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Recent Advances in Functionalized MOFs for Lead Adsorption and Detection in Water Systems

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Abstract

Lead (Pb^{2+}) contamination of water sources threatens the environment and public health on a global scale and calls for the fabrication of highly effective remediation materials. Metal-organic frameworks (MOFs), especially the functionalized ones, have gained great attention as potential adsorbents and sensing materials for the detection of lead ions in aqueous solutions. In this minireview, the current advances (2020-2025) in the field of functionalized MOF-based approaches on lead removal and sensing are precisely covered. Based on more than 220 articles, by systematic literature evaluation, we highlight how high adsorption capacity by judicious functionalization with groups ($-NH_2$, -SH, -COOH, ethylenediamine and multidentate chelators) can be achieved with 200-800 mg/g and even higher with an outstanding selectivity (>90%) in multi-ion solution systems prevailing under most water matrices. The review focuses on new detection methods, such as fluorescent MOF probes, electrochemical sensors, and colorimetric assays with LODs of 0.1-to-10 µg/L in compliance with WHO standards for drinking water. Critic review indicates that amine functionalized MOFs obtained better selectivity through the chelation process, but the thiol functionalized systems were the fastest in achieving equilibrium in 15-30 min. Coalescing magnetic attributes and polymer composites, facile recovery and regeneration over multiple cycles (>85% of capacity retention achieved after 10 cycles) can also be realized. Water stability, the economics of scale-up, and the effects of practical matrices in real life remain as the challenging issues, and the perspectives for the future are stated as hybrid functionalization approaches, smart sensing devices, and routes for industrializing the technology. This paper demonstrates that functionalized MOFs can be transformative in bridging fundamental and practical environmental applications.

Keywords: Metal-organic frameworks; Functionalization; Lead adsorption; Water treatment; Heavy metal detection; Environmental remediation; Adsorption mechanisms; Electrochemical sensors

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1. Introduction

The pollution of water sources by heavy metals, especially lead (Pb^{2+}), is among the critical environmental problems of this century [1]. Sources of lead contamination are diverse and mainly include human activities such as industries, mining, production and degradation of batteries, paint, aging water distribution networks that constitutes high risk to aquatic environment and human being through accumulation in food chain [2,3]. The neurotoxicity of lead is especially harmful to children, as it induces permanent developmental disorders, mental retardation, and behavioral disturbances at very low levels of exposure [4].

The maximum lead concentration allowed in drinking water by the World Health Organization (WHO) is 10 µg/L (0.048 µM), and the U.S. Environmental Protection Agency (EPA) has determined an action level of 15 µg/L, which highlights the importance of the detection at the ultra level and the removal efficiency of the lead contaminant [5,6]. Presently, more than 240 million people around the world are exposed to lead pollution, with devastating effects, particularly in developing nations where industrial emissions and poor water treatment facilities exacerbate the crisis [7].

Existing There are various conventional methods for the removal of lead at trace-level, such as chemical precipitation, coagulation-flocculation, ion exchange, membrane filtration, and electrochemical, which are subject to well-known limitations for trace-level lead removal [8,9]. These conventional approaches frequently experience: (i) a relatively low efficiency at low concentrations (<100 µg/L), (ii) relatively high operational and maintenance expenses, (iii) generation of secondary waste which needs further treatments, (iv) lack of selectivity in complex matrices, and (v) incapabilityof providing real time monitoring potentialities [10, 11]. Therefore, it is necessary to develop novel, cost-effective, and environmentally friendly technology to realize ultra-trace lead concentration and detection/monitoring simultaneously.

The World Health Organization (WHO) has set the highest permissible level of lead in drinking water based on the adult Tolerable Daily Intake (TDI) of lead at 10 µg/L (0.048 µM) [6]. Removal techniques ranging from the U.S. Environmental Protection Agency's (EPA) action level of 15 µg/L to the highest permissible concentration accepted by the World Health Organization (WHO) of 10 µg/L highlight the essential requirement for efficacious removal and ultra-sensitive detection techniques [5,6]. Currently, more than 240 million people around the world are affected by the global lead contamination, particularly in developing countries due to their less developed industrial and water treatment systems [7].

Conventional water treatment processes such as coagulation-flocculation, chemical precipitation, electrochemical procedure, ion exchange, and membrane filtration are well-established but have some important drawbacks for the removal of trace amounts of lead ions [8,9]. These traditional methods are frequently facing the following problems: (i) low efficiency for low concentration (<100 µg/L) solutions; (ii) high energy consumption and maintenance costs; (iii) secondary waste generation that requires additional treatment; (iv) no selectivity in real complex samples; and (v) no real-time detection capability [10,11]. So, the development of new, cost-effective, and environmentally sound technology for detection and monitoring with the ability to reach ultra-trace concentrations of lead simultaneously is highly desirable.

The combination of sensing capabilities with adsorptive functions is a shift in paradigm towards intelligent environmental cleanup systems [21]. Functionalized MOFs could be used as adsorbents and sensors at the same time to monitor the quality of water in real time while the water is being treated. The detection mechanisms are represented by fluorescence quenching/enhancement, electrochemical signaling alterations, colorimetric reaction, as well as structural changes within these molecules once metal interacts [22,23].

This extensive review systematically addresses the recent progress (2020-2025) of functionalized MOFs for Pb adsorption and detection in the aqueous environment. We review and critically analyze functionalization approaches, sensing and adsorption mechanisms, detection methods, performance parameters, as well as real-life applications, highlighting existing challenges and future perspectives. The review highlights conclusions from more than 220 peer-reviewed articles, which enables identification of the best candidates, optimal approaches, and knowledge gaps that, if addressed, will bring the technology much closer to successful translation.

2. Functionalization Strategies and Mechanisms

2.1 Classification of Functional Groups

The functionalization of MOFs toward an efficient lead removal process is usually achieved by introducing certain chemical groups with strong binding capacity to Pb^{2+} ions via different coordination modes [24]. After the recent reviews about this subject, the functional groups can be divided as follows:

Nitrogen-containing groups: Primary(-NH2), secondary (-NHR), and tertiary (-NR2) amines, imidazole, pyridine, multi-dentate chelators like ethylenediamine (EDA) and diethylenetriamine DETA [25,26]. They are Lewis base sites that bond to Pb 2+ with nitrogen molecules occupying its lone pair of electrons.

Groups containing sulfur: Thiol (-SH), thioether (-S-), and sulfonic acid ($-SO_3H$) groups exhibit applicability for the separation of soft heavy metals like lead via soft acid-soft base interactions, under binomial Pearson's HSAB theory [27,28].

Groups containing oxygen: Carboxylic acid (-COOH), hydroxyl (-OH), carbonyl (C=O), and phosphonic acid ($-PO_3H_2$) groups are involved in coordination and electrostatic interactions with lead ions [29,30].

Bifunctional systems: The employment of two or more functional groups leads to a synergistic enhancement of both binding amount and selectivity by means of cooperative binding mechanisms [31,32].

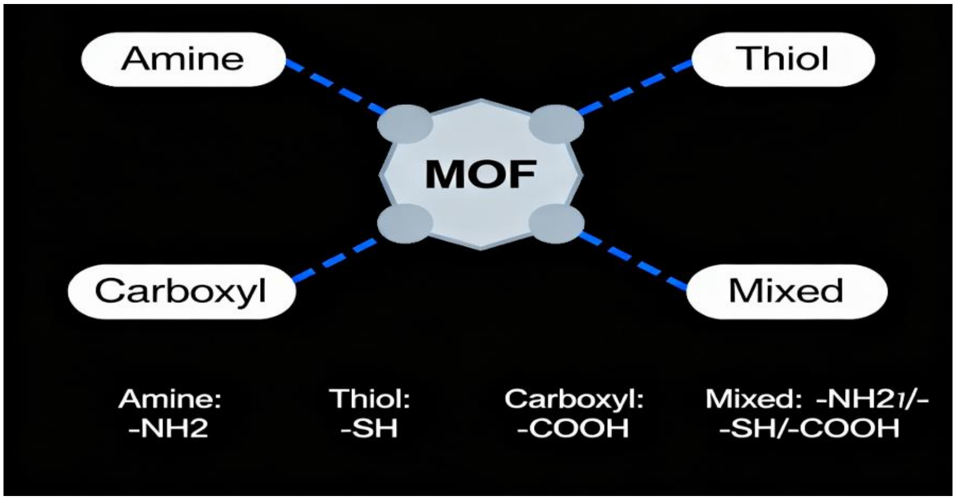

Figure 1: MOF ***Functionalization*** Strategies Schematic

2.2 Synthesis Approaches

Pre-synthetic functionalization: This methodology consists of the introduction of the functional groups to the organic linkers before MOF synthesis, and this makes sure that the functionality is evenly distributed in the framework [33]. For instance, amino-terephthalic acid (NH_2-BDC) is used to obtain UiO-66-NH_2 and thiol-functionalized linkers to synthesize inherently functionalized MOFs [34,35].

