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Machine Learning Approaches for Heavy Metal Adsorption in Water Treatment Systems: A Systematic Review

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ABSTRACT

Introduction: Machine learning (ML) techniques have been increasingly applied to model Heavy metals (HMs) adsorption from aqueous environments; however, variations in datasets, evaluation strategies, and reporting practices have limited the development of generalizable conclusions regarding model performance. This systematic review comparatively evaluated ML applications in heavy metal adsorption modeling and identified factors influencing predictive performance across heterogeneous adsorption systems.

Methods: Peer-reviewed studies published between January 2010 and December 2024 were identified through searches of Scopus, Google Scholar, ScienceDirect, and PubMed. Risk of bias was assessed using the CASP tool, and studies were classified into single-algorithm, ensemble, and hybrid intelligent models.

Results: Of 1,806 records identified, 87 studies met the eligibility criteria. Comparative analysis showed that model performance was largely context-dependent rather than algorithm-specific. Although Artificial neural networks (ANNs), ensemble methods, and hybrid models all demonstrated strong predictive capability, no approach consistently outperformed others across all conditions. Instead, predictive performance was primarily influenced by dataset size, data quality, feature selection, and system complexity. Biochar and activated carbon were the most frequently investigated adsorbents, while arsenic, lead, chromium, and cadmium were the predominant target contaminants.

Conclusions: These findings suggest that model selection should be guided by dataset characteristics and application requirements rather than presumed algorithmic superiority. Standardized reporting, external validation, and greater transparency in model development are needed to improve the reliability and transferability of ML models for real-world water treatment applications.

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Introduction

The ever-increasing demand for clean water, coupled with the progressive depletion of freshwater resources driven by industrial development, population growth, and prolonged drought conditions, has become a major global challenge[1]. Poor drinking water quality significantly affects public health[2]. HMs are among the most concerning water contaminants because of their severe impacts on human health and ecosystems. These pollutants

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are highly stable and largely non-biodegradable, resulting in the contamination of both surface and groundwater systems[3,4]. HMs originate from multiple sources, including industrial effluents, domestic wastewater, atmospheric emissions, metallurgical industries, and electronic waste [5]. Exposure to uncontrolled concentrations of HMs can lead to serious health consequences, including impaired growth and development, carcinogenicity, neurological disorders, and even mortality [6]. For instance, short-term exposure to cobalt (Co) may cause nausea, vomiting, headaches, and altered reflexes[7]. Given the need to remove HMs from water resources and mitigate their environmental and health impacts[8], various treatment methods have been developed, including chemical precipitation [9,10], ion exchange [11,12], reverse osmosis [13,14], adsorption [15,16], solvent extraction [17,18] and membrane filtration [19,20]. However, many of these technologies are limited by high operational costs, intensive chemical consumption, substantial energy requirements, and the generation of secondary waste or residual toxicity [21]. Therefore, the development of efficient, sustainable, and cost-effective approaches for metal ion removal remains essential [22]. Among the available methods, adsorption has been widely recognized as an effective and economically feasible technique for heavy metal removal at both laboratory and industrial scales because of its simplicity, environmental compatibility, and high efficiency in aqueous systems [23].

In adsorbent development and separation processes, understanding the mechanisms underlying heavy metal adsorption is crucial [24]. To characterize adsorbents, optimize operating conditions, improve the modeling and prediction of adsorption processes, and better understand their mechanisms, modern data-driven approaches, particularly ML, have emerged as powerful tools with considerable potential to enhance water treatment processes [25-28]. ML, a subset of artificial intelligence, enables the analysis of large, complex, and multidimensional datasets to develop predictive models and improve learning performance. Various algorithms, including ANNs, random forests, gradient-boosted machines, support vector machines (SVMs), K-nearest neighbors (KNN), and decision trees, have been widely applied to model heavy metal adsorption in aquatic systems[28, 29]. Despite the diversity of ML algorithms and modeling strategies, systematic comparisons and critical evaluations of their predictive performance in adsorption studies remain limited. Existing reviews have primarily focused on adsorption mechanisms, experimental performance, or specific ML applications, while comprehensive comparative assessments of ML algorithms for heavy metal adsorption in water treatment systems are still lacking. Moreover, model performance, input variable importance, and generalization capability across different datasets have rarely been systematically evaluated. Therefore, this review systematically compares and critically evaluates ML approaches used to predict heavy metal adsorption, highlights their strengths, limitations, and applicability, and identifies key research gaps to guide future developments in data-driven water treatment modeling.

Methods

The review was conducted in 2026 based on the Preferred Reporting Items for Systematic Review(PRISMA)[30] guidelines .

a. Defining the research question

Based on an adapted PICO framework appropriate for methodological systematic reviews, the research questions were defined as follows:

- **Population (P):** Adsorption systems employed for the removal of HMs from aqueous environments using various adsorbent materials.
- **Intervention (I):** Application of ML algorithms to predict adsorption performance in heavy metal removal processes.
- **Comparison (C):** Evaluation of different ML algorithms and/or adsorbent materials in terms of their predictive performance and modeling

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capabilities.

• **Outcome (O):** Prediction accuracy and overall model performance assessed using evaluation metrics such as R^2, RMSE, MAE, and other relevant indicators.

b. Developing a protocol : In the second stage, relevant keywords were identified in line with the study objectives and research questions through consultation with environmental health experts and a review of the existing literature. Inclusion and exclusion criteria were then defined in accordance with the research aims. After identifying eligible studies, data extraction and analytical synthesis were performed. The review protocol was established a priori and guided all stages of study selection, data extraction, and synthesis, with no deviations from the predefined protocol during the review process.

c. Conducting a comprehensive search: To identify relevant studies, a systematic search was conducted across four databases (PubMed, Scopus, Google Scholar, and ScienceDirect) using predefined keywords and structured search strategies. The search covered studies published from 2010 to December 2024. Search strategies were developed based on the PICO framework, applying a combination of keywords and controlled vocabulary terms with appropriate Boolean operators and logical grouping. The full search strategies and keyword combinations for each database are provided in Table 1. All databases were last searched on December 31, 2024. No additional sources, including trial registries, organizational repositories, reference lists, or institutional databases, were consulted.

Table 1. Keywords and controlled vocabulary terms combination in the search strategy based on the PICO approach.

Search strategy	Database
("Machine Learning"[MeSH Terms] OR "Machine Learning"[Title/Abstract] OR "artificial intelligence"[Title/Abstract] OR "artificial neural network*"[Title/Abstract] OR "deep learning"[Title/Abstract] OR "random forest"[Title/Abstract] OR "support vector machine"[Title/Abstract] OR "support vector regression"[Title/Abstract] OR "XGBoost"[Title/Abstract] OR "ANFIS"[Title/Abstract]) AND ("predict*"[Title/Abstract] OR "model*"[Title/Abstract] OR "estimat*"[Title/Abstract]) AND ("adsorption"[Title/Abstract] OR "adsorbent*"[Title/Abstract] OR "biosorption"[Title/Abstract]) AND ("heavy metal*"[Title/Abstract] OR "metal ion*"[Title/Abstract] OR "lead"[Title/Abstract] OR "cadmium"[Title/Abstract] OR "chromium"[Title/Abstract] OR "arsenic"[Title/Abstract] OR "mercury"[Title/Abstract] OR "nickel"[Title/Abstract] OR "copper"[Title/Abstract] OR "zinc"[Title/Abstract]) AND ("water"[Title/Abstract] OR "wastewater"[Title/Abstract] OR "aqueous"[Title/Abstract])	PubMed
TITLE-ABS-KEY ("machine learning" OR "artificial intelligence" OR "artificial neural network") AND TITLE-ABS-KEY (adsorption OR biosorption) AND TITLE-ABS-KEY ("heavy metal*" OR cadmium OR lead OR chromium OR arsenic) AND TITLE-ABS-KEY ("water treatment" OR "aqueous solution*" OR wastewater OR "water purification")	Scopus
("machine learning") AND ("heavy metal") AND ("adsorption") AND (("water treatment") OR ("aqueous solution"))	Google scholar
("machine learning") AND ("heavy metal") AND ("adsorption") AND (("water treatment") OR ("aqueous solution"))	Science direct

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d. Assessment and selection of studies: The search and screening process was independently conducted by two reviewers (RH and OY) and verified by a third reviewer (AD). Any disagreements were resolved through discussion and consensus, with arbitration by the third reviewer when necessary. The full screening workflow followed a structured multi-stage process, including title screening, abstract screening, and full-text assessment, with predefined inclusion and exclusion criteria applied at each stage. Duplicate records were removed using EndNote software and manual verification. For Google Scholar, only the first 200 results ranked by relevance were screened. Data extraction was independently performed by two reviewers (RH and OY) using a standardized form and cross-checked by a third reviewer (AD). No automation tools, ML-based screening systems, or semi-automated eligibility tools were used at any stage of study selection or data extraction. Inter-reviewer agreement during full-text screening was almost perfect (Cohen's $\kappa = 0.83$).

Inclusion criteria: Studies were included if they met all of the following criteria.

1. Published in English.
2. Investigated the adsorption-based removal of HMs from aqueous solutions.
3. ML algorithms or related data-driven predictive models, including ANN, SVM, deep neural networks (DNN), adaptive neuro-fuzzy inference systems (ANFIS), Kriging models, hybrid ML models, and ML models integrated with optimization techniques, have been applied to predict, model, or optimize adsorption processes.
4. Sufficient methodological details and model performance metrics were reported to enable data extraction.
5. Full-text articles were accessible.

Exclusion criteria: Studies were excluded if they met the following criteria:

1. It did not focus on the adsorption processes for heavy metal removal from aqueous environments.
2. ML algorithms or related data-driven predictive models were not employed for adsorption prediction, modeling, or optimization.
3. Optimization algorithms were used alone without an underlying predictive model.
4. Review articles, conference abstracts, editorials, letters, book chapters, or other non-original research publications.
5. Lacked sufficient methodological information or relevant performance outcomes.
6. Full texts were unavailable.

