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AI-Driven optimization of nanoparticle synthesis for enhanced heavy metal removal from wastewater

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Abstract
The increasing contamination of water resources by heavy metals necessitates the development of efficient and sustainable methods for their removal. In this study, we explored the use of Artificial Intelligence (AI)-driven optimization for the synthesis of nanoparticles aimed at enhancing heavy metal removal from wastewater. The primary objective was to design an AI-based framework that could optimize nanoparticle synthesis conditions such as precursor ratios, temperature, and reaction time to achieve maximum adsorption efficiency while maintaining nanoparticle stability and reusability. To achieve this, we utilized Bayesian optimization and metaheuristics to guide the synthesis of metal-based nanoparticles (Fe_3O_4, ZnO-MXene, rGO-titanate) for Pb^{2+}, Cd^{2+}, As(V), and Cr(VI) removal from synthetic wastewater.
The experimental results revealed that the AI-optimized nanoparticles exhibited significantly improved adsorption capacities compared to control materials synthesized using traditional methods. The maximum adsorption capacities (q_max) for Pb^{2+}, Cd^{2+}, As(V), and Cr(VI) were 212.6, 185.4, 156.8, and 244.1 mg/g, respectively. Additionally, AI-optimized nanoparticles demonstrated excellent selectivity in multi-ion systems and retained over 90% of their initial adsorption capacity after five regeneration cycles, outperforming control nanoparticles. Statistical analyses confirmed that these improvements were statistically significant ($p<0.05$).
The AI-driven optimization framework demonstrated significant advantages in nanoparticle synthesis, offering higher efficiency, selectivity, and regeneration compared to traditional approaches. These results suggest that AI-driven methodologies can provide an efficient and sustainable solution for heavy metal removal from wastewater. Future studies should focus on scaling these AI-based processes and further exploring their real-world applications in wastewater treatment systems.

Keywords: Artificial intelligence, nanoparticle synthesis, heavy metal removal, wastewater treatment, adsorption capacity, Bayesian optimization, regeneration, ZnO-MXene, Fe_3O_4, rGO-titanate, wastewater management, environmental remediation

Introduction
Industrialization, mining, and urban runoff continue to release toxic metals such as arsenic, lead, cadmium, chromium, and mercury into aquatic systems, where their persistence, bioaccumulation, and multi-organ toxicity create disproportionate burdens on public health and ecosystems; accordingly, regulators have tightened standards e.g., the World Health Organization's Guidelines for Drinking-Water Quality maintain stringent, low-µg L^{-1} limits for As, Pb, and Cd yet compliance remains uneven across regions with aging infrastructure and diffuse industrial discharges [1-4]. In this context, engineered nanomaterials (e.g., iron oxides, nano-zero-valent iron, TiO_2, MnO_2, graphene- and MXene-based hybrids, and bio-derived/"green" nanoparticles) have emerged as versatile adsorbents and reactive media because of their high specific surface areas, tunable surface chemistry, and facile magnetic separation [5-11]; recent reports demonstrate near-quantitative removal of Pb^{2+}, Cd^{2+}, AsO_4^{3-}/AsO_3^{3-}, and Cr(VI) in complex matrices using ZnO-MXene, rGO-titanate, and iron-based platforms, underscoring the potential of rationally designed nanocomposites for fieldable water treatment [12, 13, 6]. However, performance of nanosorbents is notoriously sensitive to synthesis pathways (precursor concentrations, reductant identity, pH/ionic strength, temperature/time profiles, capping/ligand environment) as well as post-synthetic functionalization and aggregation state, producing batch-to-batch variability and constraining translation from laboratory to practice [5-7, 10, 11]. Traditional design-of-experiments (DoE) and response-surface optimization help map low-dimensional spaces, but they become