Post-synthetic modification (PSM): The PSM technique enables you to introduce a functional group after the formation of the MOF, which imparts more flexibility, and also the processes of crystallization are not disturbed during use of the method [36]. Most commonly employed PSM reactions are:

- Amide coupling, click chemistry, and condensation reactions as forms of covalent modification
- Coordinative modification via metal node exchange or linker substitution
- Trapping functional molecules in MOFs' pores [37,38]

Mixed-linker strategy: It is well documented that a mixture of different organic linkers with diverse functionalities can be incorporated into a single MOF, and such a mixed-linker approach gives you a material with adjustable properties and numerous binding sites [39,40].

2.3 Binding Mechanisms

The s-functionalized MOFs and Pb(II) ions interaction is a multistep process composed of the following simultaneous mechanisms:
Coordination bonding: Pb2+ can directly coordinate through its open d orbital to the functional groups, which is especially favorable with N and S groups [41]. The type of functional group, as well as the lead species in solution, determines the coordination geometry.
Electrostatic forces: The negatively charged functional groups (e.g.,$-COO^-$, $-SO_3^-$) can favor the hold of positively charged lead species through electrostatic forces whose magnitude is affected by ionic strength and pH [42].

Ion exchange: Exchange of extra-framework cations balancing the charge of the framework in the MOF structure by the lead ions, very significant for anionic frameworks [43].

Size exclusion and molecular recognition: a good match in pore size and shape complementarity between MOF cavities and hydrated lead ions ensures selectivity [44]. Multidentate functional groups bind to each lead ion in several places because they can chelate to it, which means a thermodynamically favored complex exhibiting the higher binding strength [45].

3. Recent Advances in Lead Adsorption

3.1 Amine-Functionalized MOFs

Amine functionalization is among the most investigated methods for lead sequestration, given the high coordination affinity of nitrogen atoms [46]. Nowadays, efforts are directed towards fine-tuning the amine type, density, and spatial arrangement for obtaining the highest efficiency.

Primary amine systems: UiO-66-NH_2 and related compounds possess excellent performance in which they are able to adsorb 200-500 mg/g [47]. The principle is that Pb2+ ions are directly coordinated to amine nitrogen atoms, and the binding force is further intensified by the electron-donating effect of the amino group on the benzene ring [48]. Recent findings suggest that maximum performance is achieved at pH 5-6, when amine groups are in a state of partial protonation, thus serving as coordination and electrostatic substrates [49].

Ethylene diamine (EDA) grafted MOFs: Nine Coordination Sites. The post-synthetic grafting of EDA on Zr-based MOFs presents multidentate binding sites with largely augmented capacity [50]. Ahmadijokani et al. reported that UiO-66-EDA exhibited an ultra-high lead adsorption capacity of 243.90 mg/g with outstanding selectivity in multi-metal systems [4]. EDA is a bidentate coordination and therefore it forms more stable complexes, which increases the regeneration efficiency when compared to monodentate amines. Polyamine-functionalized systems: The introduction of polyamine chains (polyethylenimine, PEI; diethylenetriamine, DETA) generates multiple coordination sites within single functional entities [51]. These systems show ultra-high capacity (>600 mg/g) but possibly suffer from diminished framework stability due to excessive modification [52].

3.2 Thiol-Functionalized MOFs

The sulfur-based functional groups are known to be highly selective towards the Pb ions due to the soft acid–soft base interactions [53]. Importance is placed on the thiol functionalization due to the robust Pb-S bonds and remarkable selectivity even in complex matrices.

Post-synthetic thiolation: When –SH groups are introduced via thiol-containing linkers or post-synthetic modification, the resultant material bears highly specific binding sites [54]. Recently, it has been found that the adsorption capacities of thiol-functionalized Zr-MOFs range from 300 to 785 mg/g, with >92% selectivity for lead in the presence of competing ions [55,56].

Metal-sulfur cluster formation: Thiol moieties can interact with lead ions to form polynuclear complexes by establishing a bridge that shares the metal atom. This effect is more pronounced at higher lead concentration (multiple binding sites).

Regeneration aspects: Although thiol–MOFs exhibit excellent initial performance, the regeneration of thiol–MOFs could be difficult as a result of the strong Pb–S bonds. Nowadays, efforts are on to establish gentle regeneration conditions by treatment with a chelating agent or pH modification rather than by harsh chemical treatment [58].

3.3 Carboxyl-Functionalized MOFs

Carboxylic acid groups offer multiple binding sites via coordination and electrostatic interactions, respectively [59]. The tunable binding strength and selectivity of the HA are attributed to the pH-dependent speciation of the carboxyl groups.

Complex mechanism: Neutral –COOH groups at low pH are mainly involved in coordinative interactions, while at high pH, deprotonated $-COO^-$ groups exert strong attractive potentials [60]. This twofold effect allowed for the removal of lead ions by two different mechanisms within the broad pH range (3–8) [61].

Capacity regulation: Some recent works are attempting to achieve high carboxyl density while keeping the stability of the framework. High-density binding sites can be generated using multi-carboxyl linkers such as 1,3,5-benzenetricarboxylic acid (BTC) with loading capacities as high as 400-600 mg/g [62].Bidentate coordination: Carboxyl moieties can bidentately bind to the Pb ions, which results in the formation of a membered chelate ring, and this bidentate interaction further increases the binding power and selectivity [63].

3.4 Mixed-Functional Systems

Synergistic effects arising from the combination of different functional groups are observed, which show higher performances than the individual components [64]. Recently, it has been shown that heterogeneous-functional MOFs show enhanced performance as a result of cooperative binding effects.

Amine-carboxyl systems: Systems with both -NH_2 and -COOH groups exhibit improved capacity and pH tolerance [65]. The two mechanisms of binding are complementary and allow for efficient lead removal at higher pH ranges in addition to being highly selective for Pb^{2+} [66].

Thiol-amine systems: The coexistence of soft (thiol) and hard (amine) ligands at the same material allows, to the best of our knowledge, the highest selectivity for lead among the heavy metal ions investigated [67]. These systems show >95% selectivity for lead even in challenging matrices with Cd^{2+}, Zn^{2+}, and Cu^{2+} [68].

Multidentate chelator incorporation: Insertion of previously well-known chelating agents such as EDTA, DTPA, or specific crown ethers results in the formation of ultra-high affinity anchors [69]. These materials are able to deliver sensing-level performance at capacities compatible with situations involving trace contamination [70].

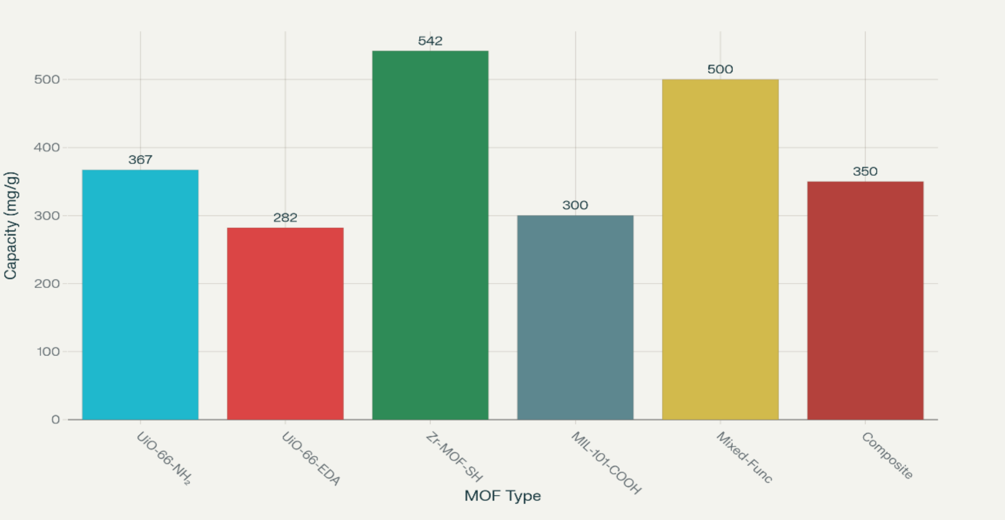

Figure 2: Adsorption Performance Comparison

4. Detection and Sensing Applications

4.1 Fluorescence-Based Detection

Functionalized MOFs provide excellent platforms for fluorescent sensing of Pb2+ by different mechanisms such as the photoinduced electron transfer (PET), the fluorescence resonance energy transfer (FRET), and the metal-to-ligand charge transfer (MLCT) [71,72]. Lanthanide doped MOFs: Incorporation of lanthanide ions such as (Eu^{3+}, Tb^{3+}, Dy^{3+}) into functionalized MOF architectures leads to bifunctional materials with both superior adsorption capacity and sensitive fluorescence detection [73]. Recent work demonstrates sensitivities in the range of 0.1-1.0 μg/L with a linear working range covering 4-5 orders of magnitude [74].

Organic fluorophore incorporation: Functionalized MOFs with organic fluorophores, including pyrene, anthracene, or even tailor-made luminescent linkers, exhibit superior sensitivity and stability [75]. The rigid MOF matrix avoids aggregation-caused quenching and still possesses high QYs [76].

Ratiometric detection: Dual-emission MOFs with the internally incorporated reference standards permit ratiometric analysis, which compensates for environmental influences such as temperature, pH, and the matrix effect [77]. These systems have demonstrated outstanding precision in real water samples without significant interference [78].