Based on the search strategies, 1,806 studies were retrieved from four databases: Scopus (329), Science Direct (1,173), Google Scholar initially retrieved approximately 16,800 records. After applying publication-type restrictions (e.g., exclusion of review articles, books, and book chapters), approximately 3,690 records remained. Due to the large number of records, the first 200 results ranked by relevance were screened for eligibility and PubMed (104). After removing duplicates and conducting systematic screening, 90 studies were selected for inclusion in the final analysis. The study selection process is illustrated in **Figure 1**.

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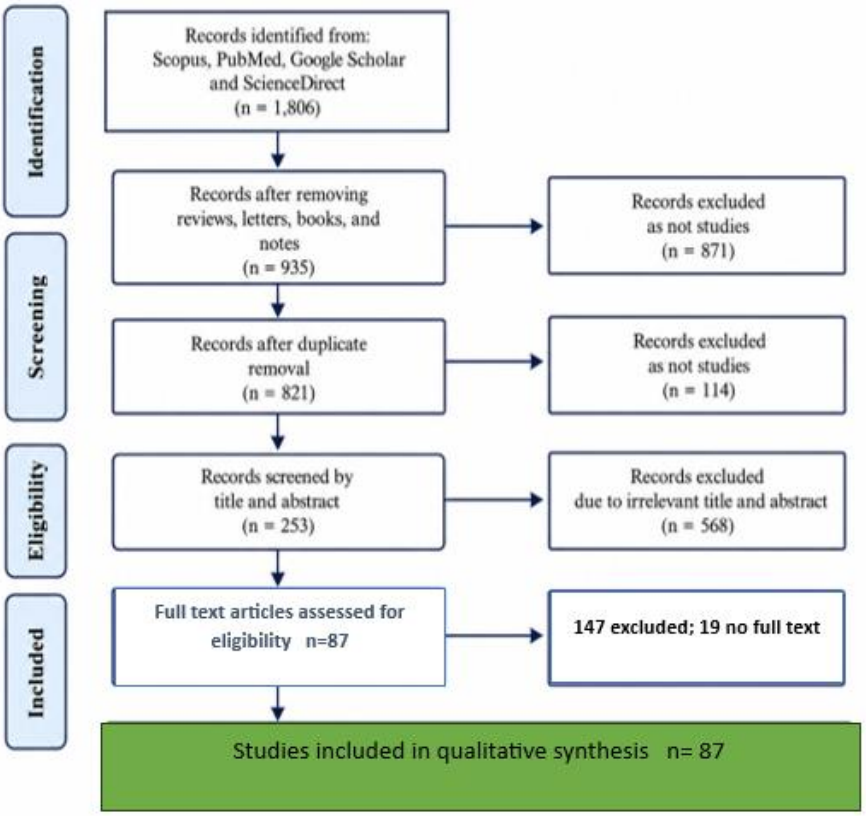

Figure 1. PRISMA diagram of the search methodology.

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e. Assessment of the quality of studies

The methodological quality of the included studies was assessed using a modified CASP-based checklist adapted for ML applications in adsorption research. Although originally developed for qualitative and health-related studies, CASP was selected due to its structured approach for evaluating methodological rigor and reporting quality, and its adaptability to predictive modeling studies. In the absence of a specific tool for ML-based adsorption studies, CASP was used as a baseline framework, although it does not fully capture ML-specific aspects such as hyperparameter tuning and model robustness.

The checklist included ten criteria covering study design, data quality, analysis rigor, and reporting clarity. Each item was scored as 1 (yes) or 0 (no/unclear), with total scores ranging from 0 to 10. The studies were categorized as low (0–3), moderate (4–6), or high (7–10) quality. These categories were used only for comparison purposes and not for exclusion from the study.

No formal publication bias or statistical heterogeneity analyses were performed owing to study heterogeneity.

A structured data extraction form was developed to collect general and technical information in line with the study objectives and research questions. The extracted variables included article title, authors, publication year, ML algorithms, adsorbent type, target HMs, dataset size, validation methods, performance metrics, study limitations, and reference details. A quality assessment field was added to evaluate the methodological rigor and reliability of the study. Data extraction was independently performed by two reviewers (RH and OY) and cross-checked to ensure accuracy and consistency of the data.

g. Data analysis

Data were first extracted using content analysis and then organized in Microsoft Excel for descriptive statistics and frequency analysis. The results summarized the characteristics of heavy metal adsorption in water treatment using ML methods, and findings were presented in tabulated form. The study protocol was approved by the Ethics Committee of Shahid Sadoughi University of Medical Sciences, Yazd (Project No. 19815; Ethics Code: IR.SSU.SPH.REC.1403.156; Approval Date: January 5, 2025). Effect measures (R^2, RMSE, MAE, and related metrics) were used solely for comparative interpretation and ranking of model performance rather than for statistical pooling or meta-analysis.

i. Risk of bias and certainty of evidence

The certainty of evidence was assessed qualitatively based on study quality, dataset size, and validation robustness. No formal GRADE assessment was performed due to heterogeneity of ML methodologies.

j. Additional analyses

No sensitivity analysis, subgroup analysis, or meta-regression was performed because of heterogeneity.

Results

The results were synthesized from 87 peer-reviewed studies. Direct quantitative comparison of performance metrics (R^2, RMSE, and MAE) across studies was not considered statistically appropriate because of substantial heterogeneity in dataset characteristics, adsorption systems, adsorbents, and validation strategies. Therefore, studies were grouped into single models, ensemble methods, and hybrid systems, and findings were synthesized based on performance trends and consistency within each category while preserving the original study context. Validation approaches, including k-fold cross-validation, hold-out testing, and independent validation datasets, were also considered when interpreting model reliability, with greater emphasis placed on studies employing more rigorous validation strategies.

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Table 2. Studies used and compared different models to predict HMs adsorption

Year	Adsorbent	Heavy metal	ML model	Dataset size	Validation method	Performance metrics	Limitations	Ref	Quality
2024	AF–Fe_2O_3 nanoparticles (green-synthesized hematite)	Cr (VI)	ANN, ANFIS	88 data points	70/15/15 train/validation/test split (random sampling)	ANN: R^2 = 0.9952, MAE = 0.0169; ANFIS: R^2 = 0.9901, MAE = 0.0187; RMSE, MSE also reported	Laboratory-scale study; no external validation dataset; limited generalization beyond experimental conditions	31	High
2024	PFMB (Porous Filter Media Block: Fe/Al salts + Moringa biomass & biochar)	As (III)	Linear regression, SVM, Ensemble trees, Gaussian Process Regression (GPR)	507 experimental data points	90/10 train-test split + 5-fold cross-validation	Best model (Optimized GPR): R^2 = 0.9429 (test), RMSE = 6.87, MAE = 5.45	Limited dataset size; model trained on batch experimental data only; potential overfitting risk in small datasets; limited generalizability to real-world systems	32	High
2023	Biochar (including pristine and Fe/Zr-modified biochar)	As(III), As(V)	AdaBoost, LightGBM (LGBoost), XGBoost	As(III): 281 final samples; As(V): 263 final samples (after cleaning) + 106 experimental validation observations	Train/test split (80/20), 5-fold cross-validation, external experimental validation	R^2 (As(III): up to 0.88 test; As(V): up to 0.97 test), RMSE (As(III): 1.40; As(V): 3.51), MAE (As(III) experimental: 3.89)	Limited generalization for As(III) before retraining; dataset heterogeneity from literature; imbalance between literature and experimental ranges; dependence on imputed data	33	High
	Silk fibroin fiber (SFF)	Pb(II), Cr(VI)	Multilayer Perceptron (MLP-ANN); Pb(II): 4–7–1 architecture, Cr(VI): 4–9–1 architecture	280 experimental data points (250 points used for sensitivity/error analyses)	Training–testing–validation split; weighted goodness function (GF) combining training, testing and validation results; regression analysis; cumulative frequency analysis; predicted R^2 (cross-validation) for	Pb(II): GF = 0.834, Total R^2 = 0.989, maximum residual = 2.68. Cr(VI): GF = 22.20, Total R^2 = 0.989, Total error = 10.98, maximum	The performance of ANN depends strongly on the dataset quality and quantity, the risk of overfitting with limited or imbalanced datasets, the extensive hyperparameter optimization required, the computationally intensive	34	High

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Year	Adsorbent	Heavy metal	ML model	Dataset size	Validation method	Performance metrics	Limitations	Ref	Quality
					PRMs	residual = 8.87. MLP predictions outperformed the polynomial regression models.	training, and the polynomial regression, which may fail to capture highly complex relationships, is sensitive to multicollinearity, and becomes impractical for high-dimensional problems.		
2024	GO/GA (Graphene Oxide / Gallic Acid functionalized GO)	Ag(I)	ANN (Cascade-forward backpropagation, Levenberg–Marquardt) + ANFIS (tested but weak)	Not explicitly reported (experimental dataset under multiple conditions: pH, dosage, time, concentration)	Train/Validation/Test split (70% / 15% / 15%) using MATLAB R2008b	ANN: R^2(train)=1, R^2(val)=0.997, R^2(test)=0.984; AAD=0.0092; ARD=0.011. ANFIS: R^2=0.54, ARD=25.52%	Dataset size not clearly reported; ANFIS performed poorly; possible overfitting risk; limited generalization beyond experimental range; outdated software (MATLAB 2008b)	35	High
2024	Metal–Organic Frameworks (MOFs: CoRE-MOFs + h-MOFs database; validated MOFs: HKUST-1, MIL-101, MOF-808, ZIF-8, UiO-66)	Pb(II)	Random Forest (RF), Decision Tree (DT), SVM, KNN, BPNN, Linear Regression (RL)	146,205 total MOFs (137,360 after prescreening; 5,000 for ML training/testing; 1,200 top candidates for screening)	80/20 train-test split + 10-fold cross-validation + grid search hyperparameter tuning + experimental validation	Best model RF: $R^2 \approx 0.94$; also RMSE, MAE, SRCC reported; HKUST-1 experimental capacity ≈ 798.68 mg/g	High computational cost for molecular simulations; dependence on simulated (GCMC/MD) data; limited experimental validation set; uncertainty in water stability of many MOFs	36	High
2024	MOFs (various metal-organic frameworks; modular organic linkers + SBUs)	As(V)	DT, RF, GBDT, HGB, XGB, CatBoost (best: XGB-Morgan)	51 MOFs, 692 adsorption isotherm data points	10-fold cross-validation + train/test split + Bayesian hyperparameter optimization	R^2, MAE, RMSE (best: R^2 = 0.97, RMSE = 11.78, MAE = 7.34)	Limited to 51 MOFs; As(V) only; feature engineering dependent on literature quality; potential bias from curated dataset	37	High
2024	Activated carbon (AC), Biochar (BC), Carbon nanotubes (CNT)	As, Cd, Cr, Cu, Hg, Ni, Pb, Zn	RF, GBDT, XGB (GBDT selected as best model)	3,674 data points from 151 studies	Random 80/20 train–test split; Grid Search (GS); Recursive Feature Elimination (RFE); external validation using	Best model (GBDT): Training R^2 = 0.9998, RMSE = 0.0126; Test R^2 =	Missing key features led to exclusion of many studies; limited coverage for some metals (especially As, Hg, Zn); different oxidation	38	High

