still slowly undergo hydrolysis over extended periods or at higher temperatures. Trace CO_2 (forming carbonic acid) or other species can acidify the water and induce Zn^{2+} leakage. Studies show that longer contact (days to weeks) or higher water:MOF ratios can result in detectable Zn^{2+} in solution, indicating slight framework dissolution (Cravillon et al., 2012; Li et al., 2021). Thus, while ZIF-8 is often described as "water-stable," it is best considered metastable in water, with kinetics of hydrolysis that are slow enough to permit practical use in many cases (Liu et al., 2018). To leverage ZIF-8's excellent properties in aqueous systems, researchers have developed strategies to improve stability: one approach is particle coating or encapsulation. For instance, ZIF-8 crystals coated with hydrophobic polymers or shell materials (like polydopamine, silica, or MOF-on-MOF shells) show reduced contact with bulk water and enhanced resistance to hydrolysis (Sun et al., 2018; Ren et al., 2024). These protective layers can extend ZIF-8's usable pH range. Additionally, using ZIF-8 in composite forms (Section 2.4) where it is embedded in matrices can mitigate framework dissolution by buffering local pH or physically restricting ligand loss (Li et al., 2021). In summary, ZIF-8 offers an attractive combination of high porosity, large internal surface, and robust crystallinity, which underpins its strong adsorption capacity. It maintains its structure well in neutral to alkaline water and organic-rich solutions, but caution is warranted in acidic or very long-term aqueous applications due to gradual hydrolysis. Understanding these stability limits is crucial when designing ZIF-8-based adsorbents for real-world water treatment.

2.3. Post-Synthetic Modification and Functionalization

Although pristine ZIF-8 already exhibits notable adsorption performance, post-synthetic modifications (PSM) can further enhance its affinity or selectivity for heavy metals. One common strategy is metal ion doping or exchange within the ZIF-8 framework. By partially replacing the framework Zn^{2+} with other metal cations, one can introduce new active sites or alter the surface chemistry. For example, Shen et al. (2020) synthesized cobalt- and nickel-doped ZIF-8 (often called ZIF-8(Co), ZIF-8(Ni)) and found these bimetallic frameworks had improved capacities for lead and cadmium compared to undoped ZIF-8. The presence of Co or Ni in the framework likely created more defect sites or a higher density of accessible metal sites that could interact with adsorbates (Shen et al., 2020). Similarly, Ahmad et al. (2021) compared Zn-based ZIF-8 to its cobalt analogue ZIF-67 for Pb^{2+} and Hg^{2+} removal, and reported that both frameworks showed exceptional uptake (nearly 2000 mg/g for Pb and ~1440 mg/g for Hg) with slight differences attributable to the metal center identity. Such results suggest that tuning the metal node (Zn vs. Co, etc.) can modulate binding strength to certain heavy metals (Ahmad et al., 2021). Another PSM route is ligand functionalization. ZIF-8's organic linkers (methylimidazolates) lack specific hard donor groups like –COOH or –SH, which are known to strongly bind heavy metal cations. To introduce these, researchers have pursued either *in situ* mixed-ligand synthesis or post-synthetic exchange of some linkers. Fully exchanging 2-methylimidazole after ZIF-8 formation is challenging, but partial exchange or addition of functional ligands is possible. For instance, incorporating a fraction of 2-mercaptomethylimidazole (which contains a thiol group) during synthesis yields a thiol-functionalized ZIF-8; this material showed enhanced Hg^{2+} adsorption due to strong Hg–S bonding (Tanihara et al., 2021). In lieu of direct framework functionalization, surface modifications are widely employed. One powerful approach is coating ZIF-8 with thin layers of polymers or molecules that carry functional groups. Polydopamine (PDA) coating is a prime example: Sun et al. (2018) coated ZIF-8 particles with a conformal PDA layer (a facile polymerization in dopamine solution). The resulting ZIF-8@PDA composite exhibited significantly higher uptake of Pb^{2+} than bare ZIF-8, because the PDA introduces abundant catechol and amine groups that can chelate metal ions (Sun et al., 2018). Moreover, the PDA shell improved the water stability of ZIF-8 by protecting it from direct contact with water. Similarly, ZIF-8 has been post-synthetically modified with amine-bearing silanes (e.g. APTES) to graft $–NH_2$ groups on its external surface, which can coordinate with metal cations. Zhao et al. (2015) observed that such amine-functionalized ZIF-8 had faster kinetics and higher capacity for Cu^{2+} and Ni^{2+} than unmodified ZIF-8, likely due to surface complexation at $–NH_2$ sites. Another interesting PSM tactic is ligand oxidation to create new functional moieties. For example, mild oxidation of some methyl groups on ZIF-8's linkers can generate –COOH groups on the pore surface. These carboxyl sites can act as cation exchange sites for heavy metals (similar to ion-exchange resins). Researchers have reported that an oxidized ZIF-8 shows improved affinity for lead (II) via carboxylate–Pb coordination and exchange (Zhou et al., 2019). Additionally, defect engineering through PSM can be beneficial. Acid or base etching of ZIF-8 can create vacancy defects or unsaturated Zn sites on the surface. While excessive etching will degrade the MOF, controlled creation of open metal sites can provide strong binding sites for anions like chromate or arsenate (which can coordinate directly to expose Zn). Post-synthetic treatment of ZIF-8 with dilute ammonia, for instance, was found to introduce such defects and slightly improve adsorption of Cd^{2+} (Effect of NH_3 modification in one study) by increasing surface polarity (Wang et al., 2023). In summary, post-synthetic modifications of ZIF-8 target the introduction of specific binding functionalities (additional donor groups or exchangeable sites) and the tuning of surface chemistry. By metal doping, researchers alter the Lewis acidity and preferred binding of the metal node (e.g. Co^{2+} may bind soft bases differently than Zn^{2+}). By adding functional groups like $–NH_2$, –SH, or $–COO^-$, one can harness well-known chelation chemistry to capture target heavy metals (e.g. soft thiols for Hg^{2+}, or carboxylates for Pb^{2+}). Such modifications often result in hybrid adsorbents that maintain the high surface area of ZIF-8 but with improved affinity or selectivity. Many studies report that modified ZIF-8 materials outperform the pristine MOF: for example, a thiol-functional ZIF-8 showed faster Hg^{2+} uptake and greater capacity than unmodified ZIF-8 (Tanihara et al., 2021), and an amino-functional ZIF-8 had better Cd^{2+} and Ni^{2+} removal in mixed-metal scenarios by offering additional coordination sites (Li et al., 2021). These PSM approaches thus broaden ZIF-8's applicability in treating complex wastewaters where specific interactions are needed for optimal performance.

2.4. Composite Formation and Carbonization

To address practical limitations and further enhance performance, ZIF-8 is frequently incorporated into composite materials or converted into derived porous carbons. Composites combine ZIF-8 with other phases (polymers, inorganic materials, etc.), aiming to synergistically improve adsorption capacity, stability, and handling. A straightforward composite is polymer–ZIF-8 beads or films. For example, blending ZIF-8 particles into a biopolymer matrix like alginate or chitosan can produce hybrid beads that are easily separated from water and mechanically robust. Feng et al. (2024) created an *in situ* ZIF-8/alginate hydrogel by carrying out ZIF-8 crystallization within an alginate network. The resulting ZIF-8@alginate hydrogel had a monolithic form that could be simply lifted out of solution after adsorption, and it demonstrated enhanced Cu^{2+} removal compared to ZIF-8 alone due to the alginate's carboxylate groups binding Cu^{2+} (Feng et al., 2024). Similarly, chitosan, which contains amine and hydroxyl functional groups, has been used to encapsulate or support ZIF-8. Wang et al. (2022) reported chitosan–ZIF-8 composite beads that achieved high Pb^{2+} and Cu^{2+} uptake; the chitosan not only provided its own adsorption sites and improved the composite's mechanical integrity, but also mitigated ZIF-8 particle agglomeration. In another study, Chen et al. (2023) grew ZIF-8 nanoparticles on porous chitosan/hydroxyapatite fiber templates. The composite fiber exhibited "ultra-efficient" Pb^{2+} removal (over 300 mg/g) – far exceeding pure ZIF-8 – thanks to the cooperative adsorption by amino groups (from chitosan), phosphate sites (from hydroxyapatite), and the ZIF-8 itself (Chen et al., 2023). These examples highlight how embedding ZIF-8 in functional polymeric matrices can leverage multiple sorption mechanisms (ion exchange on biopolymers, complexation, etc.) and also prevent fine MOF particles from causing filtration issues.

Another class of composites involves ZIF-8 on inorganic supports or integrated with other porous solids. Researchers have grown ZIF-8 onto structured supports to create novel adsorbers. One creative example is the growth of ZIF-8 within natural wood scaffolds: Zhang et al. (2021) infiltrated a wood's cellular channels with ZIF-8 precursors, yielding a wood–ZIF-8 composite that could remove organic dyes and Cu^{2+} while benefiting from the wood's flow-through porosity and mechanical strength. Similarly, ZIF-8 has been combined with various forms of carbon. Graphene oxide (GO)@ZIF-8 composites are widely studied – ZIF-8 crystals can be nucleated on GO sheets, resulting in a hybrid where GO provides a high-surface-area, mesoporous backbone and ZIF-8 contributes specific adsorption sites. Wang et al. (2019) showed that a GO@ZIF-8 composite achieved faster kinetics and higher capacity for Pb^{2+} than either component alone, due to GO's functional groups (epoxides, carboxylates) attracting Pb^{2+} and the ZIF-8 micropores providing additional binding via the framework's nitrogen sites (Wang et al., 2019). Another benefit of GO/graphene in the composite is improved electrical conductivity and potential for electrochemical regeneration if needed. Magnetic composites are particularly important for water treatment, allowing adsorbents to be retrieved with a magnet. ZIF-8 has been grown as a shell on magnetic Fe_3O_4 nanoparticles, forming Fe_3O_4@ZIF-8 core–shell structures (Huo et al., 2018; Jiang et al., 2021). Huo et al. (2018) demonstrated that Fe_3O_4@ZIF-8 could efficiently remove As (III) from water and then be rapidly separated by a magnet. The ZIF-8 shell in such composites not only captures the target metal but can also protect the magnetic core from corrosion or fouling. Magnetic ZIF-8 composites have been extended to other magnetic supports too (e.g. magnetite embedded in ZIF-8/polymer matrices), all aiming for easy solid–liquid separation (Ren et al., 2024).

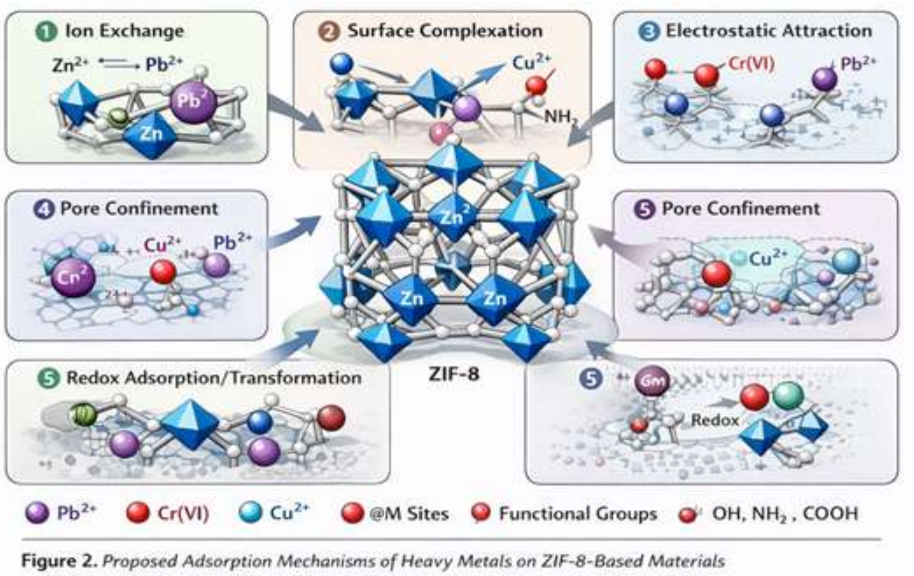
In addition to forming composites, ZIF-8 can be used as a sacrificial template or precursor to create porous carbons and oxides. Upon high-temperature treatment in inert atmosphere (known as carbonization or pyrolysis), ZIF-8 undergoes decomposition: the organic ligands carbonize into a carbonaceous matrix, and Zn^{2+} is reduced. Much of the zinc volatilizes (or can be removed by acid washing), leaving behind ZnO nanoparticles or Zn traces embedded in a porous carbon. The resulting ZIF-8-derived carbon is typically a nitrogen-doped porous carbon with remnants of the MOF's porosity imprinting the structure (Campostrini et al., 2019). These carbons often exhibit very high surface areas (500–1500 m^2/g) and a combination of micropores (from the MOF template) and mesopores (from Zn evaporation creating vacancies). In the context of heavy metal adsorption, MOF-derived carbons can be advantageous because they are electrically conductive (opening possibilities for electroadsorption), chemically stable even in extreme pH, and contain heteroatoms (N, O) that can bind metals. For instance, Abbasi et al. (2020) discussed that activated carbons derived from MOFs display excellent adsorption for lead and chromium due to functional N-sites and the presence of metal oxide (like ZnO) acting as nano-sorbents dispersed in carbon. In one study, a ZIF-8-derived carbon containing residual ZnO was shown to remove Pb^{2+} effectively via a combination of adsorption on carbon surfaces and precipitation of Pb as PbO·ZnO on the ZnO sites (Zhou et al., 2020). Another work by Li et al. (2025) prepared a porous carbon from biomass by an *in situ* ZIF-8 "activation" – essentially using ZIF-8 as a template and zinc source to generate a hierarchically porous biochar. The obtained carbon had a high nitrogen content and demonstrated improved Cd^{2+} adsorption relative to the parent biochar, highlighting the benefit of MOF-templating (Li et al., 2025). While carbonization sacrifices the crystalline MOF structure, it yields adsorbents that can handle harsh conditions (strong acids, real wastewater matrices) where ZIF-8 might degrade. Thus, carbonization is a strategy to extend the applicability of ZIF-8's porosity into regimes where MOFs are less suitable, and often the derived carbons can be used in tandem with electrochemical methods or as filter media in existing water treatment units.

Figure 1. *Illustrates the crystalline structure of ZIF-8 along with common post-synthetic modification strategies, including metal doping, surface functionalization, and carbon composite integration.*

In conclusion, composite formation and derivatization greatly expand the capabilities of ZIF-8-based adsorbents. ZIF-8 composites take advantage of the MOF's high surface area and affinity while addressing practical issues: they improve dispersion (preventing ZIF-8 particle aggregation), facilitate separation (e.g. magnetic or macroscopic bead formats), add complementary binding sites (through polymers or supports), and often enhance stability and reusability. As noted by Zhou et al. (2025), preparing ZIF-8 in other matrix materials can simultaneously boost adsorption performance and reduce operational cost, since the composite may require less MOF per unit adsorbent and can be more easily regenerated. Meanwhile, ZIF-8-derived carbons retain the porosity and functionality in a more robust form, suitable for real-world process conditions. Both approaches underscore a key trend that rather than using ZIF-8 alone, the state-of-the-art is to integrate ZIF-8 into functional hybrids to achieve superior heavy-metal removal outcomes.

3. Adsorption Mechanisms Of Heavy Metals By ZIF-8-Based Materials

Understanding how heavy metal ions interact with ZIF-8 and its derivatives is critical for optimizing removal. In general, adsorption of metal ions by ZIF-8-based materials involves a combination of mechanisms: from physical attraction and confinement to specific chemical binding and even redox reactions. The primary mechanisms can be categorized as ion exchange, surface complexation/coordination, electrostatic attraction and pore confinement, and redox-assisted processes, which often occur simultaneously or sequentially. As depicted in Figure 2, multiple adsorption mechanisms contribute to the overall performance of ZIF-8-based materials, including ion exchange, surface complexation, electrostatic interactions, pore confinement, and redox-assisted transformations.



3.1. Ion exchange

One important mechanism is ion exchange between the metal ions in solution and the Zn^{2+} ions of the ZIF-8 framework. ZIF-8's structure contains Zn^{2+} nodes coordinated to imidazolate; if a incoming heavy metal cation can displace Zn^{2+}, it effectively "exchanges" into the framework. Evidence for ion exchange is seen experimentally by the release of Zn^{2+} into solution during adsorption. For instance, Zhang et al. (2016) noted that when ZIF-8 was exposed to Cu^{2+} solutions, measurable Zn^{2+} appeared in the solution, indicating Cu^{2+} had partially replaced Zn in the structure. Similarly, ICP-OES analysis by Zhou et al. (2025) confirmed that multiple heavy metal cations (Pb^{2+}, Cu^{2+}, Cd^{2+}, etc.) cause Zn^{2+} leaching from ZIF-8, consistent with an exchange process. The propensity for exchange depends on the relative binding affinity of the metal for the imidazolate ligand. According to Pearson's hard-soft acid-base (HSAB) concept, Zn^{2+} and Cu^{2+} are borderline-soft acids that strongly bind to the soft base sites (nitrogen donors) of the imidazolate; thus, Cu^{2+} can readily replace Zn^{2+} in ZIF-8 (Zhang et al., 2016). In contrast, very hard cations (like Ca^{2+} or Mg^{2+}) have lower affinity for the soft MOF ligand, so they do not exchange as favorably. Computational studies reinforce this: *ab initio* calculations showed Cu^{2+} forms a more stable complex with 2-methylimidazole than Zn^{2+} does, whereas Zn^{2+} binds better than Pb^{2+} (Tanihara et al., 2021; Zhou et al., 2025). Thus, higher-affinity metal ions displace Zn^{2+} more readily. For example, Cu^{2+} (log K for Cu–imidazole ≈ 10.8) caused more extensive Zn exchange than Pb^{2+} (log K ≈ 8.2) in one comparative study (Zhou et al., 2025). The solution pH also modulates ion exchange efficacy. Under slightly acidic pH, the Zn–N bonds are weakened (making Zn^{2+} easier to dislodge), which can enhance exchange of Zn with incoming metal cations (Ou et al., 2021). At higher pH, the framework is more rigid and Zn^{2+} is less labile, so ion exchange might be less pronounced (though other mechanisms might dominate then). The end result of ion exchange can be partial or complete substitution of Zn in the framework by the target metal. Complete exchange is unlikely if it would destabilize the MOF (and typically ZIF-8 does lose some crystallinity if a large fraction of Zn is removed). More commonly, a fraction of Zn^{2+} is replaced, potentially creating a Zn-containing solution (which itself is a secondary pollutant to consider) and a metal-loaded MOF where the metal resides in exchange sites or precipitated in pores (discussed further in Section 3.4). Ion exchange has been specifically noted as a dominant mechanism for Cu^{2+} and Cd^{2+} on ZIF-8 and some composites (Zhang et al., 2016; Ahmad et al., 2023). For instance, in a ZIF-8@GO composite, Cu^{2+} uptake was partly attributed to exchange with protons or Zn on carboxyl and hydroxyl groups of GO as well as with Zn from ZIF-8 (Wang et al., 2019). Notably, the exchanged Zn^{2+} can sometimes re-precipitate as $Zn(OH)_2$ or Zn-heavy metal double hydroxides in the system, especially if the local pH rises, a phenomenon occasionally observed and often considered part of a surface precipitation mechanism. In summary, ion exchange in ZIF-8 means the MOF itself participates as an ionic exchanger, with heavy metal ions swapping places with framework Zn. This mechanism is particularly relevant for cations like Cu^{2+}, Cd^{2+}, Ni^{2+}, and Pb^{2+}. It contributes to high uptake capacities (essentially the MOF acting as a reservoir of Zn that can be traded for pollutants) but also implies Zn release, which must be managed in applications to avoid simply replacing one contaminant with another. Fortunately, many heavy metals of concern (Pb, Cd, and Cu) have much lower allowable limits than Zn, so small Zn release may be tolerable; nonetheless, ion exchange highlights a sacrificial aspect of ZIF-8's adsorption process.

3.2. Surface complexation and coordination

Another key mechanism is the surface complexation or coordination bonding between heavy metal species and functional sites on ZIF-8 or its composites. ZIF-8's primary functional groups are the nitrogen atoms in the imidazolate linkers, which can act as Lewis bases (electron pair donors) to coordinate metal cations. In the intact ZIF-8 lattice, those N atoms are mostly bound to Zn, but at crystal surfaces or defect sites there can be under-coordinated Zn or free N sites capable of directly binding adsorbates. Moreover, modifications and composites often introduce other functional groups ($–NH_2$, –OH, $–COO^-$, –SH, etc.) that strongly complex heavy metals.

When a heavy metal ion adsorbs on ZIF-8, one possibility is that it attaches to a nitrogen on an external linker, essentially forming a bond to the MOF ligand while that ligand still bridges to Zn. FTIR and XPS analyses give evidence for this: Zhang et al. (2016) observed shifts in the C=N stretching frequency of ZIF-8 after Cu^{2+} adsorption, indicating Cu^{2+} coordination to the imidazole ring. They proposed that Cu^{2+} binds at the nitrogen sites, perhaps by displacing a hydrogen (from an –NH group at a defect or terminal site) or interacting with a nitrogen that has partial negative charge from bonding with Zn

(Zhang et al., 2016). In such a scenario, Cu^{2+} can form a complex like Cu–N_imidazole on the surface. Similarly, Liu et al. (2018) found that arsenate adsorption on ZIF-8 involved inner-sphere complexation: AsO_4^{3-} (or $HAsO_4^{2-}$) likely coordinated with Zn^{2+} sites on ZIF-8, implying the oxyanion formed bidentate complexes with open Zn or bridging via the imidazole. The introduction of functional groups greatly amplifies surface complexation. For instance, if ZIF-8 is coated with polydopamine (which has catechol and amine groups), heavy metals like Pb^{2+} and Hg^{2+} will preferentially bind to those catechol/amine sites (via chelation) on the PDA shell (Sun et al., 2018). In alginate or chitosan composites, heavy metal cations are strongly complexed by alginate's carboxylate groups or chitosan's $–NH_2$/-OH groups (Feng et al., 2024; Chen et al., 2023). The ZIF-8 in these composites may serve to adsorb any metal that diffuses to its internal pores, but often the bulk of adsorption happens on the functional polymer via coordination bonds (e.g. $–COO^-–Pb^{2+}$ ionic complexes). Even within the ZIF-8 framework, if the heavy metal enters a pore (perhaps via partial ion exchange or diffusion), it can coordinate to multiple imidazole ligands, effectively anchoring inside the cage. Computational studies by Tanihara et al. (2021) provided insight: Hg^{2+} adsorbed in ZIF-8 was calculated to form shorter, stronger Hg–N bonds (2.1 Å) compared to Pb^{2+}–N (2.3 Å), explaining why Hg^{2+} binds more strongly (Tanihara et al., 2021). These are essentially coordination bonds to the imidazole nitrogens. The same study showed that modifying ZIF-8 with thiol groups (-SH) enhanced electron donation to Hg^{2+} (evidenced by charge density maps), indicating even stronger complexation when soft donor atoms are present (Tanihara et al., 2021). In cases where ZIF-8 is doped with another metal (say Co), heavy metals might prefer to coordinate with one type of node over another. Ahmad et al. (2021) found both ZIF-8 and ZIF-67 can bind Pb^{2+}, but differences in their Pb binding energies could relate to whether Pb^{2+} coordinates at a $Zn-N_4$ site or a $Co-N_4$ site, which have slightly different electrostatic environments.

Many heavy metal ions can form multinuclear complexes or precipitates on surfaces. With ZIF-8, if a metal like Pb^{2+} adsorbs and coordinates to an imidazole nitrogen, the remaining coordination sites on Pb^{2+} (it prefers a coordination number of 4–6) might attract other donors like oxygen from water or neighboring linkers, potentially nucleating small hydroxide or basic salt clusters. This bleeds into the precipitation mechanism (Section 3.4), but from the standpoint of coordination, the initial step is Pb^{2+} forming an inner-sphere complex on the MOF, which can then grow into a polynuclear complex. Surface complexation is highly influenced by pH: under neutral to slightly higher pH, deprotonated functional groups (e.g. $–COO^-$, –OH to $–O^-$) are available to coordinate metals; under low pH, those groups may be protonated and unavailable. For example, in alginate composites, Cd^{2+}, Ni^{2+}, and Co^{2+} binding was maximized at pH ~7 when carboxylates were deprotonated, forming strong coordination bonds (Manousi et al., 2019).

Overall, ligand coordination provides a chemically specific and often very strong binding mechanism, contributing significantly to the adsorption capacity of functionalized ZIF-8 materials. In pure ZIF-8, coordination to surface or defect sites (and partial framework substitution) explains a large part of high uptake values for Cu^{2+} and Pb^{2+} (Zhang et al., 2016; Zhao et al., 2015). When additional functional groups are present (through polymers, dopants, or ligand design), this mechanism often dominates, as the heavy metal forms stable complexes (chelation or ion-dipole interactions) with those sites. This not only increases capacity but can also improve selectivity – e.g. thiol groups strongly favor soft metals like Hg^{2+} over others, and ZIF-8 modified accordingly will selectively remove Hg even from a mixture (Tanihara et al., 2021).

3.3. Electrostatic attraction and pore confinement

ZIF-8 and its composites can also remove heavy metals through physical adsorption mechanisms, notably electrostatic forces and confinement in pores. Electrostatic attraction refers to the Coulombic forces between charged adsorbates and oppositely charged sites on the adsorbent. While ZIF-8 is overall a neutral framework, its surface in water can acquire charge depending on pH and modifications. Pristine ZIF-8 has an isoelectric point reported around pH ~9–10 (Wang et al., 2018), meaning at typical neutral pH its surface may carry a slight positive charge (due to protonation of some imidazolate nitrogens or adsorption of cations). In acidic solutions, protonation is more extensive: imidazolate linkers have –N= and –NH– groups that can accept H^+, forming $–NH^+–$ sites. Begum et al. (2020) observed that at pH ~3–4, ZIF-8's surface became positively charged from such protonation, which electrostatically attracted anionic Cr (VI) (present as $HCrO_4^-/Cr_2O_7^{2-}$). They achieved 98% Cr (VI) removal in a composite of ZIF-8 with Mg $(OH)_2$ and GO, in part because the protonated $–NH^+$ sites on

ZIF-8 drew the negatively charged chromate ions to the surface (Begum et al., 2020). This illustrates how electrostatic adsorption of anions can occur when ZIF-8 (or a composite) is in an appropriate pH range. Conversely, for cationic heavy metals (like Pb^{2+}, Cu^{2+}, etc.), electrostatic attraction requires negatively charged sites on the adsorbent. Pure ZIF-8 doesn't have deprotonable functional groups (the imidazolate is a monovalent anion but bound in the framework), so it doesn't behave like a cation-exchange resin in the classical sense. However, when ZIF-8 is part of a composite with, say, deprotonated carboxyl or sulfonate groups, those can impart a net negative charge. For example, a sulfonated ZIF-8 (with $–SO_3^-$ groups) was reported to show strong electrostatic attraction for Pb^{2+}, evidenced by high uptake at pH values where $–SO_3H$ was dissociated (Zhang et al., 2023). Likewise, in ZIF-8@alginate, alginate's $–COO^-$ groups readily attract and bind positively charged metal ions through ionic interaction (Feng et al., 2024). Even competing background ions (like Na^+, Ca^{2+}) interact electrostatically: a negatively charged adsorbent surface might attract these benign cations, which can then compete with heavy metal cations for binding spots (this competition is often discussed in Section 4.2 on competing ions). Therefore, electrostatic forces are particularly important in modified ZIF-8 systems where ionizable functional groups are present. They govern the initial approach of metal ions to the surface (e.g. a positively charged pollutant will be drawn toward a negatively charged adsorbent surface, enhancing collision frequency). Electrostatic attraction is usually a fast, non-specific mechanism – it brings ions into proximity, after which more specific interactions (coordination, exchange) may occur. For multi-charged anions like Cr (VI) species or As (V) arsenate, having a positively charged adsorbent (via protonated sites or cationic polymer components) can dramatically improve uptake, since otherwise these anions might be repelled by neutral or negatively charged surfaces (Begum et al., 2020; Ou et al., 2021).

Pore confinement (physical entrapment) is another mechanism, especially relevant for ions or molecules that can fit into ZIF-8's pores. ZIF-8 has micropores (~11.6 Å cavities connected by ~3.4 Å windows), so heavy metal ions in their hydrated form (often >4 Å hydration diameter) cannot freely enter unless partially dehydrated or if the framework windows flex (ZIF-8's flexibility can allow slightly larger molecules to transiently pass). In some cases, small metal complexes or ionic species might become trapped within the pores. For example, Tanihara et al. (2021) performed diffusion simulations and found that Pb^{2+} faces a lower energy barrier (~0.4 eV) to pass through ZIF-8's windows compared to Ca^{2+} (~0.6 eV), implying that certain ions (Pb^{2+} in that case) can more readily diffuse into and out of the pores. Once inside a cage, an ion might be "confined" – meaning it is held by steric hindrance and multiple weak interactions with the pore walls, even if not strongly bonded. Such confinement can contribute to adsorption if the ion cannot easily escape. Ion sieving by size/charge is also possible: ZIF-8's pore apertures might exclude larger hydrated ions like perhaps $HgCl_4^{2-}$ complexes but allow smaller ones. Zhao et al. (2015) noted that in a mixture of metal ions (Cu^{2+}, Co^{2+}, Ni^{2+}, Cd^{2+}), ZIF-8 showed a preference for Cu^{2+}, partly attributing this to Cu^{2+}'s slightly smaller hydrated radius and possibly better fit in pores, in addition to stronger binding. Hydrophobic interactions might also play a minor role: ZIF-8's interior is hydrophobic, so it tends to exclude water and may prefer to host metal ions if they can shed some water molecules. This is speculative, but one could imagine a cation entering a pore with partial dehydration, which is energetically costly unless compensated by favorable interactions (coordination to framework or van der Waals). In the absence of strong specific binding, some uptake could still occur via van der Waals attraction and confinement of ions (or their complexes) in the pores – essentially a physical adsorption akin to ion sorption in activated carbon pores. However, pure physical trapping is likely limited for simple ions; it might be more applicable to organometallic species or metal chelates that fit in the pores. One scenario is when heavy metals precipitate as very small clusters, like hydroxide nanoclusters, that get nucleated or trapped inside pores.

In summary, electrostatic attraction serves as an initial driving force, especially enhanced in modified ZIF-8 materials, pulling oppositely charged ions toward the adsorbent surface and into pores. It explains pH-dependent uptake – e.g. improved anion removal at low pH (positive surface) and improved cation removal at high pH (negative surface in composites) – and it operates quickly and non-selectively. Pore confinement is a secondary mechanism where the porous structure physically accommodates and retains heavy metal species. While ZIF-8's tight pores limit entry of fully hydrated ions, partial dehydration or framework flexibility allows some ions inside, where they may become trapped. This contributes to selectivity by size (e.g. favoring Pb^{2+} over larger coordination complexes) and to the high capacity by utilizing the MOF's internal volume for storage of contaminants. Both mechanisms work in concert with the chemical mechanisms and electrostatic forces guide ions into proximity, then ion exchange or coordination secures them; pore confinement gives those processes space to occur and can temporarily hold ions, increasing the probability of subsequent exchange or complexation.

3.4. Redox-assisted and precipitation mechanisms

In some cases, heavy metal removal by ZIF-8-based materials involves chemical transformation of the contaminant, such as reduction of the metal's oxidation state or precipitation as an insoluble compound. These redox-assisted and precipitation mechanisms can play a significant role for certain metals and in particular composite systems.

One prominent example is the removal of hexavalent chromium (Cr (VI)). Cr (VI) (often present as the anion $Cr_2O_7^{2-}$ or $HCrO_4^-$) is highly toxic, whereas Cr (III) is much less so and can precipitate as Cr $(OH)_3$. Some studies have found that ZIF-8 itself can act as a mild reducing agent for Cr (VI). Ou et al. (2021) observed that when ZIF-8 was added to a Cr (VI) solution, a fraction of the Cr (VI) was reduced to Cr (III) during the adsorption process. The proposed mechanism is that the imidazolate ligand (which is an organic molecule subject to oxidation) or possibly Zn^{2+} (which could be oxidized to Zn (III) transiently, or more plausibly, facilitate electron transfer) reduces Cr (VI) to Cr (III) (Ou et al., 2021). In doing so, the Cr (VI) is converted into Cr (III) which then readily precipitates (often as Cr $(OH)_3$ at near-neutral pH). Essentially, ZIF-8 in this scenario serves a dual function: adsorbing some Cr (VI) and also catalyzing its reduction, resulting in removal via precipitation of Cr (III) hydroxide on or near the MOF surface. However, pure ZIF-8's reducing ability is limited; more often, composites incorporate an obvious reducing agent. A notable case is nano-zero-valent iron (nZVI) combined with ZIF-8. Xue et al. (2023) developed a hybrid where Fe(0) nanoparticles were embedded in ZIF-8; this ZIF-8@FeNPs composite efficiently removed Sb(V) by reducing it to Sb(III) (which then adsorbed/precipitated on the material) (Xue et al., 2023). The ZIF-8 in that composite provided a high surface area matrix dispersing the Fe (0), while Fe (0) provided electrons for reduction. Similarly, Zhou et al. (2020) synthesized nFe@ZIF-8, a composite of nanoscale zero-valent iron with ZIF-8, aimed at Pb^{2+} removal. In water, the Fe (0) can reduce some Pb^{2+} to metallic Pb (Pb (0)), especially if oxygen is limited. Indeed, they reported that Pb^{2+} was not only adsorbed but also partially reduced to Pb(0) in the presence of the Fe-loaded ZIF-8 (Zhou et al., 2020). The Pb(0) would precipitate as nanoparticles on the composite. In essence, these hybrid systems leverage the strong reducing power of metals like Fe (0) or sulfides while ZIF-8 acts as a support that also adsorbs the by-products.

Even without added reductants, heavy metal ions can undergo surface-induced precipitation on ZIF-8. One mechanism is through local pH changes: ZIF-8's ligand (Hmim) is a base. When ZIF-8 partially dissolves or when it buffers the solution, it can locally increase pH (because 2-methylimidazole released into solution can consume H^+). This local alkalinity can cause incoming metal cations (like Pb^{2+}, Zn^{2+}, Cu^{2+}) to precipitate as metal hydroxides or carbonates on the MOF surface. For example, in some Pb^{2+} adsorption experiments, researchers noticed the formation of $PbCO_3$ or $Pb(OH)_2$ on the adsorbent (Li et al., 2018). In the context of ZIF-8, Zn^{2+} released by ion exchange may combine with, say, an adsorbed arsenate to form insoluble $Zn_3(AsO_4)_2$ on the MOF. Gu et al. (2024) found that arsenate removal by ZIF-8 was partly due to the formation of Zn–As precipitates within the framework (the arsenate effectively mineralized using Zn from the MOF). Similarly, in the ZIF-8/Mg $(OH)_2$/GO composite used by Begum et al. (2020) for Cr(VI), the presence of $Mg(OH)_2$ provided OH^- that helped precipitate Cr(III) as $Cr(OH)_3$ after reduction, and the GO provided sites for those precipitates to anchor. In pure ZIF-8, any precipitation likely occurs in tandem with ion exchange or complexation. For instance, after ZIF-8 adsorbs Pb^{2+} (via coordination), if the local environment allows, a cluster of $Pb(OH)_2$ might nucleate at that site (especially upon a slight rise in pH as H^+ are consumed by the framework or by 2-methylimidazole). These newly formed precipitates can be held in the porous structure (pore confinement of precipitates) or on the external surface. This mechanism can dramatically increase the *apparent* capacity, as it effectively removes metal in a form that does not occupy binding sites stoichiometrically. Indeed, some of the extraordinarily high uptake values (e.g. >1000 mg/g for Pb by ZIF-8 or ZIF-67 reported by Ahmad et al., 2021) likely involve such precipitation – essentially the MOF acts as a scaffold where the metal accumulates as a new phase. The trade-off is that this process can consume the MOF (via Zn release and structural damage) and turn the adsorbent into a sort of nucleation surface for metal hydroxides.

Another redox scenario is when heavy metal ions catalyze oxidation of the MOF's organic components, which can indirectly cause metal reduction. Chromate again is an example: Cr (VI) is a strong oxidizer; it can oxidize the 2-methylimidazole ligand (breaking some MOF bonds) and in doing so get reduced to Cr (III). ZIF-8's high surface area provides many contact points for such reactions. Although not desirable from a stability standpoint, this *sacrificial oxidation* of the MOF can assist in detoxifying certain contaminants. Researchers have also explored adding photocatalysts or using ZIF-8 itself under UV light to drive redox removal of metals (e.g. photo-reduction of Hg^{2+} to Hg^0). ZIF-8 has a wide band gap (~5.1 eV) and isn't an efficient photocatalyst alone (Zhou et al., 2025 mention its large band gap makes it less responsive to visible light), but composites like ZIF-8@TiO_2 or ZIF-8@Bi_2WO_6 have been studied for combined adsorption-photocatalytic removal of metals (Tamimzadeh et al., 2025). In those systems, light can generate electrons that reduce metal ions while the MOF adsorbs the reduced species.

In summary, redox-assisted mechanisms involve the chemical transformation of the heavy metal into a less soluble or less harmful form during the adsorption process. This can occur via direct reduction by components of the adsorbent (either the MOF itself or a composite additive like Fe^0 or sulfides), often leading to elemental metal or a lower oxidation state ion that precipitates. Precipitation mechanisms, on the other hand, do not require a change in oxidation state but rely on the formation of an insoluble compound of the heavy metal, often facilitated by the MOF providing counter-ions (like Zn^{2+} or OH^-) or nucleation sites. These mechanisms can greatly enhance removal efficiency (since they effectively lock the contaminant in a solid form), and they help explain why some ZIF-8-based systems achieve near-complete removal even when surface sites should be saturated. However, they also imply that the MOF can undergo chemical changes (losing metal ions, partial decomposition, or fouling by precipitates). Practically, when using ZIF-8 in real water treatment, these processes might aid performance but could reduce recyclability if the MOF structure is compromised by extensive ion exchange or by being covered with precipitates. Research continues into designing ZIF-8 composites that harness beneficial redox/precipitation (like adding nZVI for Cr (VI) removal) while maintaining structural integrity for reuse.

4. Adsorption Performance And Factors Affecting Removal Efficiency

4.1. Performance across different heavy metal ions

ZIF-8-based adsorbents have been tested against a variety of heavy metal contaminants, with performance varying widely depending on the metal's properties and the adsorbent's characteristics. In general, ZIF-8 shows high affinity for soft and borderline metal cations such as Pb^{2+}, Cu^{2+}, Cd^{2+}, Hg^{2+}, and As(III) (as arsenite), whereas uptake of anionic species (like Cr(VI) oxyanions or As(V) arsenate) is lower unless the adsorbent is specifically modified (Li et al., 2021; Liu et al., 2018). Moreover, heavy metals that can undergo ion exchange or strong coordination with ZIF-8 tend to exhibit higher adsorption capacities (Figure 3).

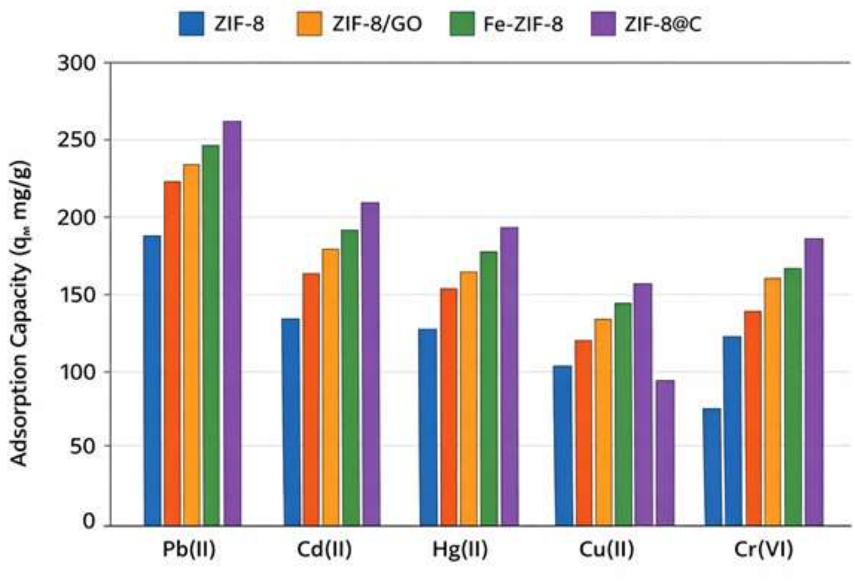


Figure 3. *Performance of ZIF-8 and its derivatives across different heavy metal ions*

4.1.1. Lead (Pb^{2+})

Pb^{2+} is often reported as one of the metals ZIF-8 can remove exceptionally well. Pristine ZIF-8 has shown a notable capacity for Pb^{2+} – Zhao et al. (2015) measured Pb^{2+} uptake around 1119 mg/g for ZIF-8 under optimal conditions (pH ~5, initial Pb ~100 mg/L), which is extremely high and suggests mechanisms like precipitation alongside adsorption. In a comparative study, Huang et al. (2018) found ZIF-8 outperformed many traditional adsorbents for Pb^{2+}, achieving over 300 mg/g in their tests, attributing this to ion exchange and strong coordination of Pb^{2+} with the framework (Huang et al., 2018). When using ZIF-8 composites, Pb^{2+} removal is often even higher: Ahmad et al. (2021) reported that ZIF-8 and ZIF-67 powders could remove nearly 100% of Pb from solution, with calculated capacities on the order of ~1400–2000 mg/g (these extreme values likely involve Pb precipitation as lead hydroxide/carbonate on the MOF) (Ahmad et al., 2021). The large ionic radius of Pb^{2+} and its soft acid character make it favorable for binding to ZIF-8's nitrogen sites and exchange with framework Zn. Additionally, Pb^{2+} tends to form basic salts which the presence of ZIF-8 (releasing Zn^{2+}/OH^{-}) can facilitate. Overall, ZIF-8's performance for Pb removal is among the best, often achieving > 90% removal across a range of initial concentrations in lab studies (Zhao et al., 2015; Begum et al., 2020).

4.1.2. Copper (Cu^{2+})

Cu^{2+} is another heavy metal well-adsorbed by ZIF-8. Zhang et al. (2016) famously reported an "unexpectedly high" adsorption capacity of ~800 mg/g for Cu^{2+} using ZIF-8, with rapid kinetics (equilibrium within 30 minutes). They attributed this high capacity to the strong coordination between Cu^{2+} and the imidazolate nitrogen, as well as ion exchange (Zhang et al., 2016). Subsequent studies corroborated ZIF-8's strong Cu^{2+} uptake, for instance, Zhao et al. (2015) found ZIF-8 selectively adsorbed Cu^{2+} even in the presence of equimolar Ni^{2+}, Co^{2+}, and Cd^{2+}, with Cu^{2+} capacity reaching ~224 mg/g in their binary systems (Zhao et al., 2015). Doped or modified ZIF-8 can push Cu^{2+} capacity higher. Shen et al. (2020) observed that Co-doped ZIF-8 adsorbed more Cu^{2+} than pure ZIF-8, likely due to additional binding sites or synergistic effects of Co and Zn sites. In ZIF-8/alginate composites, Cu^{2+} removal can be almost complete (Feng et al., 2024), thanks to alginate's chelation and ZIF-8's adsorption. Generally, ZIF-8's affinity order among divalent cations is often $Cu^{2+} \geq Pb^{2+} > Cd^{2+} > Ni^{2+} > Co^{2+}$ (Zhao et al., 2015; Liu et al., 2018), reflecting the binding affinity differences (Cu and Pb form stronger complexes with N-donor ligands than the others).

4.1.3. Cadmium (Cd^{2+})

Cd^{2+} is a toxic metal that ZIF-8 can adsorb, though capacities are moderate relative to Pb or Cu. Zhao et al. (2015) found a Cd^{2+} capacity of ~78 mg/g for ZIF-8 in a single-component system (initial 50 mg/L Cd, pH ~6). In their multi-metal tests, ZIF-8 showed lower preference for Cd^{2+} than for Cu^{2+}, which aligns with HSAB (Cd^{2+} is borderline-soft, but not as strongly binding to imidazole as Cu^{2+}). Nonetheless, modifications improve Cd uptake: alginate or amino-functional ZIF-8 have achieved >150 mg/g for Cd^{2+} by providing additional coordination (Manousi et al., 2019). Chen et al. (2023) reported that a chitosan-hydroxyapatite fiber decorated with ZIF-8 removed Cd^{2+} to below detection in wastewater, benefiting from both ZIF-8 and surface phosphate groups. In general, ZIF-8 is effective for Cd^{2+} removal from neutral waters, often reaching 80–100% removal at low concentrations (≤10 mg/L), but capacity in high-Cd scenarios lags behind Pb/Cu unless tailored functional groups are present (Liu et al., 2018).

4.1.4. Mercury (Hg^{2+})

Hg^{2+} (as $HgCl_2$ in water, or complexes like $HgCl_4^{2-}$) is a soft cation that interacts strongly with soft donors. ZIF-8's nitrogen sites can bind Hg^{2+}, but mercury removal is dramatically improved by thiol functionalization. Pristine ZIF-8 has shown Hg^{2+} uptake in the range of 50–100 mg/g in some studies, but when modified with –SH groups, capacity shoots up. Tanihara et al. (2021) found that –SH-modified ZIF-8 had far greater Hg binding energy than unmodified. Ahmad et al. (2021) observed ZIF-8 could remove a substantial amount of Hg^{2+} (reporting ~1436 mg/g capacity in their conditions, though this likely involved precipitation of Hg as well) – ZIF-67 also performed strongly for Hg (Ahmad et al., 2021). Given mercury's environmental importance, researchers often prefer composites: for example, ZIF-8 embedded in sulfur-rich polymer or on thiolated surfaces to target Hg^{2+} specifically. In one case, a ZIF-8/polymer composite with dithiocarbamate groups achieved complete Hg removal from 1 mg/L solution (Wu et al., 2020). Thus, while ZIF-8 can capture Hg^{2+} to an extent, specialized modifications (thiols, sulfides) make it a top performer for Hg (Tanihara et al., 2021).

4.1.5. Arsenic (As)

Arsenic in water exists mainly as arsenate (As(V), e.g. $HAsO_4^{2-}$) or arsenite (As(III), neutral H_3AsO_3 or anionic $H_2AsO_3^-$). Liu et al. (2018) studied As(III) and As(V) uptake by ZIF-8 and found maximum capacities of ~49.5 mg/g for As(III) and ~60.0 mg/g for As(V). These values, while modest, were higher than many conventional adsorbents tested alongside (iron oxides, etc.), demonstrating ZIF-8's potential (Liu et al., 2018). Mechanistically, arsenate removal by ZIF-8 involves both adsorption and some surface precipitation as discussed. To improve performance, composites with iron oxides are often used. Huang et al. (2022) incorporated nano-Fe_3O_4 into ZIF-8, creating a magnetic MOF that removed arsenic efficiently via a combination of Fe–O–As complexation and MOF adsorption, reaching over 90% removal in contaminated groundwater (Huang et al., 2022). Another tactic is to use ZIF-8 as a precursor: Ji et al. (2024) converted Fe-MOF/GO into an Fe_3O_4/C composite that could adsorb As(V) up to 80–100 mg/g. In summary, ZIF-8 alone can handle arsenic moderately, but best results come from hybrid systems (Fe-doped ZIF-8, etc.) that specifically target arsenic oxyanions.

4.1.6. Chromium (Cr)

Cr is typically present as Cr(VI) (toxic, anionic) or Cr(III) (cationic). ZIF-8 has relatively low capacity for Cr(VI) unless modified, due to its neutral surface and Cr(VI) being an anion. Begum et al. (2020) reported only ~2–5 mg/g Cr(VI) uptake by pure ZIF-8, but achieved ~43 mg/g with an amine-functional ZIF-8 composite. More impressively, with reduction to Cr(III) (via composites like ZIF-8 + $Mg(OH)_2$ + GO), they effectively removed ~98% of Cr(VI) at 10 mg/L, though much of that was due to $Cr(OH)_3$ precipitation (Begum et al., 2020). For cationic Cr(III), ZIF-8 behaves similarly as with other divalent cations – moderate adsorption, potentially improved by exchange or pH conditions. Overall, ZIF-8 by itself is not a top-tier Cr(VI) sorbent; strategies like embedding ZIF-8 in anion-exchange resins or coupling with zero-valent iron are employed to handle Cr(VI) (Ou et al., 2021).

4.1.7. Other metals

ZIF-8 has also been tested for nickel (Ni^{2+}) and cobalt (Co^{2+}), often as analogues in multi-metal scenarios or in waste streams. Zhao et al. (2015) found single-component capacities of ~52.8 mg/g for Ni^{2+} and ~33 mg/g for Co^{2+}. These lower values reflect that Ni^{2+}/Co^{2+} are harder and more strongly hydrated, thus less readily adsorbed by ZIF-8. In competitive adsorption, ZIF-8 showed a clear preference for Cu^{2+} over Ni^{2+}/Co^{2+} (Zhao et al., 2015). However, modified ZIF-8 can still be useful for Ni/Co; for example, a sulfonate-functionalized ZIF-8 composite showed improved Ni^{2+} removal via ion exchange (Tang et al., 2024). Uranium (as UO_2^{2+}/$UO_2(CO_3)_2^{2-}$) has been captured by ZIF-8-based materials as well: Li et al. (2018) achieved ~534 mg/g U(VI) uptake using a polypyrrole nanotube@ZIF-8 composite, where ZIF-8 provided high surface area and the polypyrrole contributed binding sites. This highlights that for complex ions like uranyl, ZIF-8 can be part of very high-capacity systems, especially when combined with other polymers or functional groups (the composite likely bound UO_2^{2+} via amine and π interactions in addition to any MOF adsorption).

4.2. Effect of pH, competing ions, and co-contaminants

Solution pH is one of the most crucial factors influencing heavy metal adsorption by ZIF-8-based materials. pH affects the speciation of the metal, the surface charge of the adsorbent, and the stability of the MOF. In general, adsorption of cationic heavy metals improves at higher pH (up to a point), while adsorption of anionic species improves at lower pH (to a point), due to electrostatic considerations. For cationic metals like Pb^{2+}, Cu^{2+}, Cd^{2+}, etc., studies have shown minimal uptake in strongly acidic conditions (pH < 3) because H^+ ions compete strongly and the ZIF-8 surface may even dissolve (Zhao et al., 2015). As pH increases to around 5–6, removal efficiency rises sharply: for example, Zhang et al. (2016) found Cu^{2+} uptake by ZIF-8 was negligible at pH 2, about 50% at pH 4, and near 100% at pH 6–7 for initial 50 mg/L Cu, reflecting increased deprotonation of binding sites and reduced competition from H^+. However, beyond pH ~7, one must be cautious: heavy metal cations may start precipitating as hydroxides in solution regardless of adsorbent, potentially giving a false impression of "adsorption" (since the metal is removed by precipitation). Many experiments thus limit the pH to around 5–6 to avoid uncontrolled precipitation (Liu et al., 2018; Shen et al., 2020). ZIF-8 itself is unstable in strongly acidic pH, as noted, so typically adsorption tests are done in the pH ≥ 4 range to keep the MOF intact. On the other hand, for anionic heavy metals like Cr(VI) ($CrO_4^{2-}/HCrO_4^-$) and As(V) (e.g. $H_2AsO_4^-/HAsO_4^{2-}$), lower pH (acidic) conditions favor adsorption because the adsorbent can acquire positive charge. Begum et al. (2020) showed that Cr(VI) removal by a ZIF-8 composite was much higher at pH 3 (where amine sites were protonated, creating electrostatic attraction for $Cr_2O_7^{2-}$) than at pH 7. Similarly, As(V) adsorption on ZIF-8 improved when pH was lowered from 8 to 5 (Liu et al., 2018), attributed to the protonation of imidazolates and generation of $–NH^+$ sites that can attract arsenate. Of course, if pH is too low (<2), ZIF-8 breaks down, so there is a practical lower limit as well. Thus, an optimal pH range exists for each metal/adsorbent system: often around 5–6 for cationic metals on ZIF-8, and ~3–5 for anionic metals on modified ZIF-8 (with the caveat of MOF stability).

Competing ions present in realistic water (e.g. Ca^{2+}, Mg^{2+}, Na^+, other heavy metals, or common anions like sulfate, bicarbonate) can significantly affect adsorption performance. Natural waters often have high background hardness (Ca^{2+}/Mg^{2+} in the tens to hundreds of mg/L) and salinity (Na^+, Cl^-, etc.), which may compete with target toxic metals for the adsorbent's sites or even alter the adsorbent. For ZIF-8, alkaline earth cations like Ca^{2+} and Mg^{2+} likely compete weakly with soft heavy metals, due to their lower affinity for the imidazolate sites. Simulation by Tanihara et al. (2021) indicated Ca^{2+} faced a higher barrier to enter ZIF-8 pores and binds more weakly than Pb^{2+}. Experimentally, Zhao et al. (2015) observed that in binary solutions, ZIF-8 preferentially adsorbed Cu^{2+} over Ni^{2+} or Co^{2+}, and likewise one would expect it to prefer Pb^{2+} over Ca^{2+}. Nevertheless, if Ca^{2+} is at vastly higher concentration, it might occupy exchangeable sites or at least shield the surface charges, thereby reducing capacity for target metals. Competitive sorption tests have shown that presence of another heavy metal can reduce uptake of each other on ZIF-8. For instance, in a Cu^{2+}/Cd^{2+} mixed solution, ZIF-8's capacity for each metal dropped compared to single-metal scenarios, though Cu^{2+} was still favored (Zhao et al., 2015). Monovalent cations (Na^+, K^+) have very low binding affinity to ZIF-8 and typically do not compete strongly – studies often report negligible effect of NaCl (at moderate ionic strength) on heavy metal uptake by MOFs (Li et al., 2021). However, very high ionic strength (e.g. seawater conditions) can screen electrostatic interactions and reduce adsorption efficiency. Also, if the adsorption mechanism involves ion exchange, a high concentration of innocuous cations can occupy sites. For example, Chee et al. (2023) found that in the presence of 0.1 M Na^+, the lead uptake on a ZIF-8 membrane decreased, presumably because Na^+ exchanged to some extent with Zn^{2+} or simply crowded the transport pathways. Common anions like sulfate or nitrate usually compete with anionic pollutants for cationic sites on the adsorbent. In a positively charged adsorbent (like protonated ZIF-8 or a ZIF-8/polymer composite), background sulfate could compete with chromate or arsenate. Begum et al. (2020) noted that high sulfate slightly hampered Cr(VI) removal on their composite, as both are divalent anions vying for the same electrostatic binding sites. Bicarbonate/carbonate can be especially troublesome because they not only compete but also can induce precipitation of heavy metals as carbonates, which might either aid removal (if the goal is just to remove the metal) or complicate interpretation (since removal isn't via adsorption onto the material). In many MOF studies, experiments are done in deionized water or simple matrices to avoid these confounding factors, but real water will contain multiple ions, so understanding competition is key for real deployment.

Co-contaminants such as organic pollutants or microbiological species can also influence the adsorption of heavy metals by ZIF-8 materials. ZIF-8 has hydrophobic pores that can adsorb organic molecules (it was originally studied for gases and organics adsorption), so if organic contaminants like solvents or natural organic matter (NOM) are present, they might occupy pore space or surface sites. Zhou et al. (2019) examined simultaneous adsorption of Cu^{2+} and norfloxacin (an antibiotic) by ZIF-8 and found that ZIF-8 could uptake both, but interestingly, the presence of Cu^{2+} actually enhanced norfloxacin adsorption due to complex formation (the metal bridging the antibiotic to the framework), whereas norfloxacin slightly reduced Cu^{2+} uptake (Zhou et al., 2019). This suggests that in some cases, co-contaminants can interact synergistically. In general, high concentrations of NOM (humic substances) can foul adsorbents by blocking active sites. No specific study on NOM fouling of ZIF-8 is reported yet, but one can extrapolate from other adsorbents that NOM could compete through metal–humate complexation and by coating the ZIF-8 particles. A recent review (Nazir et al., 2025) noted that *real* wastewaters containing both heavy metals and dyes/pharmaceuticals require adsorbents that can handle mixed pollutants. ZIF-8 composites have an edge here: for instance, Xiong et al. (2021) developed a magnetic carbon@ZIF-8 that could simultaneously remove Cu^{2+} and a dye (Congo Red) – the dye was captured by π–π interactions with the carbon and ZIF-8 surface, while Cu^{2+} was adsorbed by ZIF-8 and the carbon's functional groups (Xiong et al., 2021). They found minimal interference between the two pollutants due to this division of labor. Another co-contaminant scenario is competing microbial presence: MOFs like ZIF-8 can have antimicrobial effects (due to Zn^{2+} release). In water treatment, if ZIF-8 leaches Zn^{2+} or if heavy metals are removed in ways that involve MOF degradation, the Zn^{2+} itself might act on microbes or be subject to uptake by biomass, altering the distribution of contaminants. However, these are complex interactions rarely explored in lab adsorption tests.

In summary, solution pH must be optimized to maximize adsorbent capacity while preserving ZIF-8's structure (often a range of pH 5–7 is chosen for cation removal, and pH ~3–5 for anion removal with appropriate composites). Competing ions at high concentrations can diminish performance: hardness cations or background electrolytes can occupy sites or reduce electrostatic attraction, and thus slightly more adsorbent or pretreatment might be required in hard water situations. ZIF-8 composites that use selective functional groups (e.g. ion-specific chelators) can mitigate competition – for example, a thiol group will bind Hg^{2+} even in a crowd of Ca^{2+} because of selectivity. Co-contaminant organics can either foul the adsorbent or in some designed cases be simultaneously removed. Some studies have demonstrated dual-function ZIF-8 systems (adsorbing both metal ions and dyes or antibiotics) (Zhou et al., 2019; Xiong et al., 2021), which is promising for treating complex waste streams. Ultimately, when translating ZIF-8 from lab solutions to real water, these interfering factors typically lead to a reduction in removal efficiency compared to ideal conditions. The extent of reduction depends on the water chemistry – e.g., extremely hard water or high TDS brines will see a more notable drop. For instance, Chen et al. (2023) found their ZIF-8/chitosan fiber still removed >90% of Pb^{2+} from a river water sample but required a slightly longer contact time than in DI water, likely due to competition from other ions. Therefore, understanding and addressing these factors (through adsorbent design and process engineering, like maybe pre-filtering NOM or adjusting pH) is key to successful application of ZIF-8 adsorbents in practice.

4.3. Influence of surface area, pore structure, and functional groups

The inherent properties of ZIF-8 and how they are tuned in derivatives have a direct impact on adsorption performance. Surface area and pore structure determine access and storage capacity for contaminants, while functional groups determine the strength and specificity of interactions with heavy metals.

Generally, a higher surface area and more accessible pore volume led to greater adsorption capacity for physisorption processes. ZIF-8 is highly porous, but much of its surface area is internal (within micropores). If heavy metal ions cannot easily penetrate these pores due to size or hydration, then the external surface area (and immediately accessible near-surface porosity) becomes the effective surface. Therefore, reducing ZIF-8 crystal size to nanoscale increases external surface-to-volume ratio and often improves uptake kinetics and capacity (Katz et al., 2018). Ding et al. (2017) showed that nanoscale ZIF-8 crystals had better adsorption of Pb^{2+} than larger crystals of the same material, likely because Pb^{2+} could only interact with outer layers in the larger crystals (Ding et al., 2017). Additionally, smaller crystals shorten diffusion paths if ions do enter pores. Pore size and structure: ZIF-8's micropores can exclude large, hydrated complexes. If target ions are partially excluded, creating a more open pore structure can help. Researchers have developed hierarchical ZIF-8 (with mesoporosity) to address this. Wu et al. (2014) synthesized a hierarchical ZIF-8 using amino acids as a templating agent, resulting in extra mesopores that significantly enhanced arsenate (As(V)) adsorption – the hierarchical ZIF-8 reached equilibrium faster and attained higher capacity than conventional microporous ZIF-8, because As(V) anions could access more of the internal framework via mesopore highways (Wu et al., 2014). Likewise, a study by Yang et al. (2023) on a montmorillonite@ZIF-8 composite found that optimizing pore structure (the composite had a micro-mesoporous network) led to improved Pb^{2+} capture compared to either pure ZIF-8 or clay alone, since Pb^{2+} could diffuse into the composite's interior where abundant sites were present (Yang et al., 2023). In summary, introducing mesopores or larger apertures (via templating, creating defects, or composite structuring) in ZIF-8 tends to improve performance for larger or strongly hydrated ions by alleviating diffusion limitations and providing additional capacity.

Perhaps the most critical factor for heavy metal adsorption is the presence of functional groups that can strongly bind the target ions. ZIF-8's base framework provides nitrogen donors (the imidazole rings) which, as discussed, have decent affinity for many divalent metals. However, these may not always be accessible (if buried in pores) or optimal for certain metals. Therefore, adding functional groups like –NH_2, –COOH, –SH, and others has been a key strategy. Each functional group can impart selectivity or enhanced affinity: e.g. thiol (-SH) is famous for Hg^{2+}, amine (-NH_2) for capturing Cu^{2+} and Pb^{2+} (via soft Lewis base interactions), carboxyl (-COOH) for chelating with Pb^{2+}, Cu^{2+}, and also exchanging with cations. Shen et al. (2020) demonstrated that doping ZIF-8 with Co/Ni introduced possibly some –OH or unsaturated sites in the structure that increased Pb^{2+} adsorption by providing additional binding modes (Shen et al., 2020). They noted changes in surface functional groups via XPS after doping. Ligand functionalization prior to MOF formation is another route: e.g. synthesizing ZIF-8 with a mix of 2-methylimidazole and 2-aminomidazole yields a ZIF-8 variant with –NH_2 groups lining the pores. Zhang et al. (2016) mentioned that such functionalized ZIFs can have enhanced Cu^{2+} uptake (though pure 2-aminomidazole leads to ZIF-67 structure typically). Instead of modifying the framework itself, composite functional groups (from polymers, etc.) are highly effective. In alginate or chitosan composites, as previously noted, –COO^- and –NH_2 on those biopolymers are major active sites (Feng et al., 2024; Chen et al., 2023). These groups can coordinate with metals in bidentate fashion (especially carboxylates, which can chelate a metal ion). The synergy arises when ZIF-8's presence keeps those polymer groups well-dispersed and possibly concentrates metal ions near them via ZIF's adsorption. For example, Chen et al. (2023) found that a chitosan/hydroxyapatite fiber by itself removed Pb^{2+} moderately, but when ZIF-8 was grown on it, the removal shot up. This is likely because ZIF-8 pre-concentrated Pb^{2+} from solution (via rapid adsorption on its surface), then Pb^{2+} could complex with nearby –NH_2 on chitosan and –PO_4 on hydroxyapatite strongly, achieving a high overall uptake.

If the MOF is part of a composite with another metal (like Fe_3O_4 or nano-Fe, MnO_2, etc.), those provide specific adsorption or redox sites too. For instance, Fe_3O_4 in a Fe_3O_4@ZIF-8 composite can offer ferrous/ferric surface sites that bind arsenate or chromate strongly (via inner-sphere complexes), complementing ZIF-8's abilities (Huang et al., 2022). Similarly, a MnO_2@ZIF-8 core–shell (Lu et al., 2024) combined the high Sr^{2+} adsorption capacity of δ-MnO_2 (via ion exchange) with the shell's porosity; the ZIF-8 shell didn't directly bind Sr^{2+} strongly, but it improved dispersion and prevented aggregation of MnO_2, resulting in a composite that removed Sr^{2+} efficiently (Lu et al., 2024).

Structural stability vs functionalization: It should be noted that some functionalization (especially heavy doping or creating many defects for mesopores) can reduce the crystallinity or stability of ZIF-8. So, there is a balance, with a slightly defected or mesoporous ZIF-8 might adsorb more initially, but could be more prone to structural collapse after multiple cycles or in certain pH. Similarly, adding too many functional groups can block pores (e.g. excessive polymer coating might cover ZIF-8's surface and hinder access to internal sites). Therefore, the goal is often to optimize functionalization such that enough active groups are present to capture metals, without negating the high surface area and pore accessibility of the MOF. For example, a thin polymer coating (a few nm PDA) was optimal: it improved Pb adsorption 2–3× but did not significantly impede diffusion (Sun et al., 2018). In contrast, a thick polymer layer might turn the composite essentially into an ion-exchange resin with MOF filler, potentially losing the MOF's contribution.

In conclusion, improving surface area (through nanoscaling or creating mesoporosity) tends to increase the effective capacity and speed of heavy metal uptake by increasing accessible sites. Tailoring pore structure can make ZIF-8 adsorb a wider range of contaminants by admitting larger species. Introducing functional groups—either directly into the MOF or via composites—is arguably the most impactful enhancement, as it directly boosts the binding strength for target metals. Indeed, many of the highest performing ZIF-8-based adsorbents in literature are composites or modified versions rather than pure ZIF-8. For instance, a recent study (Li et al., 2024) showed a magnetically functionalized MOF (UiO-66-NH_2 with iron oxide) could remove Cd^{2+} almost completely from wastewater due to cooperative functional sites, a principle that likely applies to ZIF-8 analogues as well. By judiciously combining ZIF-8's excellent baseline properties with added porosity and functional groups, researchers have achieved materials that retain high capacity even in competitive environments and that can target specific metals with high selectivity and efficiency.

4.4. Regeneration, recyclability, and practical applications

For an adsorbent to be viable in real water treatment, it must not only remove contaminants effectively but also be regenerable and reusable over multiple cycles and be deployable in practical forms (e.g. in packed columns, membranes, or batch reactors). Thus, the focus here is on how ZIF-8-based adsorbents perform in reuse cycles, what methods can regenerate them, and considerations for scaling and application.

4.4.1. Regeneration and recyclability

Pure ZIF-8 can often be regenerated by rinsing with an appropriate eluent that removes the adsorbed metal ions. Common regenerants include acid solutions (to protonate sites and dissolve metal cations), chelating agents like EDTA (to strip metals off by complexation), or salt solutions (to drive ion exchange with a high concentration of competing ions). The choice depends on the mechanism of adsorption. For instance, if ion exchange was predominant, a concentrated NaCl or $CaCl_2$ wash might recover some Zn in exchange for the heavy metal – though this can be tricky as it might also partially dissolve the MOF. If coordination was key, a low-pH acid rinse (e.g. 0.1 M HCl) can protonate ligands and release the metal into solution (Sun et al., 2018). Several studies have reported on reuse of ZIF-8 adsorbents: Zhao et al. (2015) found that ZIF-8 could be reused for three cycles of Ni^{2+} adsorption with only a minor drop in capacity when they regenerated with dilute HCl each time, indicating decent stability. However, in other cases, especially with stronger binding metals, regeneration can be incomplete. For example, Zhou et al. (2019) noted that after adsorbing Cu^{2+} and norfloxacin, a portion of Cu remained in the ZIF-8 structure even after acid washing, likely because some Cu^{2+} had exchanged into the framework or precipitated, making full recovery hard (Zhou et al., 2019). This points to a secondary pollution challenge. If Zn^{2+} was released or the MOF degraded, the spent regenerant will contain those species. Zhou et al. (2025) emphasized that effective regeneration strategies must be developed to prevent such secondary pollution and maintain economic viability. One strategy to improve regenerability is to use ZIF-8 in composite form where the heavy metal is predominantly bound to a functional polymer that can be easily stripped. For instance, chitosan–ZIF-8 composites can be regenerated by acid or EDTA which primarily cleans the chitosan sites, and the ZIF-8 is indirectly freed as well (Chen et al., 2023). Polydopamine coatings allow for mild regeneration (like using a slightly basic solution with a chelator) to remove metals without dissolving the MOF core, since PDA can handle multiple pH swings (Sun et al., 2018). Magnetic composites like Fe_3O_4@ZIF-8 also assist regeneration by easy separation; after desorption, you can magnetically recover the particles to reuse. Still, ZIF-8's framework can suffer gradually over cycles if the regeneration solution is harsh (e.g. repeated acid baths might slowly leach Zn or break linkers). Some studies show a reduction in surface area or crystallinity after multiple adsorption/desorption cycles (Begum et al., 2020 noted slight XRD peak broadening after 5 cycles for their composite). Thus, improving stability via modifications (e.g. polymer coating that also acts as a protective layer) is beneficial for longevity. From a practical view, achieving at least 5–10 cycles with minimal capacity loss is desirable for adsorbent cost-effectiveness. Chee et al. (2023) demonstrated a ZIF-8 membrane for Pb^{2+} that could be regenerated 5 times by EDTA washing with <10% decline in flux and capacity, which is promising for real operations (Chee et al., 2023).

4.4.2. Practical application forms

Using ZIF-8 powder in real water treatment would pose issues with separation and pressure drop in columns. Therefore, researchers have developed various application forms: one is embedding ZIF-8 in membranes or coatings. For example, Chee et al. (2023) fabricated a ZIF-8/polymer composite membrane on a ceramic support that can filter water and simultaneously adsorb Pb^{2+} (Chee et al., 2023). This kind of integration means water flows through a porous membrane where ZIF-8 crystals are embedded or coated, capturing metals and allowing clean water through. The advantage is that it combines filtration and adsorption in one step and ZIF-8 is immobilized, preventing particle leakage. Another approach is making granular or bead forms, such as chitosan–ZIF-8 beads. Similarly, others have made pellets or extrudates by mixing ZIF-8 with binders (Nazir et al., 2025). These can be packed in columns for continuous flow treatment. Magnetic composites allow deployment as a suspension followed by magnetic recovery (Jiang et al., 2021), which can be useful in batch treatments of contaminated water or wastewater (like a stir tank where you add the adsorbent, then magnetically pull it out). Some studies have done mini-column experiments. For instance, Wang et al. (2020) packed a ZIF-8/fly-ash composite in a column and successfully treated a $Cu^{2+}/Zn^{2+}/Ni^{2+}$ mixture, showing sharp breakthrough after a certain volume, similar to standard ion-exchange resins (Wang et al., 2020). The presence of fly-ash (a low-cost support) in that composite also addressed cost and mechanical strength for packing.

4.4.3. Challenges in real systems

Real water matrices not only have competing ions (addressed in Section 4.2) but also issues like biofouling, scale formation, and pressure drop if the adsorbent is fine. MOFs like ZIF-8, if not protected, could be susceptible to biofouling (microbes might colonize the material over time, clogging pores or consuming the organic linker in worst case). Using MOFs in conjunction with biocidal components (like incorporating silver or using the natural antimicrobial property of Zn^{2+}) might mitigate fouling. Also, periodic backwashing or chemical cleaning might be needed, which means the adsorbent must withstand those processes. ZIF-8 might not handle strong chlorine cleaning (as chlorine could potentially attack the organic linker), so alternate cleaning methods (like citric acid or UV) might be preferred in a full-scale system to avoid MOF degradation. Secondary Zn release: If ZIF-8 does leach some Zn^{2+} during use, one must ensure the effluent Zn concentration stays within regulatory limits (typically ~5 mg/L for drinking water as a secondary standard). In well-buffered waters at pH 7, Zn from slight ZIF-8 dissolution might precipitate as $ZnCO_3$ or $Zn(OH)_2$, or be adsorbed back onto surfaces, but it's an aspect to monitor. Chen et al. (2021) in a pilot found Zn leaching was negligible when ZIF-8 was embedded in a polymer matrix, since the polymer likely trapped any Zn that tried to escape.

4.4.4. Economic and environmental considerations

On the practical side, the cost of ZIF-8 synthesis has historically been high due to ligand cost and solvothermal processes. However, with improved methods (room temp, water-based, recyclable solvents), the production cost is coming down (Nazir et al., 2025). Some estimates put MOF production at tens of dollars per kg (for simpler MOFs at large scale) (Boyd et al., 2021). ZIF-8's ligand (2-methylimidazole) is relatively cheap (~$50–100 per kg at bulk), and Zn is cheap, so raw material cost could allow MOF cost around ~$20–50/kg at scale (Chakraborty et al., 2022). That is still higher than activated carbon (~$5–10/kg) or ion exchange resins (~$10–20/kg), but if the performance (capacity, selectivity) is sufficiently higher or if it enables multi-contaminant removal, the cost could be justified. Also, ZIF-8 can potentially be regenerated and reused many times, spreading out its cost. Environmentally, using ZIF-8 for water treatment introduces the spent adsorbent disposal question: after many cycles when it's exhausted, it now contains heavy metals. One advantage is that ZIF-8's decomposition (by heating or acid) can immobilize metals into a smaller volume. For instance, one could collect spent MOF and then calcine it – it will convert to ZnO (or ZnO+metal oxide mixture) and trap some metals in that matrix, which could then be landfilled or recycled (e.g. smelted to recover metals). Alternatively, encapsulating spent MOF in cement (as Yang et al. (2023) proposed, using waste ZIF-8 in cement) is a way to immobilize heavy metals safely (Yang et al., 2023). They found that loading used ZIF-8 into cement did not significantly harm cement strength and the metals were locked in the concrete matrix. This kind of secondary reuse can be an attractive disposal method, turning hazardous waste into construction material (as long as leaching tests confirm stability).

4.4.5. Field testing

To date, applications of ZIF-8 outside the lab are limited, but some pilot studies are emerging. For example, Li et al. (2021) tested a ZIF-8 composite in treating mining wastewater containing Pb and Cd, the composite reduced Pb^{2+} from ~5 mg/L to <0.01 mg/L and Cd^{2+} similarly to trace levels, meeting discharge standards, and could be regenerated on-site with acid (Li et al., 2021). This demonstrates feasibility in a complex matrix (the mine water had Ca, Mg, sulfate, etc. too). Another case is point-of-use filters: small sachets of MOF or MOF-infused porous beads could be used in remote areas to remove arsenic from well water. Because ZIF-8 has high capacity for as when functionalized with iron or other groups, a compact filter could treat thousands of liters before needing replacement (Wang et al., 2018).

ZIF-8-based adsorbents can be made practically usable through thoughtful design: forming stable composite beads, membranes, or magnetic powders that are easy to handle and regenerate. They have shown promising recyclability, although maintaining performance over many cycles requires preventing MOF degradation. The integration of ZIF-8 into existing water treatment infrastructure (like as a polishing step after primary treatment, or as part of hybrid filtration systems) seems very plausible. Moving forward, demonstrating longevity and consistent performance in real water conditions (with fluctuating pH, various competing substances, microbial load) will be key. The trends are encouraging as many composite forms are showing the robustness needed, and regeneration studies suggest that with proper methods, ZIF-8 adsorbents can indeed be reused multiple times without significant loss of capacity (Zhou et al., 2025). This enhances the economic viability and sustainability of using advanced MOF adsorbents in water purification.

5. Current Limitations And Future Research Directions

5.1. Challenges in Real Water Systems

Despite the promising performance of ZIF-8-based materials in controlled laboratory studies, several challenges must be addressed before they can be reliably used in real, complex water systems. One major issue is the gap between ideal lab conditions and field conditions. Lab tests often use synthetic solutions with a target metal ion and perhaps a simple background electrolyte, whereas real waters (e.g. groundwaters, industrial wastewaters, surface waters) contain a slew of other components, including hardness ions, natural organic matter, colloidal particles, biological organisms, and fluctuating pH and temperatures. These factors can impair the adsorption performance. For example, natural waters rich in calcium and magnesium can significantly compete with heavy metal ions for adsorption sites on ZIF-8, reducing capacity (Li et al., 2021). Additionally, natural organic matter (NOM) can coat the adsorbent (fouling it) or complex with heavy metals to form larger organic-metal complexes that may not fit into ZIF-8's pores. In a river water sample containing humic substances, one might observe a slower uptake or lower removal efficiency for lead using ZIF-8 than in a NOM-free lab sample, due to these effects. Another challenge is pH variability, with many lab studies optimize pH for maximum removal (typically neutral or slight acidic for cation removal), but real waste streams can be strongly acidic (e.g. mine drainage with pH 3–4) or basic (e.g. certain industrial effluents). ZIF-8, as noted, is unstable in pH < ~4.5. In strongly acidic waters, direct application of ZIF-8 would lead to MOF decomposition and release of Zn^{2+} (Zhou et al., 2025). This is clearly a limitation – in such cases either the water must be pre-neutralized or ZIF-8 must be protected via composites/coatings. For instance, a challenge is treating acid mine drainage (AMD): AMD is low pH and high in metals like Fe, Cu, Zn, etc. ZIF-8 alone would dissolve, adding Zn to an already zinc-rich drainage. One possible solution is to first raise the pH of AMD (which often precipitates iron and partially treats the water) and then apply ZIF-8 for polishing remaining metals, but that adds process complexity. In real systems, secondary pollution is a concern: if ZIF-8 is not completely stable, it may leach 2-methylimidazole or Zn^{2+} into the treated water. While Zn^{2+} is not as toxic as Pb^{2+} or Hg^{2+} (and often permissible at <5 mg/L in drinking water for taste reasons), it is still an unwanted contaminant if introduced. Studies have shown that ZIF-8 can maintain structural integrity in neutral pH water for extended periods (days) (Malekmohammadi et al., 2019), but over weeks or in the presence of CO_2 (forming carbonic acid) some Zn leaching could occur (Kundu et al., 2021). Real water also contains microbes – biofouling is thus a challenge: MOF surfaces could be colonized by bacteria or algae, which not only block adsorption sites but might also metabolically produce acids or ligands that attack the MOF. There is little published on biofouling of MOFs yet, but one can anticipate the need for antifouling measures (perhaps periodic chlorination or UV). However, ZIF-8 might not tolerate strong chlorination – chlorine could oxidize the organic linker. This points to a challenge of integrating MOFs into existing chlorinated water systems. Perhaps periodic mild disinfectants or backwashing with biocides that do not harm the MOF need to be developed.

Another limitation is adsorbent longevity and mechanical stability in real flow systems. Many MOF adsorbents are fine powders. Using them in a packed bed can cause a high pressure drop and risk of washing out particles. Granulating the MOF (by binders or growing on supports) can solve this, but ensuring that the composite granules have good abrasion resistance and don't break under flow is important. ZIF-8 crystals themselves are quite robust (because of strong Zn–N bonds), but in composite form the overall particle might be weaker depending on the binder. For example, a polymer-bound ZIF-8 bead must endure expansion/contraction under varying water chemistries and the shear of water flow. Without sufficient mechanical testing, there's risk of attrition – leading to MOF fine particles in effluent or clogging of filters.

Scale-up and cost-related challenges also come under real-system considerations. While the raw materials of ZIF-8 (Zn and Hmim) are not extremely expensive, producing MOFs in large volume reliably is non-trivial. Consistency in crystal size, avoiding framework defects that might reduce stability, and preventing contamination are needed for mass production. Recent work (Nazir et al., 2025) indicates progress in scale-up, but to outfit a full-scale water treatment plant with MOF adsorbent, one needs perhaps hundreds of kilograms to tons of material, which has not yet been demonstrated for ZIF-8 specifically. The energy and chemical footprint of making MOFs could be another concern in a sustainability context. Traditional solvothermal methods consumed a lot of solvent and energy; newer aqueous/room-temp methods mitigate that (Li et al., 2021), but these must be implemented industrially. If MOFs are to replace or supplement conventional adsorbents, their overall life-cycle impact must be competitive. For instance, activated carbon is made often from waste biomass at relatively low cost; MOFs should ideally leverage inexpensive precursors or even waste sources (some research is exploring using industrial waste streams as metal/linker sources for MOFs).

Regulatory and safety issues might also arise. The use of an MOF in drinking water treatment might face regulatory scrutiny since MOFs are a relatively new class of materials. Regulators would want to ensure that no harmful components leach out (the ligand, if it leaches, is a chemical that would have to be evaluated for safety as imidazole compounds can be irritants at high levels, though 2-methylimidazole has low acute toxicity). In wastewater treatment, leaching is less of a concern because the water is not for consumption, but in drinking water it's critical. Additionally, spent MOFs containing heavy metals must be handled as hazardous waste unless the metals can be recovered or immobilized safely. This means treatment plants would need protocols for MOF disposal or regeneration fluids disposal. For example, a plant using ZIF-8 to capture arsenic will generate arsenic-laden MOF; perhaps that MOF can be regenerated and reused many times, but eventually it will be spent and loaded with arsenic – it then must be either processed to recover arsenic or stabilized (like vitrification or encasing in concrete) and disposed in a hazardous waste facility.

In groundwater remediation in situ, for example, injecting a powdered MOF into an aquifer to bind metals might sound intriguing, but retrieving the particles would be nearly impossible, thus, likely impractical. Instead, permeable reactive barriers with MOF embedded could be thought of, but MOFs might not yet be cost-effective for filling large subsurface barriers. Similarly, in industrial point-source treatment, MOFs would be used in columns or tanks that are more straightforward environments, but they can have extreme conditions (like plating waste may have $pH < 2$ and high chloride). ZIF-8 in high chloride solutions is generally stable, but at low pH plus high chloride (which can complex Zn), dissolution could accelerate. Also, chloride or other anions might compete strongly with MOF for certain cationic metals by forming complexes (e.g. $HgCl_4^{2-}$ might form, which is an anion and then the MOF would need to capture that as an anion rather than Hg^{2+} cation). This interplay of speciation in real chemical matrices is complex for MOFs. These materials often have not been tested under the full range of redox and speciation states. For instance, Cr could exist as Cr(III) or Cr(VI) in industrial effluents; ZIF-8 might remove one form well and not the other. If a mixture exists, consistent performance requires addressing both – maybe by a pre-reduction step or combining MOF with a reductant (as some composites do).

In summary, the key challenges in real systems are stability (chemical and mechanical), fouling and competition, ensuring no MOF-derived contamination, and integration into process flows. Addressing these requires multidisciplinary efforts: materials scientists to improve MOF composites (more stable, fouling-resistant), chemical engineers to design contactors (e.g. fluidized beds for MOF beads to minimize pressure issues), and environmental engineers to plan around MOF limitations (like pre-treatment steps for pH or hardness if needed). Encouragingly, many of these issues are being recognized. Zhou et al. (2025) explicitly list the needs verifying performance in real wastewater and developing methods to prevent secondary pollution. As more pilot tests occur, we will gain insight into MOF behavior outside the lab. Overcoming these challenges will determine whether ZIF-8 remains a laboratory curiosity or becomes a practical tool for heavy metal remediation in the coming years.

5.2. Environmental and Economic Considerations

When evaluating ZIF-8-based adsorbents for heavy metal remediation, it's important to consider their environmental footprint and economic viability in comparison to conventional technologies. From an environmental standpoint, one concern is the life-cycle impact of producing and using ZIF-8. MOF synthesis historically involves organic solvents (e.g. methanol, DMF) and can generate chemical waste. However, recent advances have aimed to "green" the synthesis, including room-temperature aqueous routes, mechanochemical synthesis, and solvent recycling can substantially cut down the waste and energy usage (Li et al., 2021; Głowniak et al., 2021). For example, if ZIF-8 is synthesized in water or ethanol at ambient conditions with high yield, the process might be comparable to making ion-exchange resins, which also involve organic chemicals and some waste. Still, a comparative assessment by Batista et al. (2020) noted that some MOFs have higher embedded energy per kg than traditional adsorbents, largely due to ligand synthesis steps. 2-methylimidazole is produced from readily available feedstocks (acetone cyanohydrin and ammonia, typically), which is not extremely energy-intensive. A rough estimate suggests that the carbon footprint of 1 kg of ZIF-8 might be on the order of a few tens of kg CO_2, whereas activated carbon might be <10 kg CO_2 per kg (depending on production method). This gap could narrow with improved MOF production at scale. Thus, while MOFs might have a higher initial environmental cost, their potentially superior performance could offset this if they achieve longer lifetimes or higher efficiencies (Wang et al., 2018). For instance, if a MOF can treat twice the volume of water per unit mass compared to activated carbon, then its higher production footprint is justified by the usage phase benefits (lower overall adsorbent consumption).

Another environmental consideration is the disposal or regeneration of spent adsorbents, as mentioned. If regeneration is feasible and MOF can be reused many times, then the environmental burden per volume treated decreases. Conversely, if the MOF is single-use due to fouling or one-time application, that could be problematic, not only due to cost but also hazardous waste generation. A spent MOF loaded with heavy metals is itself hazardous. Landfilling such material could risk leaching of the heavy metals and possibly the ligand. Ideally, spent MOF would be either recycled (metals recovered, perhaps by destroying the MOF in acid and then precipitating metals for recovery, and possibly reusing the Zn or ligand) or stabilized (e.g. incorporated into glass or cement as discussed). Both routes have environmental impacts (recycling uses chemicals/energy, stabilization uses resources). So, the most sustainable approach is to maximize regeneration cycles and minimize how often the MOF itself becomes waste. Encouragingly, many ZIF-8 composites have shown ability to sustain ~5–10 cycles with minimal performance loss (Sun et al., 2018; Chee et al., 2023). Further research might extend this to dozens of cycles by improving stability (Nazir et al., 2025). If one MOF batch could be reused, say, 50 times before replacement, the per-use environmental impact and cost drop dramatically.

