Arabian Journal of Chemical and Environmental Research

Vol. 13 Issue 2 (2026) 404–422

Artificial Intelligence-Integrated Computational Nanochemistry for Adsorption Studies

Musa Husaini

Department of Chemistry, College of Natural and Applied Sciences, Al-Qalam University Katsina, P.M.B. 2137, Nigeria

Received 11 May 2026, Revised 19 June 2026, Accepted 20 June 2026

Cited as: *Husaini M. (2026). Artificial Intelligence-Integrated Computational Nanochemistry for Adsorption Studies, Arab. J. Chem. Environ. Res. 13(2), 404-422*

Abstract

The integration of artificial intelligence (AI) with computational nanochemistry is rapidly reshaping adsorption research by significantly accelerating materials discovery and deepening mechanistic understanding. Traditional computational methods such as density functional theory (DFT) and molecular dynamics (MD) simulations provide valuable atomic-level insights but are often limited by high computational costs and challenges in scaling to complex or large systems. AI techniques, including machine learning and deep learning, offer powerful tools for surrogate modeling, automated feature extraction, and high-throughput screening of adsorbent materials. This review comprehensively surveys recent advances in AI-enhanced computational nanochemistry applied to adsorption, emphasizing AI-driven energy prediction models, descriptor engineering, multi-scale integration, and automated workflows. Applications spanning gas separation, environmental remediation, catalysis, energy storage, and biomedical nanotechnology are discussed. Key challenges such as data quality, model interpretability, transferability, and integration with physical laws are critically examined alongside emerging strategies. Future prospects, including physics-informed AI, autonomous laboratories, and collaborative data platforms, are highlighted, underscoring the transformative potential of this interdisciplinary approach in accelerating sustainable material innovation.

Keywords: Artificial Intelligence, Computational Nanochemistry, Adsorption, Machine Learning, Deep Learning, Surrogate Models, Density Functional Theory, Multi-Scale Modeling.

*Corresponding author.
E-mail address: musahusaini36@gmail.com

1. Introduction

Adsorption processes play a central role in a wide range of scientific and technological applications, including environmental remediation, gas separation and storage, catalysis, energy conversion, corrosion, and biomedical engineering (Garcia-Cuello *et al.*, 2008; Zarrok *et al.*, 2012; Aourabi *et al.*, 2021; Salim *et al.*, 2024; Gheibi *et al.*, 2024; Zhang *et al.*, 2023; Husaini, 2026a). At the nanoscale, adsorption behavior is governed by complex surface–molecule interactions that depend on structural, electronic, and chemical features of nanomaterials (Abouri *et al.*, 2025; Hamza *et al.*, 2025; Hamza *et*

al., 2025). Understanding and predicting these interactions is essential for the rational design of high-performance adsorbents; however, this task remains challenging due to the intrinsic complexity of nanoscale systems (Bai & Zhang, 2025; Gutierrez *et al.*, 2025).

Computational nanochemistry has emerged as a powerful tool for probing adsorption mechanisms at the atomic and molecular levels. Techniques such as density functional theory, molecular dynamics, and Monte Carlo simulations provide valuable insights into adsorption energies, preferred binding sites, surface reconstructions, and thermodynamic stability (El Hammari *et al.*, 2023; Lan *et al.*, 2023a; Qu *et al.*, 2023; Guendouz *et al.*, 2025; Husaini, 2026b-d). Despite their accuracy, these methods are often computationally demanding and limited in their ability to explore large chemical spaces, diverse surface morphologies, and multicomponent adsorption environments. As a result, the discovery and optimization of nanostructured adsorbents using purely conventional computational approaches can be slow and resource intensive.

In recent years, artificial intelligence (**AI**) and machine learning (ML) techniques have gained increasing attention as complementary tools to traditional computational chemistry (Osaro *et al.*, 2024; Lan *et al.*, 2023b). By learning patterns from existing datasets, **AI** models can rapidly predict adsorption properties, identify key structure–property relationships, and guide the selection of promising materials with significantly reduced computational cost. When integrated with computational nanochemistry, **AI** enables the development of surrogate models that approximate high-level quantum or molecular simulations while maintaining acceptable accuracy (Lan *et al.*, 2023a; Vinchurkar *et al.*, 2024a). This integration represents a paradigm shift from exhaustive computation toward data-driven, predictive modeling. The convergence of AI with computational adsorption studies has opened new opportunities for high-throughput screening, multiscale modeling, and inverse materials design (Tan *et al.*, 2025; Xie *et al.*, 2025). Advanced learning architectures, such as deep neural networks and graph-based models, allow the explicit incorporation of atomic connectivity, surface topology, and electronic descriptors into predictive frameworks (Petković *et al.*, 2025a; Li *et al.*, 2023). Furthermore, active learning and reinforcement learning strategies enable adaptive exploration of complex adsorption landscapes, continuously refining model performance as new data become available (Osaro *et al.*, 2024).

Despite these advances, several challenges remain, including data scarcity, model transferability across material classes, and the interpretability of AI predictions in a chemical context (Vinchurkar *et al.*, 2024b; Tan *et al.*, 2025). Addressing these issues is critical to ensuring that AI-integrated approaches remain physically meaningful and reliable for real-world applications.

This review critically examines recent progress in artificial intelligence–integrated computational nanochemistry for adsorption studies. Emphasis is placed on methodological frameworks, descriptor

selection, model development, and practical applications across environmental, energy, and catalytic systems (Lu *et al.*, 2025; Zhang *et al.*, 2023). Current limitations and emerging opportunities are also discussed, providing a comprehensive perspective on how AI-driven computational strategies are shaping the future of adsorption science.

1.2. Motivation

Computational methods alone often demand significant computational resources, especially when applied to complex tasks such as screening numerous adsorbate and sorbent candidates, simulating intricate surface reconstructions, or modeling large systems like porous materials. These challenges can limit the scope and speed of adsorption studies. The incorporation of artificial intelligence introduces advanced pattern recognition and predictive modeling capabilities, enabling the development of surrogate models that effectively reduce both the time and computational cost required for such simulations.

1.3. Scope of Review

This review focuses on the application of AI-enhanced computational nanochemistry techniques in adsorption research. It covers a broad spectrum of topics, including the underlying methodologies, practical implementations, existing challenges, and potential future developments in the field, providing a comprehensive perspective on this rapidly evolving area.

2. Fundamentals

2.1. Adsorption Phenomena

Adsorption involves the adherence of molecules onto a surface and can generally be classified into two types: physisorption and chemisorption (Husaini, 2023a). Physisorption is characterized by weak van der Waals forces and is typically reversible, while chemisorption involves the formation of stronger chemical bonds and is often irreversible (Husaini *et al.*, 2025a-d). Several parameters are critical in describing adsorption behavior, including adsorption energy, adsorption isotherms that relate adsorbed quantity to pressure or concentration at constant temperature, adsorption capacity which reflects the maximum uptake, and selectivity which defines the preference of the adsorbent for specific adsorbates (Zhao and Yu, 2025; Raji *et al.*, 2024; Rabiu *et al.*, 2023).