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Year	Adsorbent	Heavy metal	ML model	Dataset size	Validation method	Performance metrics	Limitations	Ref	Quality
					108 independent data points from 9 studies	0.9707, RMSE = 0.1420	states of As and Cr were not modeled separately; absence of some adsorbent characteristics (e.g., pHpzc, surface functional groups)		
2024	Ammonia-functionalized magnetic humic acid (AF-MHA)	Pb(II)	RF, SVR, ANN, CatBoost (best)	Not explicitly stated (experimental batch dataset; multiple adsorption runs under varying conditions)	Train-test split (70/30) + model comparison; no external validation reported	R^2, MAE, RMSE (CatBoost best: $R^2 \approx 0.91$ test, RMSE lowest, MAE <10 mg/g error)	Limited dataset size; only Pb(II) studied (no multi-metal generalization); lab-scale batch experiments; no external validation dataset	39	High
2023	Metal–Organic Frameworks (MOFs) (44 types of MOFs including MIL-101(Fe), UiO-66, MIL-53(Al), ZIF-8, etc.)	As(III), As(V)	RF, Gradient Boosting Regression Tree (GBRT), Extreme Gradient Boosting (XGBoost), ANN	Total As: 1508 cases; Inorganic As: 1075 cases; Organic As: 433 cases; External validation: 42 cases	80/20 train–test split; Hyperparameter optimization using GridSearchCV with 5-fold cross-validation; External validation using an independent dataset from five recent studies	XGBoost (best model): Total As: Test $R^2 = 0.93$, RMSE = 0.22; Inorganic As: Test $R^2 = 0.94$, RMSE = 0.22; Organic As: Test $R^2 = 0.96$, RMSE = 0.18; External validation (inorganic As): Validation $R^2 > 0.81$	Database size still limited; important descriptors such as pore volume and functional groups of MOFs were not included; some input values in the external validation dataset fell outside the confidence interval of the training dataset; adsorption mechanisms of different As species require further investigation	40	High
2023	Nano zero-valent aluminum (nZVAl)	Cu(II)	ANN, SVR, LR	108	Hold-out validation (80% training, 20% testing)	ANN: MSE < 10^{-5}; LR: MSE ≈ 10^{-3}; SVR: MSE ≈ 10^{-2}	Synthetic aqueous solution only; no real wastewater validation; reusability/regeneration of nZVAl not evaluated; limited external validation/generalizability	41	High

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Year	Adsorbent	Heavy metal	ML model	Dataset size	Validation method	Performance metrics	Limitations	Ref	Quality
2023	Lanthanum-modified bentonite (B-La)	Pb(II), As(V)	ANN, ANFIS, RSM (quadratic and cubic polynomial models)	63 experimental runs	ANN: train–validation–test split with 15% validation set; ANFIS: train–test evaluation; RSM: ANOVA and correlation analysis	ANN: Train R^2 > 0.99, Test R^2 > 0.94 (~0.97 best). ANFIS: Train/Test R^2 > 0.90. RSM: Pb(II): R^2 = 0.9307; As(V): R^2 = 0.9539. Quadratic model outperformed linear model; cubic model achieved R^2 = 0.9978 for As(V). The NRMSE comparison showed that the ANN had the lowest prediction error.	Small experimental dataset (n = 63); evidence of overfitting after ~25,000 ANN epochs requiring validation; quadratic models showed artificial reverse trends at prolonged contact times that were not experimentally observed; ANFIS performance was lower than ANN; model generalizability to external datasets was not evaluated.	42	High
2023	ZIF-60	Pb(II)	ANN, SVM, RF	20	N-fold cross-validation	RF: R = 0.9632, RMSE = 9.13; ANN: R = 0.9494, RMSE = 9.79; SVM: R = 0.8907, RMSE = 14.04	Small dataset derived from RSM experiments; experiments conducted using synthetic Pb solutions; no external validation on independent datasets; model performance may improve with larger datasets	43	High
2023	ZSM5/Silica Aerogel (ZSM5/SA) composite	Pb(II)	MLP-ANN, SVR (MLR used as a baseline statistical model)	875	ANN: 70% training, 15% validation, 15% testing; SVR: 70/30 and 80/20 train–test split	ANN (trainlm): Test R^2 = 0.9962, MSE = 0.0003; ANN (trainbr):	Single heavy metal (Pb) and single adsorbent system; external validation was not performed; data were	44	High

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Year	Adsorbent	Heavy metal	ML model	Dataset size	Validation method	Performance metrics	Limitations	Ref	Quality
						Test R^2 = 0.9944, MSE = 0.0003; SVR: Test R^2 = 0.9705, MSE = 0.0083 (70/30 split)	obtained from one experimental dataset, limiting generalizability		
2023	Ocimum sanctum leaves powder (OSL) and Syzygium cumini seed powder (SCS)	(Fe)	ANN (MLP 7:10:1:1); SVM (Bayesian optimizer, Quadratic kernel)	75 data points	ANN: 85% training (65), 15% testing (10), plus 10 unseen experiments; SVM: 85% training (65), 15% testing (10), 10-fold cross-validation, plus 10 unseen experiments	ANN: Training R^2 = 0.9964, MSE = 3.70; Additional testing R^2 = 0.9933; Overall accuracy = 99.65%. SVM: Training R^2 = 0.99, MSE = 2.633; Testing R^2 = 0.99, MSE = 0.153. SVM outperformed ANN based on lower MSE.	Small dataset derived from laboratory batch experiments; no external validation; limited to Fe removal using two biosorbents, and not evaluated using real wastewater systems.	45	High
2023	Nano-nickel hydroxide (n-$Ni(OH)_2$)	Cr(VI)	ANN	Not explicitly reported	Train–test–validation split	MAE, MSE, R^2, Maximum Error, Explained Variance	Small experimental dataset; ANN and nonlinear models showed poor performance; model developed using laboratory data only; external validation and pilot-scale verification were not conducted	46	High
	Hydrochar (99 hydrochar types derived from various feedstocks	Pb(II), Cd(II), Zn(II), Cu(II),	ANN, RF, XGB, GBDT (best-performing model: GBDT)	169 adsorption datasets from 29 studies (99 hydrochars)	85:15 train–test split with 5-fold cross-validation; external validation using 14 experimental datasets	GBDT (Test set): R^2 = 0.93, RMSE = 25.65; Training set: R^2 = 0.98,	Relatively small dataset; modification methods were simplified into binary categories	47	High

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Year	Adsorbent	Heavy metal	ML model	Dataset size	Validation method	Performance metrics	Limitations	Ref	Quality
	including agricultural waste, sewage sludge, and microalgae)	Sb(III), Sb(V), Cr(VI), U(VI)			(6 new experiments + 8 literature datasets)	RMSE = 12.67; External validation: R^2 = 0.92, RMSE = 23.77	(modified/unmodified), preventing evaluation of individual modification strategies; Zn adsorption prediction was less accurate because of limited Zn data; heterogeneous experimental conditions among studies		
2023	BWPS, BCMDS (beaded aluminum/iron-based adsorbents)	Fluoride (F^-), As(V)	XGBoost + SHAP	722 samples	Train/test split (9:1, 8:2, 7:3, 6:4) + repeated optimization	R^2 = 0.93, RMSE = 0.429, MAE = 0.33, MAPE = 0.26	Missing features in dataset, reliance on literature data, outlier removal sensitivity, incomplete feature coverage, need for larger datasets	48	High
2022	Rice husk (biochar-based systems)	Hg(II), Ni(II)	Elastic Net, Decision Tree, Gradient Boosting	18 samples	Train/test split (hold-out validation)	R^2 = 0.998 (best GB model), RMSE ≈ 0.103, MAE ≈ 0.086	Very small dataset, limited generalizability, potential overfitting risk, lack of large-scale experimental validation	49	High
2022	Biochar systems (BSs)	Cu(II), Pb(II), Zn^{2+}, As(III), Cd(II), Ni(II)	ANN and optimized ANN (QSA-ANN)	353 experiments (after preprocessing ~282 train / 71 test)	Train-test split + normalization + RMSE optimization + statistical evaluation (R^2, VAF)	Best model: QSA-ANN (RMSE = 0.074, R^2 = 0.960, VAF = 95.882%)	Data heterogeneity across studies, complex real-world BS variability, optimization dependency on dataset quality	50	High
2021	Biochar	Pb(II), Cd(II), (also Zn(II), Cu(II), Ni(II), As(III))	KELM, Kriging (also compared with ANN, RF)	353 datasets	Train/test split + point/group selection + sensitivity & stepwise regression	R^2 up to 0.980, RMSE as low as 0.009 (best in optimized models)	Similarity of data within studies, limited generalization, dependence on experimental conditions	51	High
	Various adsorbents/bio-sorbents (from 7 literature datasets)	(As)	RF, SVR	7 datasets (expanded via natural cubic spline	80/20 train-test split + 10×10 repeated k-fold cross-validation	RF: SRCC = 97.3%, R^2 = 95.9%; SVR: SRCC = 96.3%,	Limited experimental datasets; data scarcity; reliance on interpolated (synthetic) data points;	52	High