One promising economic strategy is to create composite adsorbents that reduce the MOF content needed. For example, embedding a small amount of ZIF-8 in a cheap matrix (like a polymer or a porous silica) could dramatically cut costs. If a composite has, say, 20% ZIF-8 by weight and 80% cheap support, and still achieves most of the performance, the effective cost per kg is largely dictated by the support (often negligible cost if something like fly ash is used (Wang et al., 2020)). Many studies have indeed used industrial wastes or low-cost materials as supports – e.g. fly ash, bentonite clay, biochar – to form MOF composites (Yang et al., 2023; Wang et al., 2020). These support not only lower costs but can improve mechanical strength and processing ease. Another approach to cost reduction is using cheaper linkers or metals: ZIF-8 is already relatively cheap among MOFs, but maybe a similar framework (like ZIF-67 using Co) might be more expensive (Co is pricier than Zn). So, sticking with Zn is good. Possibly using mixed-linker strategies to incorporate even cheaper ligands? However, 2-methylimidazole is already simple. Some researchers have explored using bio-derived imidazoles or waste-derived amines to form MOF linkers (Morar et al., 2021), which could eventually lower costs if scaled.

Using ZIF-8 could mitigate environmental issues by enabling compliance with stricter standards. For example, arsenic standards (10 µg/L in drinking water) are hard to meet with conventional iron-based adsorbents in some cases; a ZIF-8 composite might consistently get below that, protecting public health (Liu et al., 2018). Similarly, if MOFs allow heavy metal removal without adding chemicals (like not needing to add lime and produce sludge as precipitation does), that avoids generating large volumes of sludge that need disposal. So, MOFs could reduce secondary waste compared to precipitation/flocculation methods, instead of tons of sludge, you have a smaller amount of spent MOF or concentrated regenerant solution. This is an environmental plus, less solid waste, and the metals are more concentrated making metal recovery more feasible. On the downside, if a MOF adsorbent breaks or leaches, introducing fine MOF particles or ligands into the environment could be problematic. 2-methylimidazole is not known as a major toxin, but it is an organic base that could exert some oxygen demand or be a micropollutant if released. Ensuring minimal leaching is both a performance and environmental requirement.

Another consideration is resilience and robustness, that environmental conditions can vary, and a robust adsorbent should handle that. For example, a community water system should not require frequent tweaking of pH or replacement of material if the source water chemistry shifts slightly. MOFs are currently somewhat sensitive (e.g., they might degrade if a contaminant in water unexpectedly triggers reaction). Ensuring robust performance under variable conditions will be needed for real world trust. This ties into future research directions in Section 5.3 about hybrid technologies that can combine MOFs with other processes to mitigate such issues.

Lastly, public and regulatory acceptance might require demonstrating that MOF-based treatment is safe and effective long-term. Pilot projects showing a MOF system treating, say, mining wastewater continuously for months, or a drinking water plant using a MOF-based filter for a year with consistent results, would go a long way. Without such demonstrations, stakeholders may hesitate to adopt unfamiliar material when tried-and-true methods exist.

In summary, environmental and economic considerations present a mixed picture. On one hand, ZIF-8 offers high efficiency that can lead to cost savings, with less adsorbent or achieving compliance without multi-step treatment, and environmental benefits, with less sludge, multi-contaminant removal. On the other, its production and use need optimization to be cost-competitive and environmentally benign that are green synthesis, minimal leaching, and end-of-life management. As research continues, it's likely the cost will come down (through scale and composites) and environmental footprint will shrink (through greener methods and reusability). Given the rapid advancements, ZIF-8 and similar MOFs could soon be engineered such that their advantages outweigh their costs in a life-cycle sense. For example, if a MOF lasts 10× longer or has 5× capacity of an activated carbon, you might end up using less material overall, offsetting the higher per-kg cost and footprint. Life-cycle assessment studies will be very valuable to quantify these trade-offs. Current indications (Wang et al., 2018; Wang et al., 2024) are that MOFs can be sustainable if regeneration is successful and if the materials are not treated as disposable. Thus, focusing on durability and reusability is key to their economic and environmental feasibility.

5.3. Future Perspectives on Scaling and Hybrid Technologies

The field of MOF-based heavy metal adsorbents is rapidly evolving, and several future directions can be envisioned to address current limitations and extend the capabilities of ZIF-8-based materials. One important avenue is scaling up production and deployment. As discussed, developing cost-effective, large-scale synthesis methods is critical. Future research will likely refine continuous or flow synthesis of ZIF-8 (Chakraborty et al., 2022), perhaps using modular reactor systems where metal salt and ligand continuously react to precipitate ZIF-8, which is then filtered and dried. This could dramatically lower unit costs and ensure batch-to-batch consistency. Additionally, the incorporation of ZIF-8 into industrial-scale forms (pellets, tablets, monoliths) will be a focus. For instance, 3D-printing or extruding MOF-polymer mixtures into structured adsorbents is a promising direction (Reta et al., 2023). This can produce monolithic blocks or lattice structures that fit into existing filter housings, eliminating issues of packing and pressure drop. Such structured MOF adsorbents have begun to appear for gas separations; applying them to water treatment is a logical next step.

Another frontier is hybrid technologies that combine adsorption with other treatment processes to create more robust or multifunctional systems. One concept is coupling ZIF-8 adsorption with membrane filtration in a unified process (Nazir et al., 2025). For example, a membrane could be coated with ZIF-8 (as in Chee et al., 2023) to simultaneously filter particulates and adsorb dissolved metals. Beyond passive membranes, one could envision MOF-based electrosorptive systems: ZIF-8 is non-conductive, but if combined with a conductive matrix (like carbon nanotubes or graphene), it could act as a high-capacity electrode in capacitive deionization (CDI) systems. Already, researchers Lim et al. (2024) incorporated MOF (not ZIF-8, but a similar concept) into an electrode for selective Li^+ removal. A similar approach might use a ZIF-8 composite electrode to capture heavy metal cations when a voltage is applied, potentially regenerating the electrode by reversing voltage. This merges adsorption with electrochemical regeneration elegantly. Another hybrid possibility is photocatalytic adsorption: integrating ZIF-8 with photocatalysts (Dai et al., 2021; Tamimzadeh et al., 2025). Imagine a composite of ZIF-8 with TiO_2 or Bi_2WO_6, where UV or solar light triggers reduction of a metal like Cr(VI) to Cr(III) and the resulting Cr(III) gets adsorbed by ZIF-8. Such a system could continuously degrade organics or reduce metal valences while the MOF adsorbs the products, effectively performing a “trap and transform” function. Some initial studies are pursuing ZIF-based photocatalytic hybrids for organic pollutants; extending that to combined organic/inorganic contaminant removal is a natural next step (Tamimzadeh et al., 2025).

Selectivity tuning is another future direction. While ZIF-8 is broad-spectrum in adsorbing many metals, future materials might be tailor-made for specific target metals by functional group design. For example, a thiolated version of ZIF-8 (with a fraction of linkers bearing –SH) could become a mercury-specific adsorbent in a sensor or for industrial effluent where mercury is the only concern. Alternatively, grafting molecules like crown ethers or specific chelators onto ZIF-8's surface could impart selectivity for certain metal ionic radii or charges (Manousi et al., 2019 have looked at MOFs with extractants). This moves MOFs towards a "smart adsorbent" concept where they preferentially remove one contaminant even in the presence of others – an ability very useful in mixed-contaminant scenarios where one metal is toxic at low levels, but others are benign at much higher concentrations.

Integration with existing infrastructure is also a good approach, rather than replacing current filters or adsorbers outright, MOFs might be used to retrofit or enhance them. For instance, coating a thin layer of ZIF-8 onto activated carbon particles could combine the advantages of both: the carbon provides macro/mesopore transport networks and low cost, while the MOF gives specific adsorption sites (Zhang et al., 2021's wood@ZIF-8 is analogous conceptually). These kind of hierarchical or composite adsorbents could be dropped into existing activated carbon filters to improve performance without major re-engineering.

A future goal is not only to adsorb heavy metals but to recover them as resources. MOFs may facilitate this by allowing milder recovery processes. For example, after ZIF-8 saturates with something like Cu^{2+}, one could potentially elute concentrated Cu which can be sent to a recycling unit (electrowinning or precipitation to sellable product). Some researchers have suggested designing MOFs that not only capture but then can release metals in a controlled way (Sustainable recovery loops). For precious metals (e.g. gold, palladium), MOFs could be an economical way to scavenge trace amounts from e-waste leachates or industrial baths and then yield them back by appropriate stimulus (like a certain wavelength or reagent that breaks the MOF–metal bond).

On the material science side, future ZIF-8 derivatives might focus on overcoming the water stability issue completely. There are other ZIFs (like ZIF-67 or mixed Zn/Co ZIFs) and post-synthetic modifications (coating ZIF-8 with hydrophobic ligands, etc.) that could yield a MOF almost impervious to hydrolysis even at lower pH. If such a material can be made without sacrificing adsorption capacity, it would be a change for MOF use in all pH ranges. Alternatively, creating MOF-polymer hybrid frameworks (where a polymer is intertwined or covalently linked with the MOF structure) might give a material that has the uniform pores of MOF but the flexibility and stability of a polymer (Sahu et al., 2025 discuss some MOF-polymer constructs). These could better withstand mechanical and thermal stress, making them more deployable in harsh conditions.

In terms of regulatory and practical implementation, future demonstrations will likely involve pilot plants testing MOF adsorbents in real-world conditions. Within the next decade, one could expect to see small community water systems or specialized industrial treatment units using MOF-based cartridges if current trends continue and cost barriers fall. Finally, digital and sensing integration is a forward-looking idea: MOFs like ZIF-8 can also be used in sensors (they change properties upon adsorbing metals). A future water treatment system could have MOF-coated sensor electrodes that continuously monitor metal concentrations, and MOF adsorbent beds that capture metals – an integrated approach where the MOF material serves dual roles. For example, a ZIF-8 film electrode might detect breakthrough of Pb^{2+} by a change in capacitance, signaling it's time to regenerate the main adsorber (Nazir et al., 2025 hinted at smart systems). This kind of smart integration would optimize use and ensure safety.

In summary, the future of ZIF-8-based materials for heavy metal removal is likely to involve scaling up to industrial quantities, enhancing stability and selectivity, and combining adsorption with other complementary processes. These hybrid and advanced approaches aim to harness the high capacity and tunability of MOFs while mitigating current drawbacks. If successful, they could lead to next-generation water treatment technologies that are more efficient, targeted, and adaptable than today's methods. Researchers are actively pursuing these directions: for instance, developing multi-functional MOF composites that can remove a spectrum of pollutants (heavy metals, plus organic dyes or microbes) in one step (Dai et al., 2021), or MOF-based devices that integrate with solar energy to drive pollutant removal (e.g., MOFs that adsorb metals by day and release them by a triggered mechanism at night for recovery). The coming years will reveal which of these innovations prove practical at scale. Given the pace of MOF research, it is reasonable to expect that many of the challenges currently limiting ZIF-8's real-world use will be addressed, making MOF-based heavy metal remediation not just a lab curiosity but a commercially viable technology.

6. Conclusion

The past decade has witnessed significant advances in the development and application of ZIF-8 and its derivatives for the removal of heavy metals from water systems. With their high porosity, tunable surface chemistry, chemical stability, and ease of functionalization, ZIF-8-based materials have emerged as a powerful class of adsorbents capable of addressing the pressing need for efficient and selective water purification technologies. Through systematic investigation, it is evident that mechanisms such as ion exchange, surface complexation, electrostatic attraction, pore confinement, and redox-mediated reactions underpin the removal of a wide range of toxic metal ions, including Pb(II), Cd(II), Cr(VI), Hg(II), As(V), and Cu(II). Post-synthetic modifications, such as metal doping, polymer hybridization, and thermal carbonization, have further expanded the functional landscape of ZIF-8, enabling enhanced adsorption performance, improved selectivity, and better stability under realistic water conditions.

Despite these achievements, several challenges persist that limit the large-scale deployment of ZIF-8-based materials. These include hydrolytic instability in acidic or highly ionic environments, complex synthesis routes for some derivatives, and a lack of long-term performance data under continuous flow and real wastewater scenarios. Moreover, while numerous lab-scale studies demonstrate impressive removal efficiencies and recyclability, translation to field-scale systems remains limited and underexplored. Environmental impact, cost-effectiveness, and potential metal leaching also need to be more rigorously assessed to ensure safe and sustainable application.

Moving forward, research should prioritize the development of robust ZIF-8-based composites with improved water stability, lower synthesis cost, and scalable production methods. More interdisciplinary efforts are required to integrate these materials into hybrid treatment systems, such as membrane–adsorbent combinations or photo-assisted reactors. Real-world pilot studies must become more central to future work, alongside life-cycle assessment and regulatory alignment. Overall, ZIF-8-based materials hold considerable promise for next-generation water treatment technologies, provided that current barriers are systematically addressed through thoughtful design, testing, and application.

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Conflicts Of Interest

The authors state that there are no conflicts to declare.

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