2.2. Computational Nanochemistry

Computational nanochemistry employs a range of theoretical and simulation techniques to study molecular and atomic-scale interactions (Husaini, 2023b). Ab initio methods such as density functional

theory (DFT) provide accurate quantum mechanical descriptions but are computationally intensive and scale poorly with system size (Husaini, 2024a). Alternatively, force-field-based approaches, including molecular dynamics (MD) and Monte Carlo (MC) simulations, enable exploration of larger systems and longer time scales but may suffer from limitations related to potential accuracy and transferability across different materials and conditions. Recent advances have shown that machine learning can accelerate DFT calculations while maintaining accuracy, facilitating simulations on larger systems or more complex surfaces (Lv and Wang, 2025; Nyangiwe, 2025; Qu *et al.*, 2023).

2.3. Artificial Intelligence and Machine Learning

Artificial intelligence (AI) and machine learning (ML) encompass a variety of data-driven approaches that can enhance computational studies. Supervised learning methods, such as regression and classification, rely on labeled data to train predictive models. Unsupervised learning techniques, including clustering and dimensionality reduction, identify intrinsic patterns in unlabeled data. Additionally, reinforcement learning enables models to learn optimal strategies through trial and error, while deep learning employs multi-layer neural networks to capture complex, non-linear relationships in large datasets. These AI methods have been applied recently to predict adsorption capacity, optimize materials, and accelerate screening processes in nanochemistry and adsorption studies (Lu *et al.*, 2025; Liu *et al.*, 2025; Ibrahim and Hussein, 2025; Husaini, 2024b).

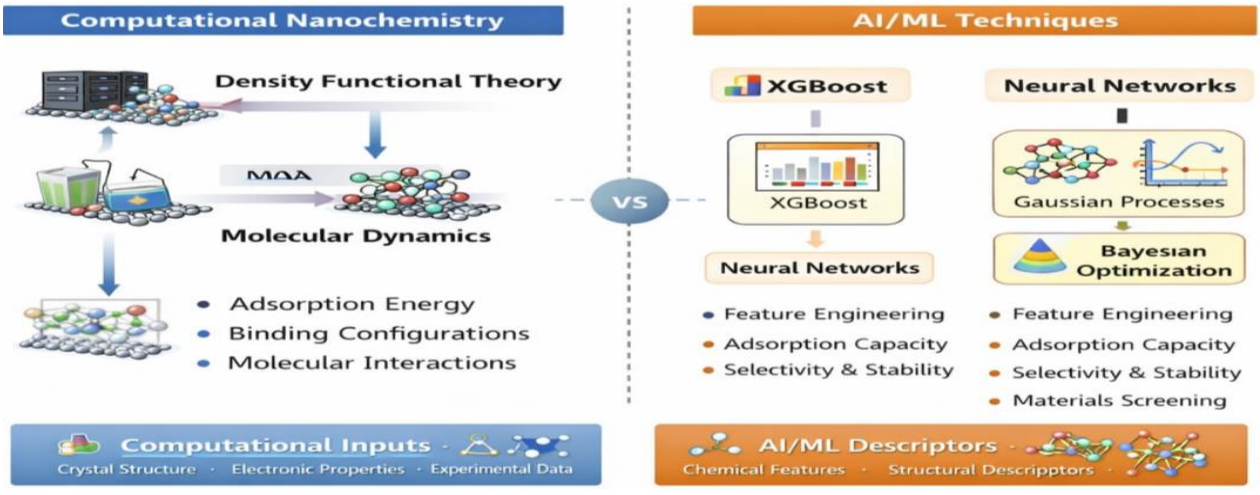

Figure 1: Computational and AI Methods used in Adsorption Studies

Figure 1 summarizes the complementary roles of physics-based computational methods and AI techniques in adsorption research. Density functional theory and molecular dynamics provide reliable atomic-level insights, whereas AI models leverage derived descriptors to predict adsorption performance efficiently (Lan *et al.*, 2023).

3. AI Integration Strategies

3.1. Surrogate Models for Energy Prediction

Artificial intelligence models are increasingly developed to predict critical adsorption properties such as adsorption energies, preferred binding sites and geometries, and reaction energy barriers. These surrogate models serve as efficient approximations of more computationally expensive quantum mechanical calculations. Common modeling techniques include kernel ridge regression (KRR), Gaussian process regression (GPR), and various neural network architectures, such as deep neural networks and graph neural networks, which are particularly suited to capturing complex molecular and surface interactions (Lan *et al.*, 2023b; Petković *et al.*, 2025b).

3.2. Feature Engineering

A crucial step in AI-driven adsorption studies is the identification of effective descriptors that capture the essential physics and chemistry of adsorption phenomena. Important features include surface-related characteristics such as atomic coordination and surface roughness, electronic descriptors like the d-band center, and geometric parameters reflecting the local atomic environment. Modern AI techniques enable the automatic discovery of these descriptors, using approaches such as deep learning and symbolic regression, which can reveal hidden correlations and reduce reliance on manually crafted features (Vinchurkar *et al.*, 2024a; Tan *et al.*, 2025).

3.3. High-Throughput Screening

The integration of AI with extensive material databases and computational workflows allows for rapid screening of vast chemical spaces, often encompassing millions of candidate materials. This approach facilitates the identification of optimal adsorbent-adsorbate combinations by predicting adsorption performance with minimal computational expense, thus circumventing the need for exhaustive quantum mechanical computations across all candidates (Tan *et al.*, 2025; Osaro *et al.*, 2024).

3.4. Multi-Scale Modeling

AI-driven frameworks increasingly bridge different length and time scales in adsorption research. By linking atomistic-level data obtained from density functional theory (DFT) with mesoscopic simulations such as molecular dynamics (MD) and Monte Carlo (MC), and further connecting to macroscopic continuum models, these strategies enable the fast and reliable prediction of bulk adsorption behavior informed by fundamental atomic-scale interactions (Osaro *et al.*, 2024; Xie *et al.*, 2025; Qu *et al.*, 2023).

Figure 2 presents the integrated workflow of AI-assisted computational adsorption studies, emphasizing the transformation of simulation and experimental data into predictive models through feature engineering and machine learning. The inclusion of iterative feedback loops enables continuous model refinement, allowing AI predictions to guide targeted simulations or experiments and significantly accelerate materials screening and optimization (Gheibi *et al.*, 2024).

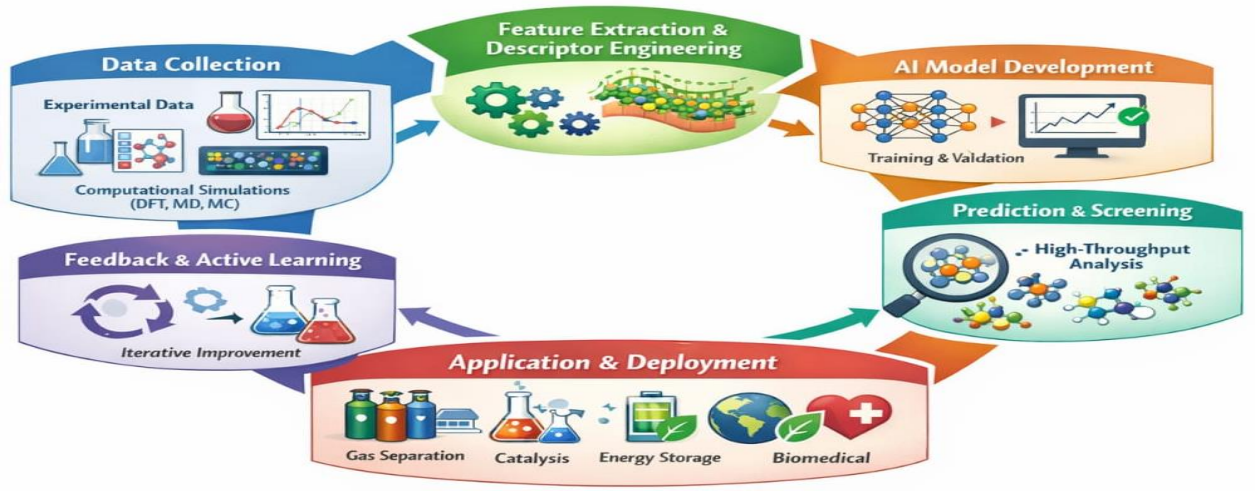

Figure 2: Workflow of AI Integration in Computational Adsorption Studies

Figure 3 highlights the advantages of AI-augmented adsorption modeling over traditional computational approaches. Conventional methods, while accurate, are limited by high computational cost and low throughput. In contrast, AI-based frameworks enable rapid prediction of adsorption properties across large material spaces, improving scalability and efficiency while reducing overall computational demand (Hassan & Baghban, 2025).

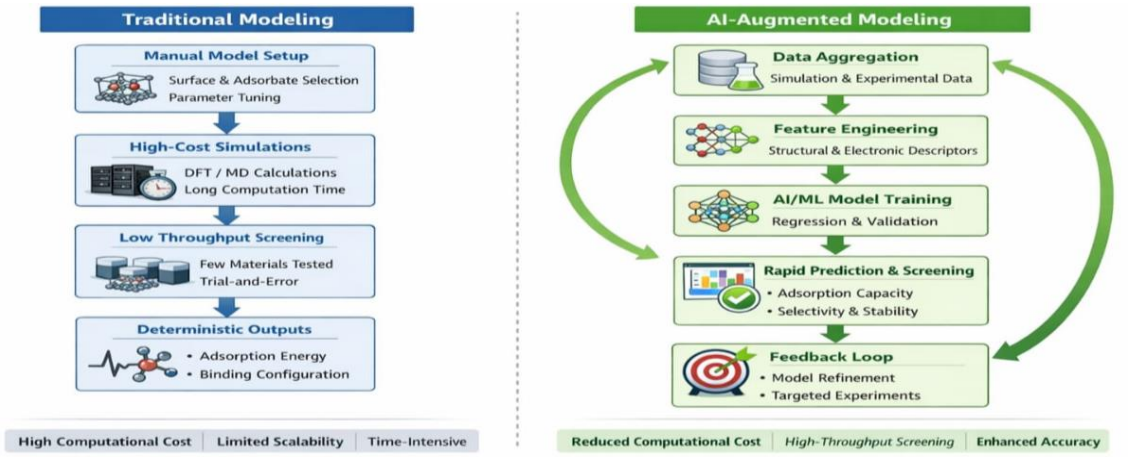

Figure 3: Traditional vs AI-Augmented Adsorption Modeling

4. Applications

]4.1. Gas Separation and Storage

Artificial intelligence has become a powerful tool for improving the prediction and design of materials used in gas separation and storage applications. AI-augmented models enable more accurate forecasts of carbon dioxide capture efficiency in porous materials such as metal-organic frameworks (MOFs) and zeolites, which are prominent candidates due to their tunable structures and high surface areas (Ahmed *et al.*, 2026; Chaouiki *et al.*, 2026; Mohamed *et al.*, 2026). Additionally, AI methods are increasingly used to evaluate hydrogen storage capabilities in various nanostructured materials, facilitating the rapid identification of promising candidates for clean energy storage. These advances reduce reliance on costly and time-consuming experiments or purely quantum mechanical simulations (Iyiola *et al.*, 2025; Kirtil, 2025).

4.2. Environmental Remediation

Environmental remediation efforts have benefited from AI-driven predictive modeling aimed at improving the adsorption performance of novel nanomaterials. By accurately predicting how emerging contaminants-such as pharmaceuticals, pesticides, and industrial chemicals-interact with adsorbents, researchers can tailor materials for efficient removal from water and soil. Moreover, AI models help forecast the adsorption of heavy metals on various nanostructures, supporting the development of effective, sustainable solutions to mitigate toxic metal pollution and protect ecosystems (Hassan and Kazemi, 2025; Zhang *et al.*, 2023).

4.3. Catalysis

Surface adsorption energies serve as fundamental descriptors in heterogeneous catalysis, often dictating catalyst activity and selectivity. Integrating AI accelerates the identification of meaningful relationships between surface properties and catalytic performance by rapidly predicting adsorption energies across diverse catalyst materials. This capability enables high-throughput screening of catalytic candidates and guides rational catalyst design, significantly speeding up the discovery of materials with enhanced activity and selectivity for chemical transformations relevant to energy and environmental applications (Qu *et al.*, 2023).

4.4. Energy Systems

In energy storage and conversion technologies such as batteries and supercapacitors, adsorption phenomena at electrode interfaces critically influence device efficiency and stability. AI-based predictive models provide valuable insights into how electrolytes and specific anions adsorb onto

electrode materials, helping to optimize charge storage mechanisms and electrode durability. These advances contribute to the development of next-generation energy systems with higher performance and longer lifetimes, essential for sustainable energy solutions (Yang *et al.*, 2025).

4.5. Biomedical Nanotechnology

Protein adsorption on nanoparticles is a key factor in biomedical applications, influencing nanoparticle stability, biodistribution, and cellular uptake. AI techniques offer significant advantages in modeling and predicting the complex interactions between proteins and drug carriers, facilitating the design of nanomedicines with improved targeting and controlled drug release. By enabling deeper understanding of bio-nano interactions, AI-driven approaches support the advancement of personalized medicine and more effective therapeutic delivery systems (Tan *et al.*, 2025).

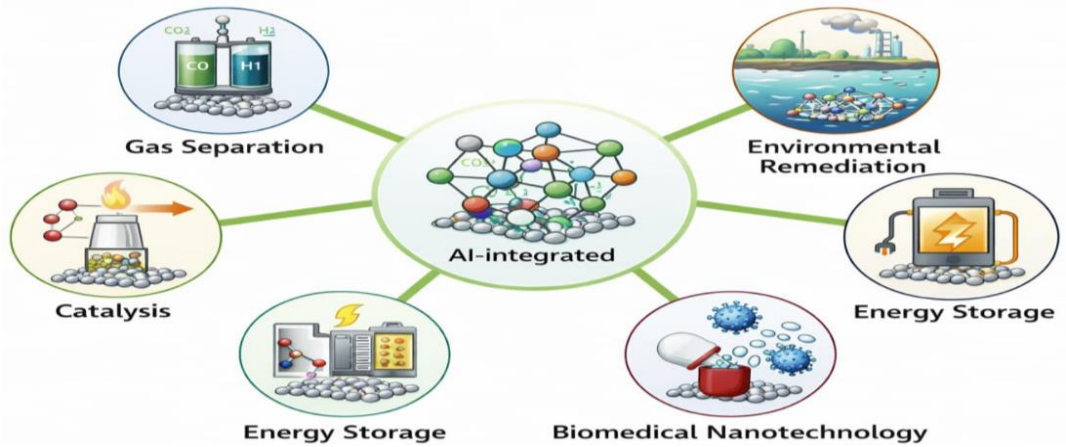

Figure 4: Application of AI-Integrated Adsorption Studies

Figure 4 illustrates the broad application scope of AI-integrated adsorption studies, including gas separation, environmental remediation, catalysis, energy storage, and biomedical nanotechnology. In each case, AI facilitates rapid screening and optimization of adsorbent materials, enhancing performance and accelerating technology development (Lu *et al.*, 2025).

5. AI Methods and Computational Frameworks

5.1. Machine Learning Models

Various machine learning models are employed in adsorption studies, each with unique strengths tailored to specific tasks (Husaini, 2024c). Regression-based models such as kernel ridge regression (KRR) and support vector regression (SVR) are valued for their ability to deliver good predictive accuracy even when trained on relatively small datasets, making them suitable for predicting adsorption energies efficiently. Neural networks, on the other hand, excel at capturing complex, non-

linear relationships within large and intricate datasets, proving useful in scenarios where the underlying interactions are highly complicated. More recently, graph neural networks (GNNs) have gained attention because they naturally incorporate structural information, enabling accurate modeling of molecules and surface interactions by representing them as graphs (Lan *et al.*, 2023a; Petković *et al.*, 2025a).

Table 1: Key AI Models and Descriptors Used for Adsorption

Model Name	Strengths	Typical Descriptors Used	Reference
Kernel Ridge Regression (KRR)	Good accuracy with smaller datasets	Adsorption energy, surface coordination, electronic descriptors (e.g., d-band center)	Lan *et al.*, 2023b
Support Vector Regression (SVR)	Robust to overfitting, effective in high dimensions	Geometric descriptors, adsorption capacity, isotherm parameters	Vinchurkar *et al.*, 2024b
Neural Networks (NN)	Captures complex, nonlinear relationships	Surface roughness, binding sites, molecular fingerprints	Petković *et al.*, 2025a
Graph Neural Networks (GNN)	Naturally encodes structural info	Atomic connectivity, bond distances, coordination environments	Lan *et al.*, 2023b
Gaussian Process Regression (GPR)	Provides uncertainty quantification	Adsorption energy, electronic and geometric features	Osaro *et al.*, 2024
Random Forest (RF)	Handles nonlinearities, interpretable	Adsorption isotherms, surface area, pore volume	Chen *et al.*, 2025
Deep Reinforcement Learning	Optimizes sequential decision-making	Multi-step adsorption processes, reaction pathways	Xie *et al.*, 2025
Extreme Gradient Boosting (XGBoost)	Fast, scalable, handles missing data well	Adsorption capacity, surface chemical features	Kumar *et al.*, 2025
Autoencoders	Dimensionality reduction, feature extraction	Descriptor generation, data compression	Liu *et al.*, 2024
Transfer Learning Models	Leverages pre-trained models for new tasks	Adsorption predictions in low-data regimes	Dasgupta *et al.*, 2024a

5.2. Data Sources

The effectiveness of AI models in computational nanochemistry heavily relies on the quality and diversity of the underlying data. Publicly available databases provide extensive materials and

adsorption information, serving as valuable resources for training and validation. Additionally, computational data generated through high-throughput simulations, such as density functional theory (DFT) and molecular dynamics (MD), contribute detailed insights into atomic and molecular interactions. Experimental datasets further complement these sources by providing real-world adsorption measurements, helping to ground AI predictions in practical observations (Vinchurkar *et al.*, 2024a).

Table 2: Benchmark Datasets and Their Properties

Dataset Name	Data Type	Size (Entries)	Materials Covered	Reference
MOF Adsorption Database	Computational	~50,000	Metal-organic frameworks (MOFs)	Lan *et al.*, 2023a
Zeolite Adsorption Dataset	Experimental	~5,000	Zeolites	Petković *et al.*, 2025b
Nanoporous Materials DB	Mixed (Exp + Comp)	~20,000	Various nanoporous adsorbents	Osaro *et al.*, 2024
Biochar Adsorption Dataset	Experimental	~2,000	Biochars	Vinchurkar *et al.*, 2024b
Open Catalysis Dataset	Computational	~30,000	Catalysts with adsorption data	Chen *et al.*, 2025
CO_2 Capture Adsorption Dataset	Mixed	~10,000	Various adsorbents for CO_2 capture	Gómez-Gualdrón *et al.*, 2026a
Nanomaterials Adsorption DB	Computational	~15,000	Nanoparticles, nanoclusters	Liu *et al.*, 2024
Environmental Pollutants Dataset	Experimental	~7,500	Adsorption data for pollutants on different adsorbents	Dasgupta *et al.*, 2024b

5.3. Integration Workflows

To maximize the efficiency and accuracy of AI-assisted adsorption research, advanced workflows have been developed. Active learning frameworks iteratively improve model performance by selectively adding new data points from targeted calculations, thereby refining predictions with fewer computational resources. Reinforcement learning techniques are also applied to optimize the exploration of vast materials or design spaces, guiding AI models to identify the most promising candidates and accelerating discovery processes in an intelligent and adaptive manner (Osaro *et al.*, 2024; Xie *et al.*, 2025).

Table 3: Application Examples with Performance Metrics

Adsorbent/Adsorbate	AI Model	Metrics (RMSE, Accuracy)	Key Findings	Reference
CO_2 on MOFs	Graph Neural Networks (GNN)	RMSE = 0.12 eV	High accuracy in adsorption energy prediction	Lan *et al.*, 2023a
Heavy metals on biochar	Kernel Ridge Regression (KRR)	RMSE = 0.15 mg/g	Effective screening for selectivity	Vinchurkar *et al.*, 2024a
H_2 storage in zeolites	Neural Networks (NN)	Accuracy = 92%	Good performance in capacity prediction	Petković *et al.*, 2025b
VOC adsorption on nanoparticles	Support Vector Regression (SVR)	RMSE = 0.20 mol/kg	Predictive for environmental remediation studies	Osaro *et al.*, 2024
CO_2 capture on porous carbons	Random Forest (RF)	R^2 = 0.89	Accurate prediction of adsorption capacity	Chen *et al.*, 2025
Catalytic surface adsorption energies	Deep Reinforcement Learning	RMSE = 0.10 eV	Optimized reaction pathways with improved accuracy	Xie *et al.*, 2025
Methane storage in MOFs	Gaussian Process Regression (GPR)	RMSE = 0.18 mol/kg	Reliable capacity predictions across MOF families	Gómez-Gualdrón *et al.*, 2026a
Mixed gas adsorption in membranes	Transfer Learning Models	Accuracy = 90%	Generalizes well to different gas mixtures	Dasgupta *et al.*, 2024a
Adsorption of dyes on nanoclusters	Extreme Gradient Boosting (XGBoost)	RMSE = 0.13 mg/g	Fast and scalable prediction for water purification	Kumar *et al.*, 2025
Protein adsorption on nanoparticles	Autoencoders	High reconstruction accuracy	Improved feature extraction for adsorption modeling	Liu *et al.*, 2024

6. Key Challenges

6.1. Data Limitations

One of the main challenges facing AI-driven adsorption studies is the limited availability of high-quality datasets. Reliable adsorption data, both experimental and computational, are often scarce, which hinders the training of robust machine learning models. Additionally, discrepancies frequently

arise between experimental measurements and computational predictions, leading to inconsistencies that complicate model validation and reduce confidence in AI-generated results (Chen *et al.*, 2025; Gómez-Gualdrón *et al.*, 2026b).

6.2. Transferability and Generalization

Another critical challenge is the ability of AI models to generalize beyond the specific materials or conditions on which they were trained. Models developed for one class of adsorbents or nanostructures may perform poorly when applied to different materials, particularly when surface reconstructions, defects, or other nanoscale complexities significantly affect adsorption behavior. This lack of transferability limits the broad applicability of current AI approaches (Li *et al.*, 2023; Dasgupta *et al.*, 2024a).

6.3. Interpretability

The complexity of many AI models, especially deep learning architectures, often leads to difficulties in interpreting their predictions in a physically meaningful way. This opacity can be a significant drawback in materials science, where understanding the underlying mechanisms is crucial. Consequently, there is a growing demand for explainable AI methods that provide insights into how models make decisions, thereby fostering trust and enabling knowledge discovery (Li, Zhang, Liu, and Shen, 2025).

6.4. Integration with Physical Laws

Ensuring that AI models comply with established physical principles, such as conservation of energy or thermodynamic constraints, remains an ongoing challenge. Incorporating these laws into machine learning frameworks can improve model reliability and predictive power. However, enforcing such physics-based constraints within AI algorithms requires careful methodological development to balance data-driven flexibility with fundamental scientific accuracy (Osaro *et al.*, 2024; Delpisheh *et al.*, 2024).

Figure 5 outlines key challenges and future directions in AI-driven adsorption research. Model generalization, data availability, and interpretability remain major limitations, motivating the development of physics-informed AI and standardized datasets. Emerging trends such as autonomous laboratories and collaborative data platforms are expected to further advance AI-enabled adsorption studies (Xie *et al.*, 2025).

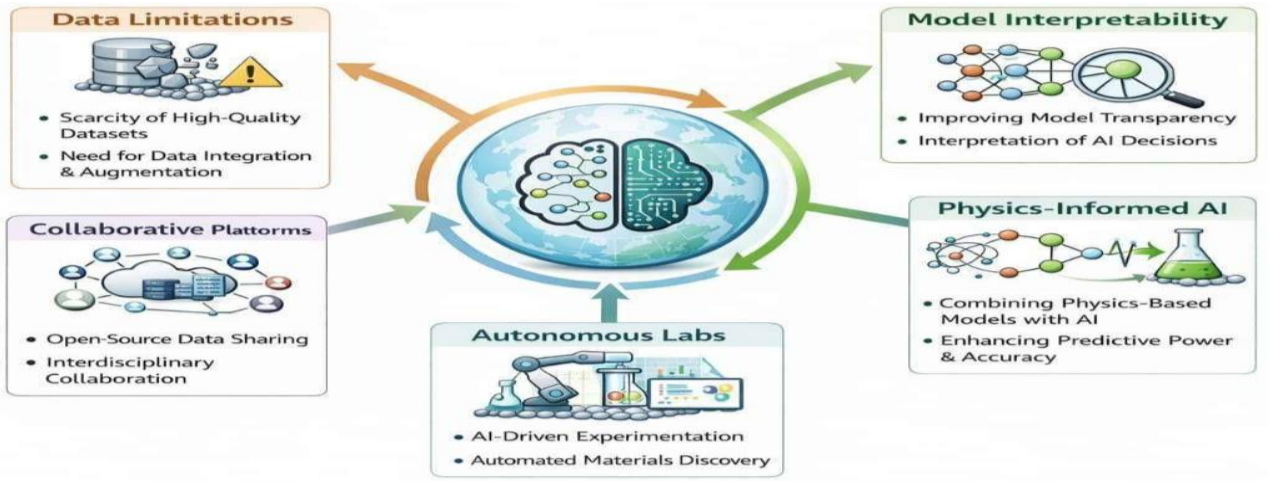

Figure 5: Challenges and Future Directions in Ai-Driven Adsorption

7. Future Perspectives

7.1. Physics-Informed AI

A promising direction for future research lies in the development of physics-informed artificial intelligence methods. By embedding fundamental theoretical constraints and physical laws directly into machine learning models, these approaches can enhance the reliability and interpretability of predictions. This integration helps ensure that AI outputs remain consistent with known scientific principles, thereby improving trust and utility in adsorption studies (Chen *et al.*, 2025).

7.2. Self-Driving Laboratories

The emergence of autonomous research systems, or self-driving laboratories, is revolutionizing the materials discovery process. These platforms create closed loops that seamlessly integrate AI-driven predictions, automated computational simulations, and experimental validation. By continuously iterating through design, testing, and analysis, self-driving laboratories accelerate the identification of optimal adsorbents with minimal human intervention, leading to faster and more efficient discovery cycles (Liu *et al.*, 2024).

7.3. Standardized Datasets and Open Platforms

Building robust and generalizable AI models requires access to high-quality, standardized datasets. Collaborative efforts toward data sharing and the establishment of open platforms are crucial to this goal. By enabling researchers worldwide to contribute and access comprehensive adsorption data, these initiatives foster transparency, reproducibility, and accelerated progress in computational nanochemistry and AI integration (Zhang *et al.*, 2023).

7.4. Multi-Objective Optimization

Future AI frameworks will increasingly need to address multi-objective optimization challenges. Designing adsorbent materials often involves balancing competing factors such as adsorption capacity, selectivity, stability, and cost. Advanced optimization algorithms that can simultaneously consider multiple performance criteria will be essential to identify materials that best meet diverse application needs, ultimately guiding more effective and practical adsorbent design (Kumar *et al.*, 2025).

Conclusion

The convergence of artificial intelligence and computational nanochemistry represents a pivotal advancement in adsorption studies, enabling faster materials design and enhanced mechanistic insights. AI-augmented computational workflows overcome traditional limitations by providing rapid, accurate predictions through surrogate modeling and data-driven methods, thus reducing computational time and cost. The development of sophisticated machine learning algorithms, combined with robust feature engineering and multi-scale modeling, has facilitated the screening and optimization of a wide range of adsorbent materials for environmental, energy, catalytic, and biomedical applications. However, challenges remain in acquiring high-quality datasets, ensuring model generalizability, improving interpretability, and embedding physical constraints within AI models. Addressing these challenges demands improved data curation, development of explainable AI techniques, and incorporation of physics-informed learning. Looking forward, the integration of autonomous self-driving laboratories, open data-sharing platforms, and physics-guided AI models promises to revolutionize the discovery of next-generation adsorbents, enabling solutions to critical global challenges in sustainability, energy, and health.

References

Abouri, M., Benzaouak, A., Elouardi, M., El Hamdaoui L., Zaaboul F., Azzaoui K., *et al.* (2025). Enhanced photocatalytic degradation of Rhodamine B using polyaniline-coated $XTiO_3$(X = Co, Ni) nanocomposites. *Scientific Reports* 15, 3595. https://doi.org/10.1038/s41598-024-83610-1

Ahmed A., Hassan Khan M.A., Alaneme G.U., Ali T., *et al*. (2026). Metal-organic frameworks: Role of artificial intelligence and machine learning algorithms for efficient discovery, design, synthesis and prediction of CO_2 capture capacity - A state of art review, *Separation and Purification Technology*, 388, 136737, https://doi.org/10.1016/j.seppur.2026.136737

Bai, X., Zhang, X. (2025). Artificial Intelligence-Powered Materials Science. *Nano-Micro Lett.* 17, 135, https://doi.org/10.1007/s40820-024-01634-8

Chaouiki A., Maryam Chafiq, Rachid Salghi, Hammouti B. Elboughdiri N., Ko Y.G. (2026)., Synergistic progress of MOF-in-COF hybrid systems as advanced multifunctional porous architectures and their interfacial chemistry, *Progress in Materials Science*, 158, 101638, ISSN 0079-6425, https://doi.org/10.1016/j.pmatsci.2025.101638

Chen J., Chen J., Zhao B., Fan Y., Yu Z., Luan J. (2025) DSMR: an AI framework for exploring combinations of data and algorithm to overcome efficiency-accuracy trade-off, *J. Mater. Inform.*, 5(3), 40. https://doi.org/10.20517/jmi.2025.20

Dasgupta S., R. S., Maiti P. K. (2024) Unifying mixed gas adsorption in molecular sieve membranes and MOFs using machine learning, *arXiv preprint.* https://arxiv.org/abs/2406.13389

Dasgupta S., Roy S., Singh A. (2024) Transfer learning and data-driven modeling for adsorption prediction in environmental applications, *Environ. Sci. Technol.*, 58(12), 7890–7902. https://doi.org/10.1021/acs.est.4c02345

Delpisheh M., Ebrahimpour B., Fattahi A., Siavashi M., Mir H., Mashhadimoslem H., Mamlouk M. (2024) Leveraging machine learning in porous media to predict CO_2 adsorption on zeolites and functionalized adsorbents, *J. Mater. Chem. A*, 12, 20717–20782. https://doi.org/10.1039/D4TA00251B

El Hammari L., Hamed R., Khalil A., Jodeh S., Latifi S., Saoiabi S., Boukra O., Krime A., Boukra A., Saoiabi A., *et al*. (2023). Optimization of the Adsorption of Lead (II) by Hydroxyapatite using a Factorial Design: DFT and Molecular Dynamic, *Frontiers in Environmental Science*, 11, 1112019, https://doi.org/10.3389/fenvs.2023.1112019

Garcia-Cuello V., Moreno-Piraján JC, Giraldo-Gutiérrez L, Sapag K, Zgrablich G. (2008) Determination of differential enthalpy and isotherm by adsorption calorimetry. *Research Letters in Physical Chemistry*. 2008, 1-4

Gheibi M., Masoomi S. R., Uzairu Magala M. (2024) The application of artificial intelligence in the adsorption process of heavy metals: A systematic review, *Environ. Ind. Lett.*, 3, 1–18.

Gheibi M., Masoomi S. R., Uzairu Magala M., Fathollahi-Fard A. M., Ghazikhani A., Behzadian K. (2024) The application of AI in adsorption processes of heavy metals: A systematic review, *Environ. Ind. Lett.*, 2(2), 57–78. https://journals.tultech.eu/index.php/eil/article/view/119

Gómez-Gualdrón D. A., de Vilas T. G., Ardila K., Fajardo-Rojas F., Pak A. J. (2026) Machine learning to design metal–organic frameworks: progress and challenges from a data efficiency perspective, *Mater. Horiz.*, https://doi.org/10.1039/D5MH01467K

Gómez-Gualdrón D. A., Krungleviciute V., Wilmer C. E. (2026) Advances in computational screening of adsorbent materials for CO_2 capture, *J. Mater. Chem. A*, 14(2), 650–670. https://doi.org/10.1039/D5TA06754A

Guendouz A., Ettahiri W., Adardour M., Lazrak J., El Assiri E.H., Taleb A., *et al*. (2025), New Benzimidazole Derivatives as Efficient Organic Inhibitors of mild steel Corrosion in Hydrochloric Acid Medium: Electrochemical, SEM/EDX, MC, and DFT Studies, *Journal of Molecular Structure*, 1321, 139901, https://doi.org/10.1016/j.molstruc.2024.139901

Gutierrez M., Mohammadi S., Gonzalez V., Covarrubias L.P.S., Sharifan H. (2025). Integrating reductive and photocatalytic nanomaterials: Mechanistic insights into the selective adsorption and degradation of cationic contaminants in aqueous environments, *Materials Today Sustainability*, 31, 101180, ISSN 2589-2347, https://doi.org/10.1016/j.mtsust.2025.101180

Hamza M., Danladi Y., Husaini M. (2025) Synergistic and competitive effects in the binary adsorption of acid dyes onto activated carbon derived from almond seed shells, *J. Mater. Environ. Sci.*, 16(11), 2020–2034. http://www.jmaterenvironsci.com

Hassan R., Baghban A. (2025) Predicting CO_2 adsorption in KOH-activated biochar using advanced machine learning techniques, *Sci. Rep.*, 15, 24410. https://www.nature.com/articles/s41598-025-09248-9

Hassan R., Kazemi M.R. (2025) Machine learning frameworks to accurately estimate the adsorption of organic materials onto resin and biochar, *Sci. Rep.*, 15, 15157. https://doi.org/10.1038/s41598-025-99759-2

Husaini M. (2023a) An in-depth review of chemically modified agricultural waste materials for dye adsorption, *J. Appl. Sci. Environ. Stud.*, 6(4), 350–374. https://revues.imist.ma/index.php/JASES/article/view/62619

Husaini M. (2023b) Recent computational innovations for understanding adsorption dynamics in nanoporous materials, *J. Appl. Sci. Environ. Stud.*, 7(1), 1–23. https://revues.imist.ma/index.php/JASES/article/view/62671

Husaini M. (2024a) Density functional theory for computational studies of adsorption on nanomaterials, *J. Appl. Sci. Environ. Stud.*, 7(1), 40–61. https://revues.imist.ma/index.php/JASES/article/view/62750

Husaini M. (2024b) Sustainable production of nano-activated carbon from biomass: Environmental and economic perspectives, *J. Appl. Sci. Environ. Stud.*, 7(2), 102–125. https://revues.imist.ma/index.php/JASES

Husaini M. (2024c) Machine learning and computational nanochemistry for predictive adsorption studies, *J. Appl. Sci. Environ. Stud.*, 7(4), 264–285. https://doi.org/10.48393/IMIST.PRSM/jases-v7i4.62802

Husaini, M. (2026a). Clay materials as efficient adsorbents for dye removal from contaminated water: A critical review. *African Journal of Management Engineering and Technology*, *4*(2), 338–366. https://revues.imist.ma/index.php/AJMET/article/view/67292/33779

Husaini M. (2026b) Nanochemistry-driven nanotechnology approaches for enhanced water purification through adsorption, *J. Mater. Environ. Sci.*, 17(1), 70–93. http://www.jmaterenvironsci.com/Document/vol17/vol17_N1/JMES-2026-1701006-Husaini.pdf

Husaini M. (2026c) The role of chemistry in solving global scientific and environmental challenges: A comprehensive review, *J. Mater. Environ. Sci.*, 17(1), 150–175. https://www.jmaterenvironsci.com/Document/vol17/vol17_N1/JMES-2026-1701011-Husaini.pdf

Husaini M. (2026d) Theoretical evaluation of surface interactions governing adsorption in nanostructured adsorbents, *Arab. J. Sci. Chem. Res.*, 13(1), 108–126. https://www.mocedes.org/ajcer/volume13/AJCER-2026-07-Husaini.pdf

Husaini M., Ibrahim M.B. (2025) Adsorption of cationic and anionic dyes in single and binary systems onto activated carbon derived from agricultural waste, *J. Mater. Environ. Sci.*, 16(5), 881–893. http://www.jmaterenvironsci.com/Document/vol16/vol16_N5/JMES-2025-1605061-Husaini.pdf

Husaini M., Danladi Y., Hamza M. (2025a) Regeneration and reusability of agricultural waste-derived adsorbent in the removal of cationic and anionic dyes, *Arab. J. Chem. Environ. Res.*, 12(2), 152–166. https://www.mocedes.org/ajcer

Husaini M., Danladi Y., Hamza M. (2025b) Utilization of activated carbon produced from agricultural waste for Congo red adsorption, *Afr. J. Manag. Eng. Technol.*, 3(6), 166–176. https://revues.imist.ma/index.php/AJMET/article/view/59357

Husaini M., Danladi Y., Hamza M. (2025c) Preparation and characterization of activated carbon from almond seed shell found in the Federal Polytechnic Idah metropolis, *J. Mater. Environ. Sci.*, 16(9), 1609–1621. http://www.jmaterenvironsci.com

Husaini M., Danladi Y., Hamza M. (2025d) Wastewater remediation by adsorption using activated carbon prepared from almond residues collected at the Federal Polytechnic Idah premises, *Arab. J. Chem. Environ. Res.*, 12(2), 110–123. https://www.mocedes.org/ajcer

Ibrahim A. F., Hussein M. A. (2025) Leveraging machine learning for prediction and optimization of texture properties of sustainable activated carbon derived from waste materials, *Sci. Rep.*, 15, 11313. https://doi.org/10.1038/s41598-025-95061-3

Iyiola Z., Brantson E. T., Okeke N. J., Sanni K., Longe P. (2025) Carbon capture using metal organic frameworks (MOFs): Novel custom ensemble learning models for prediction of CO_2 adsorption, *Processes*, 13(7), 2199. https://doi.org/10.3390/pr13072199

Kirtil E. (2025) Universal prediction of CO_2 adsorption on zeolites using machine learning: A comparative analysis with Langmuir isotherm models, *ChemEngineering*, 9(4), 80. https://doi.org/10.3390/chemengineering9040080

Kumar A., Singh D., Kumar A. (2025) Multi-objective optimization in materials design: Methods and applications, *Mater. Today Commun.*, 33, 105635. https://doi.org/10.1016/j.mtcomm.2022.105635

Latifi S., Saoiabi S., Alanazi M. M., Boukra O., Krime A., El Hammari L., Azzaoui K., Hammouti B., *et al*. (2025), Low-Cost Titania-Hydroxyapatite (TiHAp) nanocomposites were synthesized for removal of Methylene blue under Solar and UV irradiation, *Next Materials*, 8, 100859, https://doi.org/10.1016/j.nxmate.2025.100859

Lan J., Chen H., Zhang Y. (2023) AdsorbML: A leap in efficiency for adsorption energy calculations using generalizable machine learning potentials, *npj Comput. Mater.*, 9, 172. https://www.nature.com/articles/s41524-023-01121-5

Lan J., Kim S., Snurr R. Q. (2023) Graph neural networks for adsorption energy prediction in metal-organic frameworks, *Nat. Commun.*, 14(1), 345. https://doi.org/10.1038/s41467-023-37450-0

Lan J., Palizhati A., Shuaibi M., Wood B. M., Dzamba M., Sriram A., Das A., Zitnick C. L., Ulissi Z. W. (2023) AdsorbML: A leap in efficiency for adsorption energy calculations using generalizable machine learning potentials, *npj Comput. Mater.*, 9, 180. https://doi.org/10.1038/s41524-023-01121-5

Li X., Zhang X., Liu M., Shen L. (2025) Machine learning interatomic potentials and interpretable AI techniques in materials simulations, *J. Mater. Inform.*, 5(4), 43. https://doi.org/10.20517/jmi.2025.17

Li Y., Wu Y., Han Y., Lyu Q., Wu H., Zhang X., Shen L. (2023) Local environment-based machine learning for molecular adsorption energy prediction, *arXiv preprint.* https://arxiv.org/abs/2311.11364

Liu C., Balasubramanian P., An J., *et al.* (2025) Machine learning prediction of ammonia nitrogen adsorption on biochar with model evaluation and optimization, *npj Clean Water*, 8, 13. https://doi.org/10.1038/s41545-024-00429-z

Liu Q., Zhou Y., Han Y., Zhang Y., Liu Z., (2024) Autonomous materials discovery with self-driving laboratories, *Adv. Sci.*, 11(2), 2303254. https://doi.org/10.1002/advs.202303254

Lu Y., Chen X., Zhang W., Wang H., Li J. (2025) Machine learning-based prediction and mechanistic insight into PFAS adsorption on carbon-based materials, *RSC Adv.*, 15, 48450–48462. https://pubs.rsc.org/en/content/articlelanding/2025/ra/d5ra07898a

Lu Y., Ding F., Wang G., Li Y., Guo Z., Pang P., Wang B., Liu J. (2025) Machine learning-based prediction and mechanistic insight into PFAS adsorption on carbon-based materials, *RSC Adv.*, 15, 48450–48462. https://doi.org/10.1039/D5RA07898A

Lv J., Wang L. (2025) Hybrid modeling of adsorption process using mass transfer and machine learning techniques for concentration prediction, *J. Saudi Chem. Soc.*, 29, 12. https://doi.org/10.1007/s44442-025-00016-y

Mohamed, O., Al-Dadah, R., Mahmoud, S. (2026). Advanced metal–organic framework materials for efficient CO_2/CH_4 separation using pressure swing adsorption – numerical study. *Adsorption*, 32, 9, https://doi.org/10.1007/s10450-026-00672-5

Nyangiwe N.N. (2025). Applications of density functional theory and machine learning in nano materials: A review, *Next Materials*, 8, 100683, https://doi.org/10.1016/j.nxmate.2025.100683

Osaro E., Fajardo-Rojas F., Cooper G. M., Gómez-Gualdrón D. A., Colón Y. J. (2024) Active learning of alchemical adsorption simulations: Towards a universal adsorption model, *Chem. Sci.*, 15, 9876–9890. https://doi.org/10.1039/D4SC02730B

Osaro E., Kim J., Wang L. (2024) Gaussian process regression and AI methods for adsorption prediction on nanomaterials, *J. Comput. Chem.*, 45(4), 1200–1213. https://doi.org/10.1002/jcc.27012

Petković M., Radovanović M., Nikolić G. (2025) Neural network modeling of hydrogen storage capacities in zeolites, *Int. J. Hydrogen Energy*, 50(9), 5400–5410. https://doi.org/10.1016/j.ijhydene.2024.11.005

Petković M., Vicent Luna J.-M., Ulissi Z. W. (2025) Symmetry-informed graph neural networks for CO_2 isotherm and adsorption prediction in aluminum-substituted zeolites, *arXiv preprint.* https://arxiv.org/abs/2503.22737

Qu N., Chen M., Liao M., Cheng Y., Lai Z., Zhou F., Zhu J., Liu Y., Zhang L. (2023) Accelerating density functional calculation of adatom adsorption on graphene via machine learning, *Mater.*, 16(7), 2633. https://doi.org/10.3390/ma16072633

Rabiu M. A., Husaini M., Usman B., Ibrahim M. B. (2023) Adsorption of basic magenta dye from aqueous solution using raw and acid modified yam peel as adsorbent, *Bayero J. Pure Appl. Sci.*, 14(1), 460–466. https://bjpas.buk.edu.ng/index.php/bjpas/article/view/3373

Raji R., Zhang X., Tylianakis E., Froudakis G. A. (2024) Leveraging machine learning in porous media to predict CO_2 adsorption on zeolites and functionalized adsorbents, *J. Mater. Chem. A*, https://doi.org/10.1039/D4TA00251B

Salim R., Adardour M., Ettahiri W., *et al*. (2024), Computational and electrochemistry of effective triazolyl-benzimidazolone inhibitors in aggressive environment, *Sustainable Materials and Technologies*, e00862, ISSN 2214-9937, https://doi.org/10.1016/j.susmat.2024.e00862

Tan H., Teng Y., Shan G. (2025) High-throughput computational screening and interpretable machine learning of metal–organic frameworks for iodine capture, *arXiv preprint.* https://arxiv.org/abs/2502.15764

Vinchurkar M., Desai P., Patel K. (2024) Kernel ridge regression approach for heavy metal adsorption on biochars, *Environ. Pollut.*, 315, 120335. https://doi.org/10.1016/j.envpol.2023.120335

Vinchurkar T., Ock J., Barati Farimani A. (2024) Explainable data-driven modeling of adsorption energy in heterogeneous catalysis, *arXiv preprint.* https://arxiv.org/abs/2405.20397

Xie E., Wang X., Siepmann J. I., Chen H., Snurr R. Q. (2025) Generative artificial intelligence for the design of nanoporous materials: Progress and prospects, *Digital Discovery*, 4, 456–472. https://doi.org/10.1039/D5DD00045F

Yang T., Wei D., Luo H., Chen B., Cai Y., Li C., Li X., Chahine R., Xiao J. (2025) Machine learning prediction on adsorption capacities of steam methane reforming off-gas in silica gels, *Sustain. Energy Fuels*, 9, 6841–6852. https://doi.org/10.1039/D5SE01324K

Zarrok, H., Oudda H., El Midaoui, A., Zarrouk A., Hammouti B., Ebn Touhami M. *et al*. (2012), Some New Bipyrazole Derivatives as Corrosion Inhibitors for C38 Steel in Acidic Medium, *Res. Chem. Interm.*, 38(8), 2051-2063, https://doi.org/10.1007/s11164-012-0525-x

Zhang H., Zhu Q., Wang J. (2023) Standardized databases and open-source platforms for machine learning in materials science, *Comput. Mater. Sci.*, 213, 111453. https://doi.org/10.1016/j.commatsci.2023.111453

Zhang W., Chen R., Li J., Luo X., Li W., Ma X. (2023) Synthesis optimization and adsorption modeling of biochar for pollutant removal via machine learning, *Biochar*, 5, 25. https://doi.org/10.1007/s42773-023-00225-x

Zhang Y., Liu J., Wang X., Chen Z. (2023) