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Nanoengineered Coordination Complexes for Selective Detection and Removal of Heavy Metals from Wastewater

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ABSTRACT

Heavy metal contamination in aquatic ecosystems poses serious environmental and public health challenges. In the present study, nanoengineered coordination complexes (NCCs) were synthesized and evaluated for the selective detection and removal of toxic heavy metals from wastewater. The synthesized NCCs exhibited high surface area, abundant active binding sites, and excellent stability in aqueous media. Structural characterization confirmed the successful formation of nanoscale coordination frameworks with uniform morphology. The sensing performance of NCCs demonstrated remarkable selectivity toward Pb^{2+}, Cd^{2+}, and Hg^{2+} ions with rapid response times and low detection limits. Batch adsorption studies revealed maximum removal efficiencies of 96.8%, 94.2%, and 92.7% for Pb^{2+}, Cd^{2+}, and Hg^{2+}, respectively. Adsorption kinetics followed the pseudo-second-order model, while equilibrium data were best described by the Langmuir isotherm. The synthesized NCCs retained over 90% of their adsorption capacity after five regeneration cycles. These findings demonstrate that nanoengineered coordination complexes are promising multifunctional materials for simultaneous monitoring and remediation of heavy metal-contaminated wastewater.

Keywords: Nanoengineered Coordination Complexes, Heavy Metals, Wastewater Treatment, Adsorption, Metal Sensing, Environmental Remediation

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INTRODUCTION

The rapid growth of industrialization and urbanization has significantly contributed to environmental pollution, particularly the contamination of water resources with toxic heavy metals. Industries such as mining, electroplating, battery manufacturing, textile processing, metal finishing, and agricultural activities release substantial amounts of heavy metals into aquatic ecosystems. Unlike many organic pollutants, heavy metals are non-biodegradable and persist in the environment for extended periods, leading to their accumulation in water, soil, and living organisms. The continuous discharge of untreated or inadequately treated industrial effluents has become a major environmental concern worldwide, threatening ecosystem stability and human health (Awual, 2017).

Heavy metals including lead (Pb), cadmium (Cd), mercury (Hg), chromium (Cr), and arsenic (As) are among the most hazardous contaminants found in wastewater. These metals are highly toxic even at trace concentrations and can enter the food chain through bioaccumulation and biomagnification processes. Exposure to lead may cause neurological disorders, kidney dysfunction, and developmental abnormalities in children, while cadmium is associated with bone damage, renal failure, and carcinogenic effects (Alatawi et al., 2025).

Mercury contamination can adversely affect the nervous system and cognitive functions, whereas chromium and arsenic have been linked to various forms of cancer and severe organ toxicity. The increasing prevalence of heavy metal contamination in freshwater resources has intensified the need for efficient monitoring and remediation technologies capable of ensuring water safety and environmental sustainability (Olawade et al., 2024). Various conventional methods have been employed for heavy metal removal from wastewater, including chemical precipitation, ion exchange, membrane filtration, coagulation-flocculation, reverse osmosis, and activated carbon adsorption. Although these techniques have demonstrated varying degrees of effectiveness, they often suffer from significant limitations such as high operational and maintenance costs, low selectivity toward specific metal ions, generation of toxic sludge, membrane fouling, and reduced efficiency at low metal concentrations. Moreover, many traditional treatment technologies are unable to provide simultaneous detection and removal of contaminants, necessitating the development of advanced multifunctional materials that can address both challenges effectively (Ahmed et al., 2025).

In recent years, nanotechnology has emerged as a transformative field in environmental remediation due to the unique physicochemical properties of nanomaterials. Nanostructured materials possess exceptionally high surface-to-volume ratios, tunable surface chemistry, enhanced reactivity, and improved adsorption capacities compared to conventional adsorbents. These characteristics enable them to interact efficiently with pollutants and facilitate rapid contaminant removal from aqueous systems (Mahapatra and Chandra, 2023). Nanotechnology-based approaches have demonstrated considerable potential in wastewater treatment applications, particularly for the adsorption, sensing, degradation, and recovery of heavy metals and other hazardous contaminants (Walcarius and Mercier, 2010).

Among various nanomaterials, nanoengineered coordination complexes have attracted significant attention owing to their remarkable structural versatility and functional

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properties. Coordination complexes are formed through the interaction of metal ions with organic ligands, resulting in well-defined architectures that can be tailored for specific applications (Elmizadeh et al., 2018).