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Year	Adsorbent	Heavy metal	ML model	Dataset size	Validation method	Performance metrics	Limitations	Ref	Quality
				interpolation to ~250 points per dataset)		R^2 = 93.9% (also RMSE, MAE reported)	potential overfitting risk due to data augmentation		
2021	Nanotubular halloysite (weathered pegmatites, NaHWP)	Pb(II), Cd(II)	ANN, SVR, TLBO-ANN, TLBO-SVR	Pb: 53 cases / Cd: 56 cases (total experimental datasets ≈ 109) + external validation (Pb=11, Cd=12)	70/30 train-test split + external experimental validation	TLBO-ANN and TLBO-SVR showed the highest accuracy in predicting Pb^{2+} and Cd^{2+} adsorption, with R^2 up to 0.988, VAF >98%, and lower errors than ANN and SVR.	Limitations: Small dataset, dependence of performance on initial conditions (pH, initial concentration), need for larger data for better model generalization	25	High
2021	Biochar (24 types of biomass-derived biochar)	Cu(II), Cd(II), Ni(II), Pb(II), As(III)	BPNN, FCM-BPNN (hybrid clustering + neural network)	353 experimental samples	Train/Test split (70/30), clustering-based validation (FCM + Elbow method for k=4)	RMSE, R^2, MAPE, RSE, VAF (best: R^2 ≈ 0.987, RMSE ≈ 0.036 for FCM-BPNN)	Possible overfitting in small clusters (e.g., cluster 4), model complexity, dependence on preprocessing/normalization, limited interpretability of hybrid model	53	High
2021	Biochar	SEoHM (adsorption efficiency; heavy metals not single-specific, multi-ion systems)	SVM, RF, M5Tree, GP, ANN + ensemble models (BA-, SVM-, RF-, GP-, M5Tree-hybrids; best: SVM-ANN)	Not explicitly stated (multi-study dataset)	Train/test split + statistical metrics + Taylor diagram + boxplot + Q-Q plot	Best model: SVM-ANN (RMSE = 0.046, R^2 = 0.987, MAE = 0.026)	Dataset heterogeneity, GP model instability, poor generalization for some ensemble combinations (e.g., GP-based models)	54	High
2020	GO–Fe_3O_4–CS–EDTA nanocomposite	Pb(II)	RSM (CCD), ANFIS, GRNN	50 experimental runs (CCD design)	ANOVA (RSM), 70/20/10 split (ANFIS), statistical validation (R^2, error	R^2, RMSE, MAE, MSE, AAD, SSE,	Lack of generalizability to large scale, need for testing in continuous system	55	High

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Year	Adsorbent	Heavy metal	ML model	Dataset size	Validation method	Performance metrics	Limitations	Ref	Quality
					indices), GA & desirability optimization	ARE, χ^2	(column & pilot scale), dependence on laboratory conditions, effect of real water matrix, limited investigation		
2020	Nanocellulose-based Fe_3O_4 nanobiocomposites (RH-NIONs, SB-NIONs) derived from rice husk & sugarcane bagasse	As (III)	RSM + ANN (MLP)	30 experimental runs (CCD design, 4 factors, 5 levels)	ANOVA (RSM), train/test/validation split (70/15/15 for ANN)	$R^2 \approx 0.96–0.97$ (RSM), $R^2 \approx 0.99$ (ANN), MSE, RMSE, MAD, MAPE	ANN better prediction than RSM; pseudo-second-order kinetics; Sips isotherm fit	56	High
2020	44 lignocellulosic biomass-derived biochars	Pb, Cd, Ni, As, Cu, Zn	ANN; RF	353 adsorption datasets	10-fold cross-validation; external generalization tests using untrained metals (Cu and Zn exclusion experiments)	ANN: R^2 = 0.948, RMSE = 0.079; RF: R^2 = 0.973, RMSE ≈ 0.057; Generalization tests: RF RMSE = 0.0593 (Cu exclusion), substantially lower than ANN	Small dataset size; relatively high-dimensional input variables; missing data were discarded rather than imputed; only lignocellulosic biochars were included; limited to six heavy metals; ANN performance decreased for low adsorption values and untrained metals	57	High
2019	Lignocellulosic biomass-derived biochars (44 different biochars produced at 300–700 °C from 24 biomass feedstocks)	Pb, Cd, Ni, As, Cu, Zn	ANN; RF	353 adsorption datasets	10-fold cross-validation; additional external generalization tests by leave-one-metal-out (Cu and Zn excluded from training)	ANN: R^2 = 0.948, RMSE = 0.079; RF: R^2 = 0.973, RMSE ≈ 0.057; RF outperformed ANN in predicting low adsorption capacities and untrained metals	Relatively small dataset (353 observations); high-dimensional input features; missing data were excluded rather than imputed; only lignocellulosic biochars were considered; model generalizability evaluated only for Cu and Zn; ANN performance decreased with limited sample size	58	High

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Year	Adsorbent	Heavy metal	ML model	Dataset size	Validation method	Performance metrics	Limitations	Ref	Quality
2019	Oxidized and deep eutectic solvent (DES)-functionalized carbon nanotubes (Ak-CNTs) prepared using APB + glycerol (A-DES) after $KMnO_4$ oxidation	Hg(II)	NARX neural network (best performance), Feedforward Neural Network (FFNN), Linear Regression (LR)	176 samples (151 train/validation, 25 test)	MATLAB-based ANN modeling with train/validation/test split + comparison with experimental data + kinetic model fitting	R^2, RMSE, MSE, RE, MAPE, RRMSE (best: NARX R^2 = 0.9701, RE = 9.79%, MSE = 1.15×10^{-3})	Small dataset, batch system only, no external validation, ANN black-box limitation, experimental variability (pH, dosage, concentration)	59	High
2019	Graphene oxide (GO)	Cu(II)	ANN (3-layer BP), LMA optimized (trainlm)	90 samples (ANN modeling)	Train/validation/test split (70/15/15), MATLAB backpropagation	RMSE = 0.0179, $R^2 \approx 0.97+$, MSE, MAPE, RE	Model sensitivity to hyperparameters; limited generalizability beyond lab-scale batch system	60	High
2019	Nanomagnetic walnut shell–rice husk activated carbon	Cd(II)	(ANN, 4–9–1 architecture) + 2-level factorial design	16 experimental runs (DoE-based dataset)	Train/validation/test split (60% / 30% / 10%); also external comparison with experimental optimum	R^2 = 0.9967 (ANN), Average absolute error = 1.2931% (ANN), R^2 = 0.9055 (DoE model), Avg error = 4.806%	Limited dataset size (only 16 runs); single-metal system (Cd only); lack of external real wastewater validation; possible overfitting risk due to small dataset; limited generalizability to other metals/adsorbents	61	High
2019	DES-functionalized CNTs (KTEG-CNTs)	Pb(II)	FF-NN, ANFIS	158 experimental data points	Train (73%), validation (12%), test (15%)	MSE, RMSE, RRMSE, MAPE, R^2	Limited dataset size, single adsorbent system, lack of external validation, experimental variability, model dependency on lab-scale conditions	62	High
2018	Nickel oxide (NiO) nanoparticles (sol–gel synthesized)	Cr(VI) (Hexavalent chromium)	ANN, feed-forward backpropagation, 4:10:1 architecture + Response Surface	30 experimental runs (CCD-RSM design) used for modeling; ANN trained on	Data split into training/validation/testing sets; comparison of ANN vs RSM; regression analysis; error analysis	ANN: $R^2 \approx 0.93$–0.99, MSE minimized (≈ very low), strong agreement with experimental	Limited experimental dataset (small sample size); dependence on RSM-generated data for ANN training; lack of external validation dataset; potential	63	High

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Year	Adsorbent	Heavy metal	ML model	Dataset size	Validation method	Performance metrics	Limitations	Ref	Quality
			Methodology (RSM) for comparison	RSM-generated + experimental data		data; RSM: R^2 = 0.9597	overfitting risk due to limited independent testing data; only single adsorbent and single metal system studied		
2018	Palm oil kernel shell–derived activated carbon (POKS-based AC)	Zn(II)	ANN Differential Evolution optimized ANN (ANN-DE) Feed-forward ANN (5–6–1 topology) RSM (baseline statistical model)	50 experimental runs (CCD design) Expanded to ~270 data points (cubic spline interpolation) Split: 70% train / 15% test / 15% validation	Train/test/validation split Triplicate experimental averaging External validation dataset ANOVA (RSM significance testing) Residual analysis (normal probability plot, studentized residuals)	R^2 (RSM = 0.852, ANN-DE ≈ 0.994–0.995) RMSE (ANN-DE ≈ 0.248) SSE AAD (≈ 0.022 for ANN-DE) ARE Pearson Chi-square MPSD	Small experimental dataset (only 50 runs) Data augmentation required (interpolation) ANN-DE is computationally intensive Black-box nature of ANN (low interpretability) Requires parameter tuning (DE optimization) Limited generalization outside studied operating range	64	High
2017	Activated carbon (Medlar seed, AC-7)	Cr(VI)	ANN, GA-SVR	59 experimental data points	70% training / 30% testing, random split, normalization (0–1), GA optimization for SVR parameters	ANN → R^2 = 0.958 ; GA-SVR → R^2 = 0.981	ANN (overfitting risk, local minima, low generalization); SVR (parameter sensitivity, kernel dependence, computational cost of GA tuning)	65	High
2017	Peanut shell, Almond shell	Cr(VI)	ANN (Multilayer Perceptron: Gradient Descent, Levenberg–Marquardt)	1063 data points	70% training / 20% cross-validation / 10% testing	MSE, AARE, SD (σ), R, R^2, χ^2	Lack of interpretability of the model (black-box nature), dependence on fixed-bed laboratory data, lack of use of independent external validation	66	High
2017	nZVI/rGO composites (nano	Cd(II)	RSM (Response Surface	29 experiments (BBD design:	80/20 train-test split (ANN), Box-Behnken	R^2 (RSM: 0.9913; ANN-	Small experimental dataset; RSM limited to quadratic	67	High

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Year	Adsorbent	Heavy metal	ML model	Dataset size	Validation method	Performance metrics	Limitations	Ref	Quality
	zero-valent iron / reduced graphene oxide composite)		Methodology), ANN-BP + GA (ANN with Backpropagation + Genetic Algorithm)	24 training + 5 testing; plus confirmatory batch experiments in triplicate)	Design (RSM), ANOVA, confirmatory experiments (triplicate)	GA: 0.9999), MSE (~0.002461 best ANN), average prediction error (RSM: 6.47%, ANN-GA: 1.08%)	assumptions; ANN risk of overfitting and lack of interpretability; limited operating range (pH, concentration, temperature); requires additional experiments for generalization		
2017	Functionalized carbon nanotubes (mK-CNTs: $KMnO_4$ pre-oxidized and deep eutectic solvent-modified multi-walled carbon nanotubes)	As(III)	ANN, Feed-forward Backpropagation (BP-ANN, MATLAB R2014a)	213 batch adsorption experiments (188 training + 25 testing)	Train-test split (88% training / 12% testing), MSE-based training, correlation coefficient (R^2), error convergence monitoring	$R^2 = 0.9968$ (testing phase) MSE = 1.54×10^{-4} RMSE, RRMSE, MAPE also used (low error range overall) Maximum relative error ≈ 5.97%	Moderate dataset size for ANN training, limited experimental range of variables, potential overfitting risk despite good test performance, model not externally validated on independent datasets, and applicability limited to lab-scale batch systems.	68	High
2017	DES-functionalized carbon nanotubes (KTEG-CNTs: oxidized CNTs modified with choline chloride: triethylene glycol deep eutectic solvent)	Pb(II)	Feed-forward Backpropagation ANN (FBNN) + Layer Recurrent Neural Network (LRNN) ANN vs LRNN (recurrent architecture)	158 experimental data points (batch adsorption experiments)	Train-test split (best: 85% training / 15% testing), trial-and-error architecture tuning, ANOVA-like performance comparison, multiple training algorithms	- FBNN: $R^2 \approx 0.9956$ - MSE ≈ 1.66×10^{-4} - RMSE ≈ 1.28×10^{-2} - MAPE ≈ 4.10% - LRNN weaker (MSE ≈ 7.22×10^{-4}, MAPE ≈ 5.60%)	Small experimental dataset (158 points), risk of overfitting in ANN, limited generalization beyond studied ranges, model sensitivity to network structure and training function, lack of external validation dataset	69	High
2017	Steam-activated mung bean husk carbon (SAC-	As(V)	ANN (Feed-forward backpropagation),	20 experimental runs (CCD design)	Train/test based on CCD experimental matrix (MATLAB ANN training;	$R^2 \approx 0.9969$ (ANN), $R^2 \approx$ 0.9883 (RSM),	Limited dataset size (only 20 runs), lack of external validation dataset, model	70	High

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Year	Adsorbent	Heavy metal	ML model	Dataset size	Validation method	Performance metrics	Limitations	Ref	Quality
	MBH)		RSM (comparative model)		RSM ANOVA validation)	RMSE, AAD	dependent on experimental design (CCD), limited generalization		
2016	Talc / Fe_3O_4 nanocomposite	Pb(II), Ni(II), Cu(II)	Wavelet Neural Network (WNN), ANN comparison (IBP, QP, BBP, GA, LM)	19 experimental CCD runs (13 training + 6 test)	Train/test split (13/6), internal validation via RMSE minimization, repeated runs (10 times), RSM-CCRD comparison	R^2 up to 0.982 (Pb), 0.981 (Ni), 0.996 (Cu); RMSE as low as 1.36; best model IBP-3-14-3	Small dataset, no external validation, overfitting risk, dependent on CCD design, limited generalizability to real wastewater	71	High
2015	Shell dust of Lymnaea luteola (calcium carbonate-based biosorbent)	Cd(II)	ANN (Multilayer Perceptron)	69 experimental datasets	Training/validation/testing split (SPSS-based ANN modeling)	$R^2 \approx 0.924$ (predicted vs observed), Langmuir fit $R^2 = 0.997$, pseudo-second-order $R^2 \approx 0.998–0.999$	Limited dataset size, laboratory-scale batch system only, lack of external validation, no real wastewater application, model depends on limited operating conditions	72	High
2015	M-PAC (magnetite–powder activated carbon); ZnO nanoparticle–activated silica–Coriandrum sativum (ZnO-NPs-AS-Cs)	Ni(II), Co(II), Cd(II), As(III)	ANN, Multilayer Perceptron (MLP), Backpropagation (BP), Levenberg–Marquardt (LM) algorithm	Experimental data from batch adsorption studies (exact number not explicitly reported; derived from multiple operating conditions)	Train/test split, regression analysis (R), sensitivity analysis, comparison of BP vs LM performance	$R \approx 0.999$ (best model), MSE ≈ 7.06 (LM model), high agreement between predicted and experimental values	Possible overfitting due to hidden neurons selection; dataset size not clearly specified; dependence on experimental range limits generalization; sensitivity to input variable selection	73	High
2015	Dead and living Trichoderma viride biomass	Cd(II)	SVM–AGA (Support Vector Machine + Adaptive Genetic Algorithm)	Not explicitly reported (batch experimental dataset; multiple conditions of pH, time,	Cross-validation (for SVM tuning) + experimental batch validation	$R^2 = 0.919$, MSE = 0.85, removal efficiency up to 98.91% (optimized conditions)	Small-scale laboratory dataset, lack of external/independent validation, limited generalizability to real wastewater systems, potential overfitting due to	74	High

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Year	Adsorbent	Heavy metal	ML model	Dataset size	Validation method	Performance metrics	Limitations	Ref	Quality
				temperature, dosage, concentration)			limited sample size		
2012	Black cumin (Nigella sativa seeds)	Pb(II)	ANN + Response Surface Methodology (CCD-RSM)	20 experimental runs (CCD design; 70–15–15 split for ANN validation)	Central Composite Design (CCD) + ANN train/validation/test + external validation runs	ANN: $R^2 \approx 0.96$–0.98, RMSE ≈ 0.557; RSM: R^2 ≈ 0.81, RMSE ≈ 1.167	Limited experimental size; ANN prone to overfitting; RSM limited to quadratic models; no large-scale/field validation	75	High
2013	Zeolite prepared from raw fly ash (ZFA)	Cr(VI)	ANN	~30 experimental datasets (70% train, 15% validation, 15% test)	Train/Validation/Test split + early stopping	$R^2 \approx 0.98$, MSE ≈ 2.7×10^{-4}	Limited dataset size; batch experiments only; lack of external validation; possible overfitting risk due to small data	76	High
2013	Cloisite C20A–PCL clay–polymer composite (melt-blended polymer composite)	Pb(II)	ANN (feed-forward MLP; TRAINLM, TRAINBFG, TRAINOSS, TRAINCGB, TRAINGF compared; best: TRAINLM)	100 experimental data points	Training/validation/testing split (data partitioning ~70:15:15 optimal)	$R^2 \approx 0.999$–1.000; MSE ≈ 0.007–0.0075 (best model LM)	Limited generalization beyond experimental conditions; reliance on small experimental dataset; potential overfitting risk with neuron optimization	77	High

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Table 3. Studies used a special ML model to predict the adsorption of HMs.

Year	Adsorbent	Heavy metal	ML model	Dataset size	Validation method	Performance metrics	Limitations	Ref	Quality
2024	Scolecite (natural zeolite)	As (III/V)	ANN	~34 water samples (multiple sites in India)	Experimental validation + correlation analysis (R^2 over 1–7 days, batch adsorption tests)	Removal efficiency up to 80–94%; $R^2 \approx 0.77$–0.99; significant reduction to below 10 ppb in some industrial samples	Small dataset; heterogeneity of water samples; variable geochemical conditions (oxidizing/reducing environments); limited ML validation details (no k-fold/hold-out clearly reported); site-specific results may limit generalization	78	High
2024	Porous Filter Media Block (PFMB) – gypsum + Fe/Al salts + Moringa bark biochar/biomass	As (III)	ANN	507 experimental datasets (9 input features)	Train/validation/test split (70/15/15), hyperparameter tuning (LM, BR, SCG), SHAP + PDP interpretation	$R^2 = 0.95$ (train/val); RMSE ≈ 6–7.7 µg/g; removal capacity ≈ 98.29 µg/g; Langmuir $R^2 = 0.976$; PSO kinetics $R^2 = 0.998$	Limited experimental range (0.1–8 ppm); possible overfitting risk; dataset from controlled batch experiments only; limited field validation; high dependence on initial concentration bias	79	High
2024	Zeolite-embedded sheet (ZES)	Cu, Pb, Zn	RF	Experimental dataset (9 concentration levels per metal; lab-scale adsorption data)	Out-of-bag (OOB) validation + model testing	RMSE, MSR, % variance explained (99%+), OOB error	Limited dataset size, lab-scale conditions, model tuning sensitivity, RF computational complexity	80	High
2024	Bentonite (natural clay adsorbent)	Pb, Cu, Cd, Zn, Ni, Cr, Co	SVR, DT, RF, ET, GBDT, XGB (best: XGB)	556 samples	Train/test split (75/25), 10-fold cross-validation, hyperparameter tuning (GridSearchCV + RandomizedSearch	$R^2 \approx 0.95$–0.97 (test, XGB), error ≈ 1.16 mg/g	Heterogeneity of literature data; differences in adsorption methods (batch/shaking); limited handling of multi-metal competition; not	81	High

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Year	Adsorbent	Heavy metal	ML model	Dataset size	Validation method	Performance metrics	Limitations	Ref	Quality
					CV), experimental validation with lab adsorption kinetics		applicable to regenerated bentonite; possible multicollinearity with expanded features; dataset extracted from literature (not fully controlled experiments)		
2024	Cherry stalks (NCS, BCS, ACS)	Cr(III), Cr(VI)	ANN (feed-forward neural network)	90 experimental data points (62 train / remaining test)	Train/test split + MATLAB R2017a regression + RMS error evaluation	R^2 not fully reported; RMS error used; reported good regression fit and high predictive accuracy (>0.9 implied in conclusion)	Limited dataset size; lack of external validation; limited reporting of full performance metrics (RMSE/MAE/MAPE not fully provided)	82	High
2024	GO–CTS–PANI nanocomposite (Graphene oxide–Cu_2SnS_3–Polyaniline)	Hg(II)	RF	17 instances	K-fold cross-validation (K optimized = 12, WEKA 3.9, grid search)	R^2 = 0.982; MAE = 6.16; RMSE = 7.25; RAE = 38.7%; RRSE = 38.26%; Experimental removal = 95%	Very small dataset (n=17), limited input features (pH, dose, time), potential overfitting risk, lab-scale study, limited external validation	83	High
2023	Bentonite, Activated Carbon	Ni(II), Pb(II)	ANN, 6-10-1 topology, Levenberg–Marquardt algorithm	1000 samples (500 per metal)	Train/Validation/Test split (80/10/10), MATLAB validation + test set evaluation	MSE = 3.72×10^{-4}; R^2 = 0.99430 (test), 0.99439 (validation)	Limited dataset size; reliance on literature + experimental data; performance depends on data quality and may not generalize to other systems	84	High
2023	Abies bornmulleriana cones (normal & modified biosorbent)	Pb (II)	ANN – Backpropagation (7-9-2, dual-output)	160 data points	Random split: Training (80), Validation (40), Test (40)	R^2 = 0.982 (normal), 0.976 (modified); RMSE = 3.59–5.78; MAE = 0.28–1.16; SDR = 0.13–0.15	Laboratory-scale study; synthetic wastewater; limited real industrial effluent data; single-metal system (Pb^{2+});	85	High

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Year	Adsorbent	Heavy metal	ML model	Dataset size	Validation method	Performance metrics	Limitations	Ref	Quality
							dependency on experimental conditions		
2023	Cobalt hydroxide nano-flakes ($Co(OH)_2$)	Pb(II), Cu(II)	ANN (Feedforward Backpropagation ANN, LM algorithm)	25 training samples + 8 validation/test samples (D-optimal experimental design)	Train/validation/test split + additional random validation experiments	MSE = 0.020 (Pb), 0.017 (Cu); $R^2 \approx 0.99$; relative error < 1%	Small dataset; laboratory-scale study; limited generalizability without larger real-world datasets	86	High
2023	Nb_2CTx (MXene)	Pb(II), Cd(II)	Crystal Graph Convolutional Neural Network (CGCNN)	2600 crystal geometries (26 surfaces × 100 configurations each)	70% training / 30% testing split; DFT-based labels used as ground truth	R^2 (Pb: 0.990–0.993; Cd: 0.985–0.994), MAE (Pb: ~0.083–0.095 eV; Cd: ~0.029 eV), RMSE (Pb: ~0.142–0.162 eV; Cd: ~0.041–0.060 eV)	High computational cost of DFT data generation; limited generalization to defected surfaces (lower $R^2 \approx 0.78$); dataset specific to Nb_2CTx; synthesis and surface functional variability	87	High
2023	Waste tire activated carbon (WTAC)	Cr(VI)	ANN (LM, BR, SCG; best: traincgb)	79 data points	70:15:15 split (train/val/test), regression analysis	Best: $R^2 = 0.977$, RMSE = 2.384, MAE = 1.630	Limited dataset size; possible generalization uncertainty; moderate error variability	88	High
2023	Biochar derived from walnut shell and hazelnut shell	Pb(II)	ANN training algorithms: LevenbergMarquardt (LM), Bayesian Regularization (BR), and Scaled Conjugate Gradient (SCG)	14 experimental observations for each adsorption system (training:validation:testing = 6:4:4; 50:25:25 split)	Hold-out validation (50% training, 25% validation, 25% testing)	Walnut shell biochar: $R^2 = 0.97$; MSE = 0.011 (training), 0.0063 (validation), 0.0095 (testing). Hazelnut shell biochar: $R^2 = 0.98$; MSE = 0.051 (training), 0.0015 (validation), and 0.0024 (testing). The performance ranking was LM > BR > SCG.	Very small dataset size (n = 14 per adsorbent); hidden neurons selected by trial-and-error; no external or cross-validation; only Pb(II) adsorption examined; model applicability to other adsorbents and operating conditions remains uncertain.	89	High
2023	Carbon-based	As(III),	Random Forest	108 materials	80/20 train-test split	$R^2 = 0.874$–0.927;	Lack of detailed iron	90	High

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Year	Adsorbent	Heavy metal	ML model	Dataset size	Validation method	Performance metrics	Limitations	Ref	Quality
	materials (biochar, activated carbon, graphene oxide) and iron-modified forms (Fe-BC, Fe-AC, Fe-GO)	As(V)	(RF)	from 109 publications (past decade)	+ 10-fold cross-validation + external test set	RMSE reduced up to 44.7% (Model SFA) and 56.9% (Model SFB) vs baseline models	speciation; heterogeneous datasets; limited microscopic SOFG data in some samples; absence of experimental validation for predicted optimal thresholds (e.g., O/C, C–O, C=O ranges); potential bias from mixed CBMs/Fe-CBMs		
2022	Ni50Co50-LDH / UiO-66-(Zr)-$(COOH)_2$ nanocomposite	Hg(II), Ni(II)	ANN, multilayer perceptron (2 hidden layers)	~18 experimental data points (literature-derived adsorption isotherms)	k-fold cross-validation (K=3), train/test split	$R^2 > 0.999$ (training & validation), very low RMSE and SSE reported	Small dataset, limited generalization, purely data-driven model, lack of mechanistic interpretability, dependent on literature quality	91	High
2022	Clay minerals (montmorillonite, kaolinite, sepiolite, attapulgite, illite, rectorite, bentonite and others)	Multiple heavy metals (e.g., Pb^{2+}, Cu^{2+}	Deep Learning Neural Network (Feedforward ANN with two hidden layers) + Pearson sensitivity analysis	128 studies identified; approximately 78% retained for modelling (~100 studies)	Internal split validation using different training/validation schemes: First parameter set: 78% training, 12% validation; other parameter sets: 62% training and 14% validation or 39% training and 11% validation. Multiple repeated training (50, 80, or 100 iterations) were	Overall performance goals were reported as error values close to zero (0.0143–0.0452); Pearson correlation coefficients were used for sensitivity analysis. No standard predictive metrics, such as R^2, RMSE, MAE, MSE, or VAF, were reported.	External validation was not performed; testing proportions were not consistently described; adsorption data were compiled from heterogeneous literature sources; exact sample numbers used for each parameter subset were not reported; and the absence of commonly accepted predictive metrics limits direct comparison with other ML studies.	92	High

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Year	Adsorbent	Heavy metal	ML model	Dataset size	Validation method	Performance metrics	Limitations	Ref	Quality
					averaged.				
2022	Multi-walled carbon nanotubes (MWCNTs) synthesized from *Azadirachta indica* oil via CVD-assisted spray pyrolysis	Cr(VI)	ANN (MLP, feed-forward backpropagation) combined with RSM-Box–Behnken Design	27 experiments	Random split: 70% training (n=19), 15% validation (n=4), 15% testing (n=4)	Overall: R^2 = 0.9611; Best ANN: R^2 = 0.99512; MSE = 0.0324; Training R = 0.99757; Validation R = 0.99884; Testing R = 0.83074	Small dataset (27 samples); risk of overfitting due to limited observations and multiple iterations; recovery and regeneration of MWCNTs are difficult and expensive; potential secondary pollution from spent adsorbents; industrial-scale CNT production remains challenging	93	High
2022	CoAl-LDH and bentonite-CoAl-LDH (bentonite-intercalated layered double hydroxide)	Cr(VI)	ANN-LMA (Levenberg–Marquardt Artificial Neural Network); RSM (Response Surface Methodology)	17 FC-CCD experiments for adsorption capacity modeling; additional independent datasets for thermodynamic and kinetic studies (exact total sample size not explicitly reported)	ANN: 70% training, 15% validation, 15% testing; RSM: FC-CCD with duplicated randomized experiments and 3 center-point replicates	ANN (FC-CCD): R^2 = 0.995–0.997, RMSE = 3.092–2.982; RSM (FC-CCD): R^2 = 0.998–0.999, RMSE = 0.195–1.774; ANN (equilibrium): R^2 = 0.992–0.993, RMSE = 4.089–4.990; ANN (kinetics): R^2 = 0.998–0.999, RMSE = 6.75–17.32	Small FC-CCD dataset; RSM predictions restricted to the experimental design space; RSM unable to predict kinetic behavior due to absence of time as an input variable; lack of sensitivity and independent variable analyses for mechanistic predictions	94	High
2022	Carbon-based adsorbents derived from hazelnut shells (500°C biochar) and walnut shells	Cu(II)	ANN using Feed-Forward Backpropagation with Levenberg–Marquardt (LM)	Not explicitly reported (experimental data split into training/validation	Data division of 50% training, 25% validation, and 25% testing; hidden neurons selected by	Walnut shell biochar: R^2 = 0.99 (training, validation, testing); MSE = 0.43, 0.55, 0.21. Hazelnut shell	Exact number of observations was not reported; model evaluated only for Cu(II); ANN	95	High

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Year	Adsorbent	Heavy metal	ML model	Dataset size	Validation method	Performance metrics	Limitations	Ref	Quality
	(700°C biochar)		algorithm	/test sets)	trial-and-error	biochar: $R^2 = 0.99$ (training, validation, testing); MSE = 0.27, 0.22, 0.43	architecture optimized by trial-and-error; no external validation dataset was used		
2022	Rice bran	Cr(VI), Cu(II)	MLR; GA-ANN (MLP optimized with Genetic Algorithm and Levenberg–Marquardt training)	Cr(VI): 358 samples; Cu(II): 349 samples	Data randomization performed three times; 70% training, 20% cross-validation, 10% final prediction	MLR: Cr(VI): R = 0.9676, variance = 0.0540; Cu(II): R = 0.9674, variance = 0.0543. GA-ANN: Cr(VI): MSE = 1.85×10^{-8}–4.07×10^{-8}, AARE = 0.000357–0.001845, SD = 0.000740–0.004203, CCC (R) = 1.00, χ^2 = 3.60×10^{-5}–2.59×10^{-3}. Cu(II): MSE = 3.10×10^{-8}–4.07×10^{-8}, AARE = 0.000364–0.001705, SD = 0.000684–0.006762, CCC (R) = 1.00, χ^2 = 2.29×10^{-4}–2.71×10^{-3}.	Only one adsorbent (rice bran) was evaluated; pH was fixed and excluded from ANN inputs; external validation was not performed; the study focused on fixed-bed column conditions, limiting its generalizability to other adsorption systems.	96	High
2022	Spent macroalgal biomass (*Ulva prolifera*)	Cr(VI)	ANN + RSM (Response Surface Methodology + Feed-forward ANN)	31 experimental runs (CCD design)	RSM: ANOVA + optimization; ANN: 80% train / 10% validation / 10% test	R^2 (ANN)=0.9844, R^2 (RSM)=0.9721; MSE (ANN)=3.7002; RMSE (ANN)=1.9236; R=0.99219	Small dataset; limited generalization beyond experimental CCD range; single adsorbent system; lab-scale batch study	97	High
2022	Orange zest biochar	Cu(II)	FFBPNN (Feed Forward Back Propagation Neural Network), BBD (Response	15 BBD runs + experimental validation	Train/validation/test split (70:15:15), experimental verification, CV analysis, model	$R^2 > 0.9$ (ANN); CV = 3.47%; max adsorption capacity = 116.28 mg/g; removal up to 99.61%; Langmuir R^2	ANN cannot handle multi-response simultaneously (trained separately); limited experimental design (15	98	High

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Year	Adsorbent	Heavy metal	ML model	Dataset size	Validation method	Performance metrics	Limitations	Ref	Quality
			Surface Methodology)		comparison	= 0.9062; pseudo-first-order kinetics best fit	runs); model sensitivity to architecture and parameters		
2022	Mesoporous $CoFe_2O_4$/GO nanocomposites	As(III)	ANN (BP-ANN), GA-ANN, PSO-ANN, RF, RBF, RSM, GBRT, Garson feature analysis	30 CCD experimental runs	ANOVA, experimental verification, train/test split for ANN, optimization convergence (GA/PSO iterations)	R^2 = 0.9986 (best ANN-GA); R^2 = 0.9877 (RSM); MSE = 0.0028; removal efficiency up to 86.62%; absolute error ~1.98–3.08%	RF and RBF showed weaker prediction performance; possible overfitting in decision tree-based models; ANN sensitivity to architecture; limited dataset size (30 runs); model dependency on experimental conditions	99	High
2021	Calcined Mg–Fe–LDH (layered double hydroxide)	As(V) (Arsenate) in binary system with Pb(II), Ca(II), Fe(III)	ANN for multivariate adsorption modeling + binary isotherm modeling (modified Langmuir, Langmuir–Freundlich)	180 experimental datasets (univariate batch adsorption experiments; 25 additional validation runs)	Train/validation/test split (70/15/15), external validation set (25 runs), MATLAB-based ANN optimization, sensitivity analysis	$R^2 > 0.99$ (adsorption capacity and removal efficiency); low RMSE and χ^2 (0.118–1.141); F-value up to 551,319; validation $R^2 \approx 0.98$–0.99; strong agreement between predicted and experimental values	Strong co-ion interference (especially PO_4^{3-} significantly reduces As(V) adsorption); model dependent on lab-scale batch data; limited real groundwater validation; competition effects reduce generalizability; ANN sensitive to input ion matrix assumptions	100	High
2021	Mesoporous $CoFe_2O_4$/GO nanocomposites	As (III)	BP-ANN, ANN-GA, ANN-PSO, RSM, RF, RBF, GBRT	30 experimental runs (CCD design)	Train/test split (ANN), CCD-RSM design validation, experimental verification	R^2 = 0.9986 (ANN-GA), RMSE/MSE (low), removal efficiency ≈ 84–86%, absolute error ≈ 1.98–3.08%	RF and RBF had lower prediction accuracy; limited generalization of some ML models; experimental data limited to batch system; single pollutant (As III) only	101	High
2020	Nano-alumina	As(V)	Artificial Neural	96 data points (65	Hold-out validation	Training: R^2 = 0.991;	Small dataset; single	102	High

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Year	Adsorbent	Heavy metal	ML model	Dataset size	Validation method	Performance metrics	Limitations	Ref	Quality
	(Al_2O_3 nanoparticles synthesized by solution combustion)		Network (Feed-forward ANN with backpropagation)	training, 20 validation, 11 testing)	(training/validation/ testing split)	Validation: R^2 = 0.942; Testing: R^2 = 0.984; S.E. = 0.012; RMSE and MAE used for evaluation	adsorbent system; model developed only for As(V) adsorption; external validation was not performed; applicability to other contaminants and adsorbents remains uncertain		
2021	Composite $Ni_{50}Co_{50}$-LDH/UiO-66-NH_2 nanocomposite	Tl	ANN was The ANN developed in JMP software with two hidden layers and hyperbolic tangent activation functions.	24 adsorption data points were collected from literature-derived experiments, including 16 points for training and 8 points for validation.	K-fold cross-validation with K = 3	The model showed excellent predictive ability, achieving R^2 values of > 0.999 for both the training and validation datasets.	The ANN was trained on a limited dataset involving only one adsorbent–metal system, which may restrict its applicability to other adsorption scenarios.	103	High
2021	MOF–LDH (Metal Organic Framework–Layered Double Hydroxide nanocomposite)	Pb(II), Cd(II)	ANN, multilayer feedforward, trial-and-error optimized structure)	16 kinetic data points (11 training + 5 validation)	Train/validation split + regression performance analysis (JMP software)	R^2 (training) = 0.9990; R^2 (validation) = 0.9998; RMSE (validation) = 1.44; SSE (validation) = 10.39; excellent prediction of adsorption kinetics and equilibrium time	Very small dataset; only literature-based kinetic data; no experimental external validation; limited generalizability; simplified input variables (ion type + time only); potential overfitting risk	104	High
2019	Chemically and physically activated *Cajanus cajan* (pigeon pea) husk	Cd(II)	Backpropagation Artificial Neural Network (BP-ANN)	657 data points (428 training, 229 testing); 65% training and 35% testing	Hold-out validation (65% training / 35% testing)	Isotherm prediction: R^2 = 0.9967, absolute relative percentage error = 1.159%; Kinetic prediction: R^2 = 0.9863, absolute relative percentage	Single heavy metal (Cd) investigated; external validation was not performed; ANN architecture optimized by trial-and-error; dataset derived from	105	High

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Year	Adsorbent	Heavy metal	ML model	Dataset size	Validation method	Performance metrics	Limitations	Ref	Quality
						error = 1.9134%; Training R^2 = 0.9968 (isotherm) and 0.9980 (kinetic)	laboratory experiments on one biosorbent only, which may limit generalizability		
2019	Acid-activated shale	Pb(II), Mn(II)	Modular Neural Network (MNN) with Levenberg–Marquardt Backpropagation	90 experimental runs (CCD design); 54 samples for training, 14 for validation, 22 for testing	Data split into training (60%), validation (15%), and testing (25%); cross-validation using MSE and correlation analysis; predicted vs. observed regression plots	Pb(II): R = 0.977; R^2 = 0.988; RMSE = 0.03815; NRMSE = 0.04097; Max.AE = 0.02621; Min.AE = 0.00041. Mn(II): R = 0.9648	Single adsorbent evaluated; experiments conducted under laboratory batch conditions; external validation using independent datasets was not performed; performance statistics for Mn(II) other than R were not reported.	106	High
2018	*Bellamya bengalensis* shell dust (BSD)	Cd(II)	(ANN, Multilayer Perceptron)	69 experimental datasets	Data split into training, validation, and testing sets; regression analysis between predicted and observed values	ANN: R^2 = 0.943–0.948; SSE = 0.467; Relative error = 0.056; Regression equation: y = 0.37 + 0.95x	Small dataset (n=69); only Cd(II) investigated; laboratory batch experiments only; no external validation or independent test dataset reported; single adsorbent evaluated	107	High
2018	Spent *Ulva prolifera* macroalgal biomass	Cr(VI)	Feedforward Artificial Neural Network (ANN, 4–8–1 architecture, Levenberg–Marquardt algorithm) + RSM comparison	31 experimental runs (Central Composite Design, CCD)	Train/validation/test split (80/10/10) + regression analysis (MATLAB)	ANN: R^2 = 0.9844, MSE = 3.7002, RMSE = 1.9236; RSM: R^2 = 0.9721, MSE = 6.2179; Maximum removal = 99.11%	Limited dataset size; batch-scale experiments only; model trained on RSM-generated design space; no external/real wastewater validation; potential overfitting risk in ANN	108	High
2018	Bellamya bengalensis shell	Cd(II)	(ANN, Multilayer Perceptron)	69 experimental sets	Training / validation / testing	ANN: R^2 = 0.943, SSE = 0.467; Langmuir	Study at laboratory scale (batch); lack of	109	High

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Year	Adsorbent	Heavy metal	ML model	Dataset size	Validation method	Performance metrics	Limitations	Ref	Quality
	dust (BSD)				(SPSS v20); regression analysis	isotherm R^2 = 0.995; pseudo-second-order kinetics R^2 = 0.998; maximum adsorption capacity qmax = 30.33 mg/g	investigation of real systems (field/industrial scale); monometallic (Cd only); limited generalizability to environmental conditions		
2017	Biochar (rambutan peel) produced at different pyrolysis temperatures (optimum: 600°C, B600)	Cu(II)	Feedforward Backpropagation Neural Network (FFBP ANN, Levenberg–Marquardt algorithm)	480 experimental data points (adsorption + pyrolysis-related datasets)	Train/test/validation split + regression analysis; MATLAB-based ANN modeling	$R^2 \approx 0.99992$ (pyrolysis model), $R^2 \approx 0.9547$ (adsorption model); MSE very low (~0.001–15.9 depending on model); Langmuir best fit; pseudo-second-order kinetics dominant	Lab-scale batch experiments only; limited generalization to real wastewater; ANN dependent on experimental dataset quality; possible experimental error in adsorption measurements; no external validation	110	High
2016	Typha domingensis	Ni(II), Cd(II)	ANFIS (Adaptive Neuro-Fuzzy Inference System)	Experimental batch data (5 input variables; multiple operating conditions)	Hold-out cross-validation (training vs checking data), MATLAB ANFIS, 1-epoch exhaustive search	RMSE (training/checking errors reported), best input relevance ranking; R^2 not used for ML	Limited dataset size; single biosorbent type; controlled batch conditions (no real wastewater); model dependent on experimental range; lack of external validation	111	High
2016	Quartz/Feldspar/Wollastonite (riverbed sand, QFW)	Cr(VI)	ANN (Feed-forward backpropagation, Levenberg–Marquardt)	91 experimental data points	Random split: 70% training, 15% testing, 15% validation	$R^2 \approx 0.985$–0.986, MSE = 0.0056	Small laboratory dataset; batch system only; no external/field validation; single adsorbent system	112	High
2015	ZnO nanoparticles entrenched on activated silica	As(III)	ANN (FFNN / Backpropagation, 3-layer,	95 experimental data points	Random split: 70% training, 15% validation, 15%	R^2 = 0.986 (training), MSE = 0.0014, removal efficiency up	Limited dataset size; lab-scale batch system; possible overfitting risk;	113	High