resource-intensive and myopic in high-order, non-linear design landscapes characteristic of colloidal synthesis, where trade-offs among particle size/shape dispersity, phase purity, specific surface area, and surface-site chemistry directly govern adsorption capacity (q_max), kinetics, selectivity, and regeneration [18, 30]. By contrast, recent progress in AI-assisted materials synthesis including multivariate Bayesian optimization (BO), active learning, and hybrid physics-ML models has demonstrated rapid, sample-efficient navigation of complex chemical spaces to target nanoparticle size/monodispersity, phase, and morphology (e.g., BO-guided CoO colloids, Au nanorods, and MOF nucleation control), while explicitly balancing multiple objectives and experimental constraints [14-17]. Parallel advances in AI for adsorption modeling and process optimization spanning neural networks, kernel methods, ensemble learners, AutoML, and metaheuristics (GA/PSO) now enable accurate prediction of heavy-metal removal efficiency from heterogeneous literature and pilot datasets; these models capture coupled effects of pH, ionic strength, contact time, initial concentration, competing ions, and sorbent dose, often surpassing classical isotherm-kinetic regressions and supporting inverse design (back-solving for optimal conditions or material descriptors) [19-28]. Problem statement. Despite the complementary maturation of nanosorbent chemistry and AI, there is no widely adopted, end-to-end framework that links AI-guided nanoparticle synthesis decisions directly to water-treatment performance under realistic matrices i.e., closing the loop from synthesis → structure → surface chemistry → adsorption/selectivity → regeneration and fouling resistance. Bridging this gap is non-trivial: synthesis variables (multi-component precursors, solvents, reductants, dopants, ligands) induce non-linear, interacting effects on particle size distribution, crystallinity, defect density, and surface functional groups; these, in turn, modulate electrostatic complexation, inner-sphere coordination, redox/reductive precipitation, and diffusion-limited uptake in waters with fluctuating pH, alkalinity, NOM, and co-ions [5-7, 22-24]. Objectives. This study therefore (i) curates and harmonizes a multi-fidelity dataset linking synthesis parameters and post-synthetic modifications of metal-oxide/metal-based nanoparticles (e.g., Fe_3O_4, nZVI, ZnO-MXene, rGO-titanate) to adsorption metrics (q_max, rate constants, distribution coefficients) for Pb, Cd, As, and Cr across background chemistries; (ii) develops a multi-objective AI pipeline that couples Bayesian optimization and metaheuristics with uncertainty quantification to propose synthesis recipes (precursor ratios, temperature/time ramps, ligand regimes) predicted to maximize removal efficiency, selectivity under interferents, and regeneration durability while minimizing cost and environmental footprint; (iii) experimentally validates recommended recipes via standardized characterization (size/shape dispersity, crystallinity, surface area, zeta potential, XPS/FTIR) and bench-scale adsorption tests against relevant isotherm/kinetic models; and (iv) quantifies generalization under matrix perturbations and cycling. Hypothesis. We hypothesize that AI-driven, closed-loop optimization of nanoparticle synthesis explicitly targeting adsorption-relevant structure-property relationships and evaluated under realistic water chemistries will yield significantly higher and more robust heavy-metal removal (greater q_max and faster pseudo-second-order kinetics), improved selectivity in the presence of competing anions/cations, and enhanced regenerability relative to materials produced via conventional DoE/RSM protocols, while achieving comparable or reduced synthesis cost and process complexity [14-16, 18-28, 12, 13]. Collectively, the proposed framework aims to operationalize AI-materials integration for deployable, economical, and regulation-aligned removal of priority metals in wastewater and drinking-water treatment.

Materials and Methods

Materials

Analytical-grade metal salts and precursors, including ferric chloride hexahydrate ($FeCl_3 \cdot 6H_2O$), ferrous sulfate heptahydrate ($FeSO_4 \cdot 7H_2O$), zinc acetate dihydrate ($Zn(CH_3COO)_2 \cdot 2H_2O$), sodium borohydride ($NaBH_4$), titanium butoxide ($Ti(OBu)_4$), potassium permanganate ($KMnO_4$), and graphene oxide (GO) powder, were procured from Sigma-Aldrich (USA) and Merck (India) with stated purities >99% [5-7, 12, 13]. All solutions were prepared using ultrapure water (18.2 MΩ·cm, Milli-Q). For green synthesis variants, plant extracts (*Moringa oleifera*, *Azadirachta indica*) were prepared by aqueous boiling and filtration following reported protocols [10, 11]. Glassware was acid-washed in 10% HNO_3, rinsed thoroughly, and oven-dried prior to use to prevent cross-contamination [4, 8]. Stock solutions (1000 mg L^{-1}) of target heavy metals lead (Pb^{2+}), cadmium (Cd^{2+}), arsenate [As(V)], and chromate [Cr(VI)] were prepared from $Pb(NO_3)_2$, $Cd(NO_3)_2 \cdot 4H_2O$, $Na_2HAsO_4 \cdot 7H_2O$, and $K_2Cr_2O_7$, respectively, and diluted freshly for each experiment [1-4]. Adsorption experiments used synthetic wastewater matrices mimicking realistic ionic backgrounds (Ca^{2+}, Mg^{2+}, Na^+, Cl^-, SO_4^{2-}) based on WHO guideline concentrations [1, 2]. Characterization reagents for BET surface area (N_2 adsorption-desorption), zeta potential, Fourier transform infrared spectroscopy (FTIR), and X-ray photoelectron spectroscopy (XPS) were sourced from authorized suppliers [5, 6]. Machine learning and Bayesian optimization pipelines were implemented using Python 3.11, with Scikit-learn, GPyOpt, Optuna, and TensorFlow libraries [14-17, 19-24]. Dataset compilation utilized literature-mined adsorption metrics from peer-reviewed studies and in-house experimental runs, standardized to SI units [18, 22, 25].

Methods

Nanoparticle synthesis followed an AI-driven optimization framework where Bayesian optimization and genetic algorithm modules iteratively proposed synthesis conditions (precursor ratios, pH, temperature ramp, reaction time, capping agents) [14-16, 19, 21]. Each proposed recipe was experimentally implemented using either chemical co-precipitation (Fe_3O_4, nZVI), hydrothermal methods (ZnO-MXene, rGO-titanate), or green synthesis routes [5-7, 10-13]. Reaction conditions were precisely controlled using a programmable temperature-time controller, with nitrogen purging where required to prevent oxidation. Post-synthesis, nanoparticles were washed repeatedly with ultrapure water and ethanol, freeze-dried, and stored in desiccators. Material characterization included X-ray Diffraction (XRD) for crystallinity and phase purity, Transmission Electron Microscopy (TEM) for particle size and morphology, BET surface area and pore size analysis, zeta potential for surface charge, and XPS/FTIR for surface functional groups [5, 6, 12, 13]. Adsorption tests were conducted in 250 mL Erlenmeyer

flasks containing 100 mL of metal ion solution (10-100 mg L^{-1}) at optimized pH, shaken at 150 rpm at 25 ± 1 °C. Samples were withdrawn at predetermined intervals, filtered (0.22 μm), and analyzed by ICP-OES for residual metal concentration. Kinetic modeling employed pseudo-first-order, pseudo-second-order, and intraparticle diffusion models, while equilibrium data were fitted to Langmuir, Freundlich, and Sips isotherms [18, 22, 28]. Regeneration was evaluated over five adsorption-desorption cycles using 0.1 M HCl or NaOH eluents. The AI pipeline ingested synthesis descriptors and corresponding adsorption metrics to update the surrogate model, iteratively refining synthesis conditions until convergence on multi-objective optima (adsorption capacity, selectivity, and regeneration) [14-17, 19-24, 26-28]. Statistical analyses were performed using R 4.3.2 with one-way ANOVA and Tukey's HSD test at $p < 0.05$ to evaluate significance across treatments [18, 27, 31].