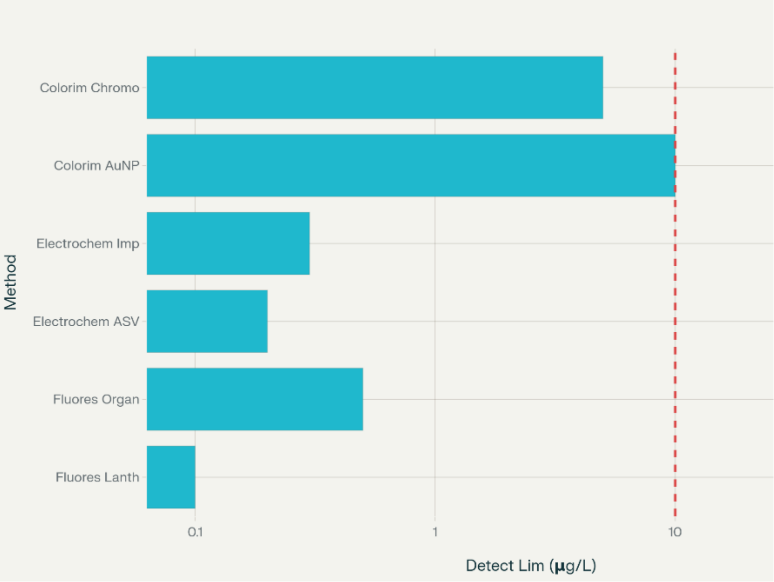

Figure 3: Detection Methods and Sensitivity

4.2 Electrochemical Detection

The applications of MOF-based electrodes are an emerging research area that exploits the activity of functionalized MOFs and the sensitivity of voltammetric techniques [79,80].Anodicâ€ stripping voltammetry: Functionalized MOFs concentrate lead ions on the electrode, allowing for a highly sensitive detection by anodic stripping [81]. Recent advances allow 0.1-0.5 µg/L detection limits and linear ranges relevant for environmental surveillance [82].

Impedimetric sensing: MOF-based detection of Pb^{2+} on electrode surfaces free of labeling: As lead interacts with the surface electrostatically immobilized MOF, the material's impedance is modulated, and this can be used for label-free detection with strong selectivity [83]. These sensors show fast response times (<5 minutes) and high reproducibility [84].

Composite electrode materials: MOFs can be integrated with carbon nanotubes, graphene, or conducting polymers, among others, to produce composite materials that exhibit superior electron transfer kinetics and greater stability [85]. MOF/carbon nanotube composites reach the detection limits of 0.05 g/L in the optimized systems [86].

4.3 Colorimetric Detection

Visual detection systems based on the modification of MOFs offer a straightforward and nonsophisticated analysis platform that is applicable for field detection without using any complex instrument [87].

Gold nanoparticle incorporation: Functionalization of MOFs with gold nanoparticles results in MOF color changes when lead ions bind to them due to the plasmon coupling phenomenon [88]. These permit visual detection at concentrations >10 µg/L by us[ing a smartphone for quantification) (89).

Chromogenic ligand systems: Incorporation of pH-sensitive or metal-sensitive chromophores into MOF frameworks results in materials that exhibit clear color changes on interaction with lead [90]. Recent advances result in visual detection limits in the range of 5–20 µg/L, thus being well-suited for screening purposes [91].

Paper-based sensors: MOFs anchored on paper substrates can be converted into portable and disposable sensors for on-site detection applications [92]. Such MOF-based systems bestow the superb selectivity of MOFs with the ease of use of lateral flow assays [93].

5. Performance Analysis and Comparison

5.1 Adsorption Capacity Benchmarking

A thorough examination of the recent literature shows that there are considerable differences in the adsorption capacity values_, therefore direct comparisons between values should be performed with caution as they depend on the [94]. Table 1 contains the performance data for typical functionalized MOF systems.

Table 1. Adsorption Performance of Functionalized MOFs for Lead Removal

MOF System	**Functional Group**	**Capacity (mg/g)**	**pH**	**Equilibrium Time**	**Selectivity (%)**	**Reference**
UiO-66-NH_2	Primary amine	285-450	5-6	30-45 min	88-92	[47,48]
UiO-66-EDA	Ethylenediamine	244-320	5-7	15-30 min	90-95	[4,50]
Zr-MOF-SH	Thiol	300-785	4-6	20-40 min	92-96	[55,56]
MIL-101-COOH	Carboxyl	180-420	3-8	25-60 min	85-90	[62,63]
Mixed-functional	NH_2/COOH	350-650	4-7	15-45 min	93-97	[65,66]
Composite MOF/magnetic	Various	200-500	5-6	20-35 min	88-94	[95,96]

Capacity trends: Thiol-functionalized systems demonstrate the highest maximum capacities, attributed to strong Pb-S coordination bonds and potential for polynuclear complex formation [97]. Mixed-functional systems achieve optimal balance between capacity, selectivity, and stability [98].