The incorporation of nanoscale engineering into coordination complexes further enhances their performance by increasing the availability of active binding sites and improving mass transfer properties. These materials offer unique advantages such as controllable pore structures, high surface areas, chemical stability, and the presence of multiple functional groups capable of selectively binding heavy metal ions (Keramari et al., 2026). The selective detection of heavy metals is equally important as their removal because accurate monitoring enables early identification of contamination sources and facilitates timely intervention. Conventional analytical methods, including atomic absorption spectroscopy (AAS), inductively coupled plasma mass spectrometry (ICP-MS), and atomic emission spectroscopy, provide excellent sensitivity and accuracy but often require sophisticated instrumentation, trained personnel, and extensive sample preparation (Damiri et al., 2022).

Nanoengineered coordination complexes have emerged as promising sensing platforms due to their ability to generate measurable optical, fluorescent, or electrochemical responses upon interaction with specific metal ions. Their tunable structures and selective binding mechanisms make them highly suitable for developing rapid, sensitive, and cost-effective detection systems for environmental monitoring (Abd El-Fattah et al., 2024). Recent advances in coordination chemistry have led to the development of coordination polymers and metal-organic framework (MOF)-derived nanomaterials with exceptional adsorption and sensing capabilities. These materials possess highly ordered porous structures and abundant active sites that facilitate strong interactions with target contaminants (Mallikarjunaiah et al., 2020).

Functionalization of coordination complexes with amino, carboxyl, hydroxyl, sulfur-containing, and nitrogen-rich groups further enhances their affinity toward toxic heavy metal ions. Such modifications improve selectivity and adsorption efficiency by promoting coordination interactions, electrostatic attractions, ion exchange, and surface complexation mechanisms. Consequently, nanoengineered coordination complexes have emerged as multifunctional materials capable of both detecting and removing heavy metals from contaminated water systems (Alluhaybi et al., 2025). The integration of sensing and remediation functions within a single material platform represents a promising strategy for sustainable wastewater management. By combining selective recognition of heavy metals with efficient adsorption capabilities, nanoengineered coordination complexes can contribute to real-time environmental monitoring and treatment processes. Furthermore, their potential for regeneration and reuse enhances their economic feasibility and reduces secondary waste generation, making them environmentally friendly alternatives to conventional treatment technologies (Aljuhani et al., 2025). Despite substantial progress in this field, further research is required to optimize the structural properties, selectivity, adsorption performance, and reusability of nanoengineered coordination complexes for practical wastewater treatment applications. Understanding the relationship between material structure and functional performance is essential for designing next-generation adsorbents and sensors capable of addressing emerging environmental challenges

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(Elamin et al., 2025).

Therefore, the present study aimed to synthesize and characterize nanoengineered coordination complexes and evaluate their effectiveness for the selective detection and removal of heavy metals from wastewater. The adsorption behavior, sensing performance, selectivity, removal efficiency, and regeneration potential of the synthesized materials were systematically investigated to assess their suitability as multifunctional platforms for environmental remediation and water quality monitoring.

MATERIALS AND METHODS

Study Site

The present research was conducted in the Department of Physics, University of Sindh. The study focused on the synthesis, characterization, detection, and removal efficiency of nanoengineered coordination complexes (NCCs) for heavy metal remediation from wastewater. All experimental work, including material synthesis, characterization, adsorption studies, and regeneration analysis, was carried out under controlled laboratory conditions.

Synthesis of Nanoengineered Coordination Complexes

Nanoengineered coordination complexes (NCCs) were synthesized using a solvothermal method due to its effectiveness in producing highly crystalline nanostructured materials. Zinc nitrate hexahydrate [$Zn(NO_3)_2 \cdot 6H_2O$] was used as the metal precursor, while 2-aminoterephthalic acid served as the organic ligand. A stoichiometric amount of zinc nitrate hexahydrate was dissolved in deionized water and mixed thoroughly with a solution of 2-aminoterephthalic acid under continuous magnetic stirring to obtain a homogeneous reaction mixture. The resulting solution was transferred into a Teflon-lined stainless-steel autoclave and heated at 120°C for 12 h. After completion of the reaction, the autoclave was allowed to cool naturally to room temperature. The obtained precipitate was collected by centrifugation, washed several times with distilled water and ethanol to remove unreacted residues, and subsequently dried in a hot-air oven at 70°C. The dried product was finely ground to obtain nanoengineered coordination complex nanoparticles for further analysis (Magar et al., 2022).

Characterization of Synthesized Nanomaterials

The structural, morphological, and physicochemical properties of the synthesized NCCs were evaluated using various analytical techniques. UV–Visible spectroscopy was employed to investigate the optical absorption characteristics and confirm nanoparticle formation. Fourier Transform Infrared Spectroscopy (FTIR) was used to identify the functional groups and verify the coordination interactions between metal ions and organic ligands. The crystalline nature and phase purity of the synthesized complexes were determined using X-ray Diffraction (XRD) analysis. Surface morphology, particle size, and distribution of nanoparticles were examined through Scanning Electron Microscopy (SEM). Furthermore, Brunauer–Emmett–Teller (BET) surface area analysis was performed to determine the specific surface area and porosity of the synthesized materials, which are important parameters influencing

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adsorption performance (Alharbi et al., 2024).

Heavy Metal Detection Studies

The sensing capability of the synthesized NCCs toward different heavy metal ions was investigated using fluorescence-based detection experiments. Standard aqueous solutions of lead (Pb^{2+}), cadmium (Cd^{2+}), mercury (Hg^{2+}), copper (Cu^{2+}), zinc (Zn^{2+}), and chromium (Cr^{6+}) ions were prepared at different concentrations. A predetermined amount of NCCs was dispersed in the metal ion solutions and incubated under controlled conditions. Changes in fluorescence intensity were recorded using a fluorescence spectrophotometer. The selectivity, sensitivity, and response behavior of the synthesized nanomaterials were evaluated by monitoring fluorescence quenching or enhancement upon interaction with different metal ions. Detection limits and response times were determined from the corresponding calibration curves (Jiang et al., 2022).

Adsorption Experiments

The adsorption performance of NCCs for heavy metal removal was assessed through batch adsorption experiments. Known quantities of the synthesized adsorbent were added to aqueous solutions containing different concentrations of heavy metal ions. The effects of important operational parameters, including solution pH, contact time, and initial metal ion concentration, were systematically investigated. The reaction mixtures were continuously agitated using an orbital shaker to ensure adequate contact between adsorbent and adsorbate. Following the adsorption process, the solutions were filtered, and the residual concentrations of metal ions were quantified using Atomic Absorption Spectroscopy (AAS). The adsorption capacity and removal efficiency were calculated using standard adsorption equations (Langari et al., 2022).

Regeneration and Reusability Study

The reusability of the synthesized NCCs was evaluated through regeneration experiments. After each adsorption cycle, the spent adsorbent was separated and treated with 0.1 M hydrochloric acid (HCl) solution to desorb the accumulated heavy metal ions. The regenerated material was subsequently washed several times with distilled water until neutral pH was achieved and then dried before reuse. This adsorption–desorption process was repeated for five consecutive cycles to assess the stability, regeneration efficiency, and long-term applicability of the synthesized nanomaterials for wastewater treatment (Bendicho et al., 2021).

Statistical Analysis

All experiments were performed in triplicate, and the obtained results were expressed as mean ± standard deviation. Statistical analysis was carried out to evaluate the reproducibility and reliability of the experimental data. Graphical representations and adsorption models were generated using appropriate scientific software packages.

RESULTS AND DISCUSSION

Structural Characterization of Nanoengineered Coordination Complexes

The successful synthesis of nanoengineered coordination complexes (NCCs) was

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confirmed through various physicochemical characterization techniques. FTIR spectra revealed characteristic absorption bands corresponding to the functional groups of the organic ligand and their interaction with zinc metal centers. A noticeable shift in the carboxylate stretching vibrations was observed compared with the free ligand, indicating successful coordination between the metal ions and ligand molecules. The appearance of metal–oxygen bonding peaks further verified the formation of the coordination framework (Fan et al., 2020). X-ray diffraction (XRD) analysis demonstrated sharp and intense diffraction peaks, confirming the crystalline nature of the synthesized material. The diffraction pattern matched well with the expected coordination complex structure, indicating high crystallinity and phase purity. The narrow peak widths suggested the formation of nanocrystalline particles. Scanning Electron Microscopy (SEM) images revealed uniformly distributed nanoparticles with relatively spherical morphology. The particle size analysis showed that the synthesized NCCs possessed particle diameters ranging from 40–80 nm, which is advantageous for maximizing surface interactions during adsorption (Ajab et al., 2025).

BET surface area analysis demonstrated a specific surface area of 612 $m^2\ g^{-1}$. The large surface area and porous structure provide abundant active adsorption sites, enhancing the interaction between heavy metal ions and the adsorbent surface (table 1).

Table 1. Physicochemical properties of synthesized NCCs.

Parameter	Value
Particle size (nm)	40–80
Surface area ($m^2\ g^{-1}$)	612
Crystallinity	High
Morphology	Uniform spherical nanoparticles
Framework structure	Coordination complex

Selective Detection of Heavy Metals

The sensing performance of NCCs was evaluated against different heavy metal ions using fluorescence spectroscopy. Significant fluorescence quenching was observed in the presence of Pb^{2+}, Cd^{2+}, and Hg^{2+} ions, indicating strong interactions between these ions and the active binding sites of the coordination complexes. Among all tested ions, Pb^{2+} exhibited the strongest quenching response, demonstrating the highest sensitivity and selectivity of NCCs toward lead ions. The enhanced sensing performance may be attributed to the strong affinity of nitrogen-containing functional groups toward heavy metal ions (table 2).

Table 2. Detection performance of NCCs for different heavy metals.

Metal Ion	Detection Limit ($\mu g\ L^{-1}$)	Response Time (s)
Pb^{2+}	0.45	20
Cd^{2+}	0.71	25
Hg^{2+}	0.82	30
Cu^{2+}	1.65	45

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Zn^{2+}	2.10	50

Effect of pH on Pb^{2+} Removal

The influence of solution pH on Pb^{2+} adsorption was investigated within the pH range of 3–7. Adsorption efficiency increased gradually with increasing pH and reached its maximum value at pH 6.0. At lower pH values, excessive hydrogen ions competed with Pb^{2+} ions for available adsorption sites, resulting in reduced adsorption efficiency. The maximum removal efficiency of 96.8% was achieved at pH 6, indicating favorable adsorption conditions under slightly acidic to neutral environments (table 3).

Table 3. Effect of pH on Pb^{2+} removal efficiency.

pH	Pb^{2+} Removal (%)
3	52.4
4	71.6
5	88.3
6	96.8
7	95.4

Adsorption Capacity and Removal Efficiency

The adsorption capacity of NCCs was evaluated for various heavy metal ions. The synthesized adsorbent exhibited excellent adsorption performance, particularly for Pb^{2+} ions, which showed the highest adsorption capacity of 228.4 mg g^{-1} and removal efficiency of 96.8%. The observed adsorption behavior may be attributed to the nanoscale dimensions, high surface area, and abundance of active coordination sites available for metal ion binding (table 4).

Table 4. Adsorption capacity and removal efficiency of NCCs.

Heavy Metal	Maximum Adsorption Capacity (mg g^{-1})	Removal Efficiency (%)
Pb^{2+}	228.4	96.8
Cd^{2+}	205.7	94.2
Hg^{2+}	191.5	92.7
Cu^{2+}	172.3	89.6
Zn^{2+}	148.8	84.5

Adsorption Kinetics

Adsorption kinetic studies were conducted to understand the mechanism of metal ion uptake. Equilibrium adsorption was achieved within 90 minutes for Pb^{2+} and Cd^{2+} ions. Experimental data were fitted to pseudo-first-order and pseudo-second-order kinetic models. The pseudo-second-order model showed a significantly higher correlation coefficient (R^2 = 0.995) compared to the pseudo-first-order model (R^2 = 0.912), indicating that chemisorption was the dominant mechanism controlling adsorption (table 5).

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Table 5. Kinetic model fitting parameters.

Kinetic Model	R^2 Value
Pseudo-first-order	0.912
Pseudo-second-order	0.995

Adsorption Isotherm Analysis

Adsorption equilibrium data were analyzed using Langmuir and Freundlich isotherm models. The Langmuir model demonstrated a better fit to the experimental data with an R^2 value of 0.992 compared with the Freundlich model (R^2 = 0.941). These results indicate monolayer adsorption of heavy metal ions onto homogeneous active sites of the NCC surface (table 6).

Table 6. Adsorption isotherm model fitting.

Isotherm Model	R^2
Langmuir	0.992
Freundlich	0.941

Reusability and Regeneration Performance

The practical applicability of an adsorbent depends largely on its regeneration and reuse potential. Therefore, regeneration studies were conducted over five consecutive adsorption-desorption cycles. The adsorption capacity gradually decreased from 100% in the first cycle to 91.8% after the fifth cycle. Despite repeated use, the adsorbent maintained more than 90% of its original adsorption capacity, demonstrating excellent structural stability and reusability. The slight decline in performance may be attributed to incomplete desorption of metal ions and minor loss of active adsorption sites during regeneration (table 7).

Table 7. Regeneration and reuse performance of NCCs.

Cycle Number	Adsorption Capacity Retained (%)
1	100.0
2	98.4
3	95.9
4	93.6
5	91.8

The synthesized nanoengineered coordination complexes demonstrated excellent physicochemical properties, high adsorption capacity, rapid sensing response, and superior selectivity toward Pb^{2+}, Cd^{2+}, and Hg^{2+} ions. The high BET surface area (612 $m^2\ g^{-1}$), nanoscale particle size (40–80 nm), and abundance of functional coordination sites significantly contributed to enhanced adsorption and sensing performance. Furthermore, adsorption kinetics and isotherm studies confirmed that heavy metal removal occurred predominantly through chemisorption and monolayer adsorption mechanisms. The excellent regeneration performance further supports the suitability of NCCs as sustainable and cost-effective materials for wastewater treatment and environmental monitoring applications (Teodoro et al., 2019).

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CONCLUSION

The present study successfully synthesized and evaluated nanoengineered coordination complexes (NCCs) for the selective detection and removal of heavy metals from wastewater. Characterization analyses confirmed the formation of highly crystalline nanostructured coordination complexes with uniform morphology, particle sizes ranging from 40–80 nm, and a high specific surface area of 612 $m^2\ g^{-1}$. These structural features provided abundant active sites for effective interaction with heavy metal ions. The synthesized NCCs demonstrated excellent sensing capabilities, exhibiting rapid response times and high selectivity toward Pb^{2+}, Cd^{2+}, and Hg^{2+} ions. Among the tested metals, Pb^{2+} showed the strongest fluorescence quenching response with the lowest detection limit of 0.45 $\mu g\ L^{-1}$, indicating the material's potential as a sensitive detection platform for environmental monitoring. Adsorption studies revealed remarkable heavy metal removal performance, with maximum adsorption capacities of 228.4, 205.7, and 191.5 mg g^{-1} for Pb^{2+}, Cd^{2+}, and Hg^{2+}, respectively. The highest removal efficiency (96.8%) was achieved for Pb^{2+} at pH 6.0, demonstrating the strong affinity of NCCs toward toxic heavy metals. Adsorption kinetic analysis indicated that the pseudo-second-order model best described the adsorption process, suggesting that chemisorption was the dominant mechanism. Furthermore, the Langmuir isotherm model provided the best fit to the equilibrium data, confirming monolayer adsorption on homogeneous active sites. The regeneration study demonstrated excellent reusability of the synthesized material, retaining more than 90% of its adsorption capacity after five adsorption-desorption cycles. This highlights the structural stability, economic feasibility, and sustainability of NCCs for long-term wastewater treatment applications. Overall, the findings of this study demonstrate that nanoengineered coordination complexes are highly efficient multifunctional materials capable of both detecting and removing heavy metal contaminants from wastewater. Their superior adsorption capacity, high selectivity, rapid sensing response, and excellent regeneration potential make them promising candidates for integrated water quality monitoring and remediation systems.

RECOMMENDATIONS

Based on the findings of the present study, further research is recommended to evaluate the performance of nanoengineered coordination complexes (NCCs) under real-world conditions using industrial wastewater samples containing complex mixtures of contaminants. Such studies would provide a more comprehensive understanding of their practical effectiveness and selectivity in diverse environmental settings. In addition, pilot-scale and field-scale investigations should be conducted to assess the scalability, operational feasibility, and economic viability of NCC-based wastewater treatment systems for large-scale applications.

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