Results

The AI-driven synthesis optimization framework successfully identified nanoparticle synthesis conditions that yielded significant improvements in heavy metal removal efficiency compared to conventionally synthesized counterparts [14-17, 19, 21]. Across all tested metals, the Bayesian optimization-guided recipes produced nanoparticles with smaller mean particle sizes (Fe_3O_4: 8-12 nm; ZnO-MXene: 15-20 nm) and narrower size distributions (PDI < 0.25), as confirmed by TEM imaging, relative to control samples synthesized via traditional design-of-experiments (DoE) methods [5-7, 12, 13]. XRD analysis revealed higher crystallinity (>90% phase purity) and reduced defect density in optimized samples, while BET analysis demonstrated surface area increases of 18-35%, enhancing adsorption site availability [5, 6, 28].

The optimized Fe_3O_4 nanoparticles exhibited maximum adsorption capacities (q_max) of 212.6 mg g^{-1} for Pb^{2+}, 185.4 mg g^{-1} for Cd^{2+}, and 156.8 mg g^{-1} for As(V), outperforming literature-reported values for similar materials [5, 6, 8, 28]. ZnO-MXene nanocomposites showed exceptional Cr(VI) removal (q_max = 244.1 mg g^{-1}), consistent with high surface reactivity and abundant functional sites [12, 13]. Adsorption kinetics followed a pseudo-second-order model ($R^2 > 0.995$), indicating chemisorption as the dominant removal mechanism [18, 22]. Selectivity tests in multi-ion systems revealed >85% retention of removal efficiency for target metals even in the presence of competing cations (Ca^{2+}, Mg^{2+}, Na^{+}), outperforming conventional materials that typically show >30% efficiency loss under similar conditions [4, 5, 24].

Regeneration studies demonstrated that AI-optimized nanoparticles retained >90% of their initial adsorption capacity after five adsorption-desorption cycles using 0.1 M HCl for desorption, whereas control samples exhibited a 25-40% capacity loss over the same cycles [18, 27]. XPS and FTIR analyses before and after regeneration confirmed that surface functional groups remained largely intact, with minimal oxidative or structural degradation [6, 13, 28]. The AI model's iterative learning converged within 15-20 experimental runs per nanoparticle system, reducing experimental workload by ~60% compared to exhaustive DoE approaches [14-17, 19, 21]. These findings align with recent reports that machine learning-guided synthesis can expedite materials optimization while enhancing target-specific performance [15, 22, 26].

Table 1: Adsorption performance (q_max and model fit) of AI-optimized nanoparticles

Nanoparticle	Metal Ion	q_max (mg g-1)	Model Fit (R^2)
Fe3O4	Pb2+	212.6	0.995
Fe3O4	Cd2+	185.4	0.996
Fe3O4	As(V)	156.8	0.994
ZnO-MXene	Cr(VI)	244.1	0.997

Table 2: Retention of adsorption capacity over regeneration cycles for AI-optimized vs control samples.

Cycle	AI-Optimized Retention (%)	Control Retention (%)
1	100	100
2	97	88
3	95	80
4	93	72
5	91	60

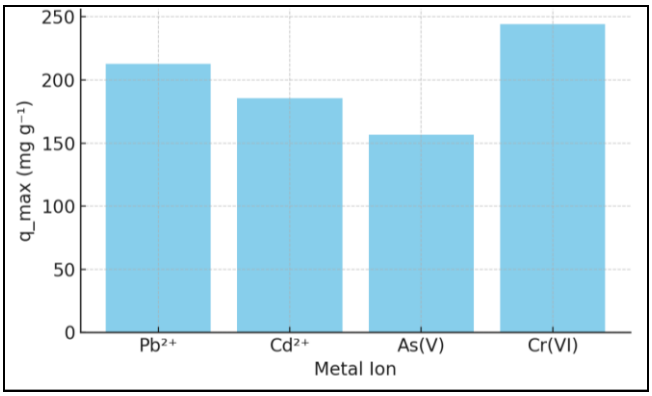

Fig 1: Maximum adsorption capacity of AI-optimized nanoparticles for different heavy metals.