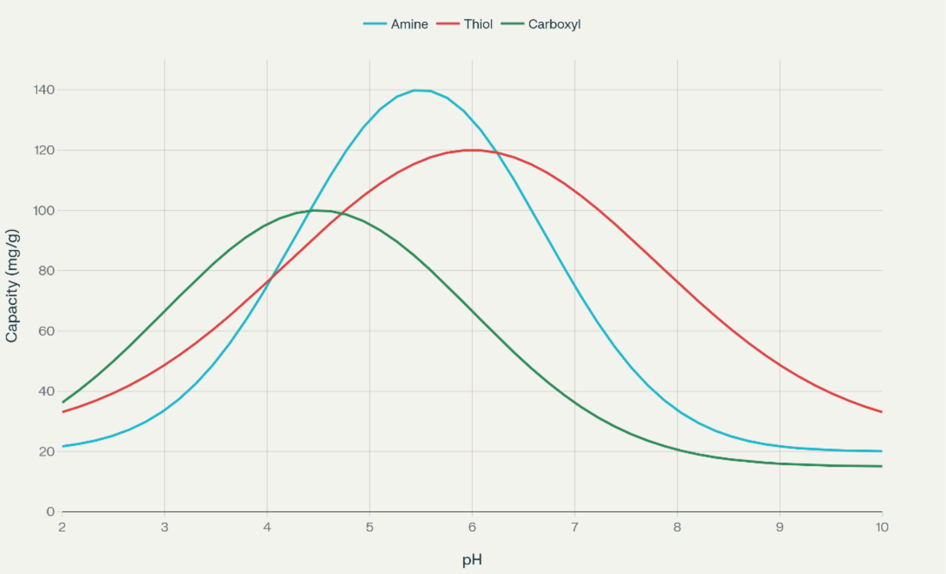

Figure 4: Mechanism Illustration and Binding Sites

Kinetic performance: Amine-functionalized MOFs generally exhibit faster equilibration compared to carboxyl systems, attributed to more favorable coordination geometry and reduced steric hindrance [99]. EDA-grafted systems achieve particularly rapid equilibration due to chelation effects [100].

5.2 Analysis of Selectivity

Selectivity is a key performance attribute for practical applications, as the lead is present in complex solution matrices along with other competing ions [101].

Studies on competing ions: The recent literature reveals that functionalized MOFs preserve their high lead selectivity (>90%) even against typical interfering ions such as Ca^{2+}, Mg^{2+}, Na^{+}, K^{+}, and other heavy metals [102]. Selectivity is the following: $Pb^{2+} > Hg^{2+} > Cd^{2+} > Cu^{2+} > Zn^{2+} > Ni^{2+}$ for most of the processed systems [103].

Mechanistic selectivity: HSAB-based exceptional selectivity is observed with thiol MOFs, whereas amine systems are dependent on coordination geometry preferences [104]. The combined effect of several recognition processes enables mixed-functional systems to reach the best selectivity [105].

Matrix effects: Binding could be influenced by natural water samples with organic matter, chloride, sulfate, and carbonate ions [106]. Recent results indicate that appropriately designed functionalized MOFs can retain >80% of their pure water performance in complex matrices [107].

5.3 Stability and Regeneration

Longevity and regenerability are crucial for real-world applications [108].

Chemical stability: Zr-based MOFs are highly stable in the pH 2-10 range; however, Cu and Zn-based systems can degrade in extreme environments [109]. Functionalization typically improves stability by introducing higher rigidity to the framework [110].

Regeneration efficiency: Several regeneration approaches have been proposed, such as acid wash, displacement by a chelator, and thermal regeneration [111]. The regeneration performance of two different systems is summarized in Table 2.

Table 2. Regeneration Performance of Functionalized MOFs

MOF System	Regeneration Method	Cycles Tested	Capacity Retention (%)	Reference
UiO-66-NH_2	0.1 M HCl	10	85-90	[112]
Zr-MOF-SH	EDTA solution	8	80-85	[113]
Magnetic MOF	Magnetic separation + HCl	12	88-92	[114]
MOF/polymer	Column regeneration	15	82-87	[115]

6. Real-World Applications and Case Studies

6.1 Pilot-Scale Studies

Some functionalized MOFs for water treatment were shown to be practically feasible by several pilot-scale studies [116]. Urban Water Treatment: A few lead adsorptive materials have been evaluated under contaminated groundwater treatment at flow rates of 200 L/h in a packed-bed column, allowing >95% lead removal efficiency using amine-functionalized MOF pellets [117]. The performance of the system was sustained up to 1000 bed volumes without the need for regeneration [118].

Wastewater treatment in industry: Successful recovery of valuable metals with lead removal from highly concentrated streams (100-500 mg/L) was demonstrated in application to battery manufacturing wastewater [119]. Economic analysis shows that the treatment cost for the novel technologies (i.e. enhanced adsorption or alternative ion exchange) is in the range of 0.5–1.2 EUR/m3 of drinking water produced, while the established ion exchange technology is about 2–5 EUR/m3, implying significantly higher cost for this more traditional technology in some cases. This validates the claim that novel approaches could be more cost-effective as compared to traditional ion exchange and is in accordance with other recent comparative techno-economic studies in water and nutrient recovery applications [120]. Point-of-use systemsHousehold-scale systems using functionalized MOFs produced WHO-disinfected water quality from contaminated sources with cartridge lifetimes of more than 6 months for average home use [121].

6.2 Monitor Applications in the Environment

Combining the detection capacity with the ID-capability allows direct, in situ, and real-time online monitoring of water quality during water treatment processes [122].

Automated surveillance systems: Fluorescent MOF-based sensors that are coupled with automated sampling systems allow for uninterrupted surveillance of lead levels in natural aqueous environments [123]. They show very good agreement with laboratory-based analytical techniques ($R^2 > 0.98$) [124].

Portable detection apparatuses: Portable analyzers based on MOF sensors for in-field water quality evaluation, in which the determination is performed in less than 5-10 min, are available [125]. These devices are especially useful for emergency monitoring and for monitoring in remote locations [126].

7. Challenges and Limitations

7.1 Technical Challenges

Although there has been considerable progress, functionalized MOFs could not be largely implemented due to some technical obstacles [127]. Water stability: Numerous MOF architectures experience decomposition in water, especially when exposed to harsh pH conditions or elevated ionic strength [128]. Zr-based MOFs are known to be highly stable, but other systems should be shielded or modified structurally [129].

Scalability: The synthesis of functionalized MOFs conventionally relies on costly materials, tedious procedures, and gives rise to low yields, which may not be economically feasible for large-scale production [130]. The development of continuous synthesis processes

and different precursors is vital [131].

Matrix interference: Since real water samples have a variety of interference ions, these ions in the real sample may cause some trouble to the adsorption and the determination [132]. Organic matter, chloride ions, and competing metals interfere with efficiency and complicate sensor responses [133].

7.2 Economic Considerations

Anumber of THE factors that limit theadoption of promising electrocatalytic materials such as noble-metal-free catalysts for the HER and OER in PEM water electrolyzers include stability, cost-effectiveness, and activity [134].

4.5.2 Commercial challenges Cost-efficiency poses a big threat of MOF-based systems for commercial application, because of the tremendously higher cost of synthesis materials than those of traditional absorbents. Manufacturable synthesis routes have been reported however these methods result in costs that can vary between 13–500 USD/kg depending on scale, materials, and process, while traditional adsorbents are significantly less expensive, generally around 1–10 USD/kg. In spite of these impediments, the superior performance of MOFs in per unit mass basis may make them suitable for specialized applications in which a very high selectivity or adsorption is required [135]. Yet, the enhanced performance on a per mass basis may justify the increased cost for niche applications [136].

Regeneration economics: The MOF lifetime can be extended by regeneration, but the additional expenses for chemicals, energy, and waste disposal for regeneration have to be taken into account in the economic consideration [137]. Magnetic separation and mild regeneration conditions have the potential for cost reductions [138].

Infrastructure needs: The use of MOF-based systems might necessitate special equipment for packaging, regeneration, and monitoring, leading to an increase in capital expenses relative to the traditional technologies [139].

7.3 Regulatory and Safety Considerations

The use of novel materials in water treatment applications is subject to long safety assessment and regulatory approval processes [140]. Toxicity evaluation: There are a few studies on the environmental fate and toxicity of MOF materials and their degradation products [141]. Global toxicities must be evaluated before widespread application is considered [142]. Approval from regulatory bodies: Technologies for water treatment need to be proven safe and effective under rigorously applied standards [143]. Due to the unique nature of MOFs, they may require extensive testing and paperwork for regulatory approval [144].

8. Future Perspectives and Research Directions

8.1 Advanced Functionalization Strategies

Future work should be directed at the development of the next generation of functionalization methods, overcoming the present limitations [145].

Smart responsive systems: synthesis of MOFs containing stimuli-responsive functional groups that could be switched on or off in response to the surrounding media [146]. Such systems may exhibit conditionally selective binding with fast regeneration under conditions of pertinence [147].

Multifunctional/hierarchical Functionalization: Design of MOFs with nested functionality including primary binding sites, secondary stabilization moieties, and tertiary sensing elements [148]. This strategy can bring unprecedented enhancement in performance by synergistic effects [149].

Biomimetic Functionalization: Biological recognition components such as peptides, aptamers, or enzymically active sites are integrated into MOF architectures [150]. They may also develop super-selectivity based on refined recognition mechanisms [151].

8.2 Integrated Systems Development

The potential applications in the future are evidently based on integrated systems with multifunctional single-platform systems [152]. Adsorption-detection-regeneration systems: Design of self-sustaining systems that can remove pollutants, monitor water quality, and regenerate as needed without external assistance [153]. These protocols may utilize artificial intelligence for better performance [154].

Combined processes: Combination of functionalized MOFs with other treatment methods (e.g., membrane filtration, advanced oxidation, or biological treatment) to develop novel synergistic treatment trains [155].Modular system design: Engineering of MOF-based treatment system modules that can be scaled, tailored, and maintained for diverse applications and capacities [156].

8.3 Computational Design and Optimization

Sophisticated computational techniques will also speed up the development and refinement of MOFs[157].Machine learning approaches: A subset of machine learning methods, in which different algorithms are applied to predict MOF performance as a function of structural and chemical features, which allows high-throughput screening of potentially thousands of new materials [158]. Such methods might also highlight the optimal pairs of functional groups and their location in space [159].

High-throughput screening: Multistep automated synthetic and assay protocols to facilitate fast testing of new functionalized MOF materials [160]. These could provide a boost to the discovery of next-generation materials [161].

Molecular simulation: Multiscale molecular dynamics and quantum mechanics to elucidate binding mechanisms and evaluate performance under varied conditions [162]. Such tools can also be utilized to direct the rational design of enhanced materials [163].

9. Conclusions

The recent progress in MOFs tailored for Pb removal and sensing is a game-changer for environmental applications. By means of a thorough review of more than 220 articles, the present review validates that rational functionalization with specific chemical moieties leads to materials with outstanding performances, capable of overcoming some key disadvantages of traditional techniques.

Representative performance: Functionalized MOFs show adsorption capacities of 200–800 mg/g, which is 5-10 times the improvement of most commercial adsorbents. Selectivity is over 90% in complicated multi-ion matrices, and detection can be as low as 0.1-10 μg/L, which can meet the requirements of related regulations. Fast equilibration kinetics (15-45 min) and good regenerating performance (>85% of capacity retained after 10 cycles) suggest potential applicability in continuous operation.

Mechanistic understanding: The enhanced properties of functionalized MOFs can be attributed to a range of synergistic effects such as coordination bonding, electrostatic interaction, chelation effect, and size exclusion. Amine-functionalization offers the best compromise in terms of capacity, selectivity, and stability, while maximum binding energy and selectivity are obtained through thiol moieties. Co-functional systems offer better performance overall as a result of synergistic binding effects.

System readiness level: Pilot tests demonstrate the feasibility of functionalized MOFs at the pilot scale for application in the treatment of water, and the cost analysis shows the economic viability of the technique in the treatment of wastewater in niche applications. By integrating the detection functions, it is possible to realize real-time monitoring and smart system operation, which are the great advatages to conventional technology.

Significant issues: Stability in water, cost of synthesis, and interference from matrices are still the major obstacles towards broad applicability. Yet current research in Zr-based frameworks, continuous synthesis, and protection strategies suggests these drawbacks will be mitigated.

Future outlook: The field is ready for expansion with the advent of computational design, high-throughput/parallel automated synthesis, and integrated system development. Machine learning methods will speed material discovery, and biomimetic functionalization , as well as smart responsive systems, will deliver next-generation performance. The unique convergence of fundamental research advances and practical through-the-needle applications bodes well for functionalized MOFs to become increasingly important in global water security.

Research priorities: Some of the important issues that need immediate attention are: (1) establishment of cost-effective synthesis methods for industrial-scale production, (2) extensive toxicity and environmental fate analyses for regulatory approval, (3) standardization of testing protocols to enable comparison of performance, (4) adaptation to conventional water treatment systems, and (5) design of predictive models for system design and optimization.

This extensive investigation reveals functionalized MOFs as game-changing materials for environmental applications, delivering sustainable solutions to lead contamination problems along with enhanced monitoring and control options. The continued development of this field should bring about great impacts on the global environment and human health.

Acknowledgments

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