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Year	Adsorbent	Heavy metal	ML model	Dataset size	Validation method	Performance metrics	Limitations	Ref	Quality
	(ZnO-NPs-AS), green-synthesized using *Azadirachta indica* extract		Levenberg–Marquardt)		testing	to 98.31%	only arsenic in synthetic solutions (not real wastewater); model mainly interpolation-based		
2014	Functionalized nanocrystalline cellulose (NCC), succinated NCC, aminated NCC	Cr(III), Cr(VI)	(ANN), MLP back-propagation, Levenberg–Marquardt algorithm	160 experimental datasets (batch adsorption data)	Train/test/validation split + cross-validation (reported K-fold-like evaluation; also 60/40 and 40/20 splits depending on ion), MATLAB/NeuroSolution modeling	R^2 = 0.994–0.999; RMSE reported for training/validation (~0.16–2.18); MSE used as optimization criterion; very high agreement between predicted and experimental data	Limited dataset size; lab-scale batch data only; model depends strongly on experimental conditions; limited generalizability to real wastewater systems; no external field validation	114	High
2012	Fenton-modified solid waste vegetable oil industry (FMSWVOI)	As(III), As(V)	(ANN), MLP (BP & LM algorithms)	~not explicitly stated (batch experiments; ANN split: ~70% train, 15% validation, 15% test)	Train/Validation/Test split + trial-and-error architecture optimization	$R^2 \approx 0.93$, low MSE (~0.0023 best model), low prediction error (<10%)	Limited dataset size; interpolation-only reliability; potential overfitting risk with hidden layer tuning; experimental variability not fully addressed	115	High
2014	Sawdust, neem bark, rice straw, rice bran, rice husk, hyacinth roots, neem leaves, coconut shell	Cr(VI)	ANN (MLP feed-forward with BP and Levenberg–Marquardt algorithms)	163 data points	Train/validation/test split (60%/20%/10%/10% + prediction set)	MSE, AARE, R, χ^2 (best R ≈ 0.96–0.97; lowest MSE ≈ 0.003–0.007 depending on model)	Limited dataset size; reliance on batch experimental data; potential overfitting risk; model sensitivity to network structure and transfer function selection	116	High

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Discussion

The critical synthesis of machine learning applications in HMs adsorption reveals that model performance is highly context-dependent rather than universally dominated by a single algorithm. While ANNs frequently achieve high predictive accuracy ($R^2 > 0.99$) in controlled laboratory settings [38, 59, 66], this performance is often contingent on dataset size and homogeneity, as seen in [84] with large experimental bases, where ANN demonstrated robustness with $R^2 \approx 0.994$. However, comparative analyses indicate that ensemble learning methods, including RF, GBDT, and XGBoost, often match or outperform ANNs in heterogeneous datasets or when dealing with complex feature interactions [36, 37, 40]. For instance, GBDT was identified as the superior model in a comprehensive study involving 3,674 data points, achieving R^2= 0.9707 and demonstrating better generalizability than simpler models when validated against independent external datasets [38]. Similarly, RF has shown superior performance in predicting adsorption on MOFs and biochars, particularly in high-dimensional spaces where ANN architectures may struggle with over-parameterization [57, 58]. In specific cases with limited data [45], SVM even outperformed ANN based on lower Mean Squared Error (MSE), highlighting the structural risk minimization advantage of SVM in small-sample learning scenarios.

A systematic evaluation of the reviewed literature highlights a pervasive methodological concern: the reliance on small datasets without adequate validation protocols, which significantly increases the risk of overfitting. As detailed in Table 3, numerous studies utilized datasets with fewer than 100 experimental points, [43, 49, 61, 70, 89], yet reported near-perfect metrics ($R^2 > 0.99$). For example, [61] shows an ANN model trained on only 16 experimental runs that achieved R^2= 0.9967; however, the absence of an independent external validation set raises serious concerns about its generalizability beyond the specific experimental design space. Similarly, [49] reported R^2= 0.998 with only 18 samples, a scenario where high accuracy often signals over-optimization rather than true predictive strength. This risk is further exacerbated by the common practice of extensive hyperparameter tuning without strict cross-validation, as observed in [32, 39, 41], where simple hold-out splits (e.g., 70/30) were used without k-fold cross-validation, potentially leading to data leakage and optimistic bias. In contrast, studies implementing robust validation frameworks, such as 10-fold cross-validation combined with external independent datasets, provided more realistic performance estimates. For instance, [40] utilized an external validation set for Arsenic adsorption, revealing a drop in R^2= 0.94 (internal test) to > 0.81 (external validation), thereby offering a more honest assessment of model utility in real-world scenarios. Other studies, such as [33] and [47], also incorporated external experimental validation, demonstrating that models like XGBoost and GBDT can maintain reasonable accuracy ($R^2 \approx$ 0.92–0.97) even when tested on completely independent data sources.

Furthermore, the majority of reviewed studies relied solely on internal validation metrics derived from random train/test splits, failing to account for structural biases in experimental data collection. Only a minority of studies employed external validation using completely independent datasets sourced from different laboratories or real-world conditions [33, 36, 40, 47, 57]. The absence of external validation limits the translational potential of these models from laboratory bench-scale to industrial applications, as seen in [44, 55, 60] where models were strictly confined to synthetic solutions. Additionally, the "black-box" nature of high-performing ANN models hinders mechanistic understanding, a limitation that tree-based models like RF and XGBoost address through inherent interpretability features. Recent studies have begun to bridge this gap by integrating SHAP (SHapley Additive exPlanations) values with ML models; for example, [48] used XGBoost coupled with SHAP analysis to identify key features influencing fluoride and arsenic removal, providing actionable insights for adsorbent design that pure ANN models could not offer. In conclusion, there is no

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single "best" ML algorithm for heavy metal adsorption modeling; while ANNs remain powerful for large, clean datasets[34, 84], ensemble methods offer a more robust and generalizable alternative for smaller or heterogeneous datasets [36, 37, 57, 58], provided that rigorous validation protocols, including external testing, are adopted to ensure real-world applicability [33, 40, 47]. Future research should prioritize the development of large, high-quality datasets, standardized validation frameworks, and hybrid interpretable models that combine predictive accuracy with mechanistic insight

Conclusion

This review establishes that the efficacy of ML in MLs adsorption is not determined by algorithmic complexity alone, but by the rigor of data curation and validation protocols. While ANNs remain powerful for capturing non-linear dynamics in controlled settings, the demonstrated robustness of ensemble methods like RF and GBDT in heterogeneous and smaller datasets necessitates a shift away from the default preference for deep learning architectures. The critical bottleneck preventing the transition of these models from laboratory explorations to industrial deployment is the prevalence of small, siloed datasets and the absence of external validation. To bridge this gap, future research must prioritize the creation of standardized, open-access repositories of adsorption data that encompass real-world water matrices, thereby enabling the development of models with true generalizability beyond synthetic conditions. Furthermore, the integration of explainable AI (XAI) techniques, such as SHAP analysis, is essential to transform ML from a "black-box" predictor into a tool for mechanistic discovery, allowing engineers to optimize adsorbent design based on interpretable feature contributions. Ultimately, the successful implementation of ML in water treatment systems will depend on hybrid frameworks that couple high-accuracy predictions with physical constraints, ensuring that digital solutions are both scientifically robust and practically scalable for sustainable environmental remediation.

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Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have influenced the work reported in this paper.

Limitations

Several limitations of this systematic review should be acknowledged. First, the review was based on studies indexed in Scopus, PubMed, ScienceDirect, and Google Scholar, and relevant studies indexed in other databases may have been missed. Second, only published studies were included, which may introduce publication bias. Third, substantial heterogeneity existed among the included studies in terms of heavy metal types, adsorbent materials, machine learning algorithms, dataset characteristics, and performance evaluation metrics, which limited direct quantitative comparison and precluded meta-analysis. In addition, the predictive performance of machine learning models may have been influenced by variations in data quality, sample size, feature selection approaches, and validation strategies across studies. The non-exhaustive nature of Google Scholar may also have contributed to potential omission of relevant studies. Furthermore, this review was limited by the absence of a standardized risk-of-bias assessment tool specifically designed for machine learning-based adsorption modeling studies, necessitating the use of a modified CASP framework. Finally, this review focused exclusively on machine learning-based approaches and did not evaluate

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other mechanistic or empirical modeling techniques that may also be relevant for adsorption process prediction. Therefore, the findings should be interpreted in light of these limitations.

Registration

The review protocol was prospectively registered in the PROSPERO database (Registration No: CRD420261422875).

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Conflict of Interest

The authors declare no conflict of interest.

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Ethical Considerations

Not applicable. (Since this study is a systematic review of existing literature).

Code of Ethics

This study was approved by the Ethics Committee of Shahid Sadoughi University of Medical Sciences (Ethics Code: IR.SSU.REC.1403.156)

Authors' contribution

O, Y: Validation; Project administration; literature review, Investigation; Data curation.

R, H: Writing – original draft, literature review, Investigation, software analysis.

A, D: Writing – original draft, Supervision, review & editing, Validation.

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