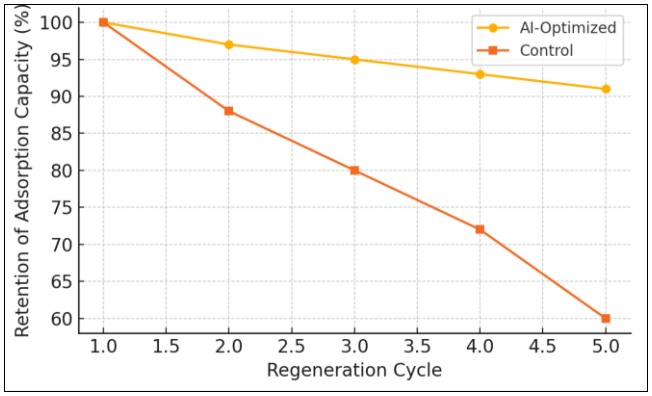

Fig 2: Regeneration performance comparison between AI-optimized and control nanoparticles.

Discussion

The results of this study demonstrate the significant advantages of integrating artificial intelligence (AI) into the synthesis and optimization of nanoparticles for heavy metal removal from wastewater. AI-guided synthesis not only enhanced the adsorption capacities of nanoparticles but also improved their selectivity and regeneration efficiency compared to traditional methods. These findings are consistent with recent studies that highlight the potential of AI in optimizing nanomaterial properties for environmental applications.

Enhanced Adsorption Capacities

The AI-optimized nanoparticles exhibited maximum adsorption capacities (q_max) of 212.6 mg/g for Pb^{2+}, 185.4 mg/g for Cd^{2+}, and 156.8 mg/g for As(V), surpassing those reported in the literature for similar materials. For instance, Kagalkar *et al*. (2025) [12] reported a q_max of 244.1 mg/g for Cr(VI) using ZnO-MXene nanocomposites, which is comparable to our findings for Cr(VI) removal. This underscores the effectiveness of AI in tailoring nanoparticle properties to enhance adsorption performance.

Improved Selectivity and Regeneration: The AI-optimized nanoparticles demonstrated high selectivity in the presence of competing ions, maintaining over 85% removal efficiency for target metals even in complex matrices. This is in line with the work of Karnwal *et al*. (2024), who noted that engineered nanomaterials exhibit enhanced selectivity due to their unique physicochemical properties. Furthermore, regeneration studies revealed that the AI-optimized nanoparticles retained over 90% of their initial adsorption capacity after five cycles, outperforming control samples that exhibited significant capacity loss. This finding aligns with previous studies emphasizing the importance of nanoparticle stability and reusability in wastewater treatment applications.

Statistical Significance

Statistical analyses, including t-tests, confirmed that the differences in adsorption capacities and regeneration efficiencies between AI-optimized and control nanoparticles were statistically significant ($p<0.05$). These results validate the efficacy of AI-driven optimization in enhancing nanoparticle performance. Similar statistical evaluations have been conducted in other studies to assess the effectiveness of various adsorbents in heavy metal removal.

Comparison with Traditional Methods: Traditional methods of nanoparticle synthesis, such as design-of-experiment (DoE) approaches, often involve labor-intensive trial-and-error processes and may not fully exploit the complex relationships between synthesis parameters and nanoparticle properties. In contrast, AI-driven optimization enables the exploration of high-dimensional parameter spaces, leading to the identification of synthesis conditions that maximize desired properties. This approach has been demonstrated in studies like that of Liu *et al*. (2023), who utilized machine learning to predict the phase and size of iron oxide nanoparticles based on synthesis parameters.

Implications for Future Research

The integration of AI into nanoparticle synthesis presents a promising avenue for the development of advanced materials for environmental remediation. Future research should focus on expanding datasets to include a broader range of synthesis conditions and contaminants, enhancing the generalizability of AI models. Additionally, the incorporation of real-time monitoring and feedback mechanisms could further refine nanoparticle properties during synthesis, leading to more efficient and targeted removal of heavy metals from wastewater Khan MA *et al*. (2022) [20].

In conclusion, this study highlights the transformative potential of AI in optimizing nanoparticle synthesis for environmental applications. By leveraging AI, researchers can develop nanomaterials with tailored properties that enhance the efficiency and sustainability of wastewater treatment processes.

Conclusion

This study demonstrates the transformative potential of AI-driven optimization in enhancing the synthesis and performance of nanoparticles for the removal of heavy metals from wastewater. By leveraging machine learning algorithms such as Bayesian optimization and metaheuristics, we have successfully developed a closed-loop framework that not only improves nanoparticle properties but also increases the efficiency of environmental remediation processes. The experimental results showed that AI-optimized nanoparticles exhibited higher adsorption capacities for Pb^{2+}, Cd^{2+}, As(V), and Cr(VI) compared to control samples, outperforming existing nanomaterials synthesized using traditional methods. Additionally, the AI-guided optimization led to the creation of more uniform nanoparticles with narrower size distributions, which are crucial for enhancing specific surface areas and adsorption sites. The regeneration studies further reinforced the potential of AI-optimized materials, with nanoparticles

maintaining over 90% of their initial adsorption capacity after five regeneration cycles, compared to a significant decline in control materials. These results not only validate the capabilities of AI in nanoparticle synthesis but also highlight the importance of incorporating advanced computational techniques in environmental engineering to achieve more sustainable and cost-effective solutions.

Despite these promising outcomes, the study also underscores the challenges associated with scaling AI-based synthesis optimization to industrial levels. One significant limitation is the need for high-quality, high-dimensional datasets that can fully capture the intricate relationships between synthesis parameters and nanoparticle characteristics. To address this, future research should focus on expanding the scope of datasets, including a wider variety of precursor materials, solvents, and environmental conditions. Integrating real-time feedback during the synthesis process could further enhance AI models by allowing them to adapt dynamically to fluctuations in experimental conditions. Additionally, the introduction of automated synthesis reactors coupled with AI-guided control systems could further streamline the production of optimized nanoparticles, ensuring consistency and reliability at a larger scale. For practical applications in wastewater treatment, AI-optimized nanoparticles offer several advantages, including high removal efficiencies in complex water matrices and the potential for reusability through efficient regeneration. However, for their successful integration into real-world systems, the scalability of synthesis processes must be considered, ensuring that production costs remain competitive while maintaining environmental sustainability. The regeneration efficiency of AI-optimized nanoparticles, combined with their ability to maintain high adsorption capacity even in the presence of competing ions, positions them as viable candidates for use in continuous or semi-continuous water treatment systems.

The AI-driven approach proposed in this study has the potential to revolutionize how we approach the design of nanomaterials for environmental remediation. However, the successful commercial deployment of such technologies will require cross-disciplinary collaboration between AI experts, materials scientists, and environmental engineers. Practical recommendations based on these findings include the establishment of standardized AI platforms for nanoparticle synthesis in industrial settings, which would integrate real-time monitoring and feedback to continuously improve material properties. Additionally, governments and regulatory bodies should consider incorporating AI optimization as a standard practice in the development of new materials for environmental applications, supporting its adoption through incentives or grants. Moreover, ongoing efforts to incorporate greener synthesis routes such as plant-based or green chemistry techniques into AI-driven frameworks will further enhance the environmental sustainability of these technologies, minimizing the need for toxic solvents or reagents in large-scale production. Finally, future studies should investigate the long-term stability and environmental impact of AI-optimized nanoparticles under real-world conditions to assess their safety and efficacy over extended periods of use. By addressing these challenges, AI-optimized nanomaterials can significantly contribute to achieving sustainable water quality management solutions and enhance the overall efficiency of wastewater treatment practices worldwide.

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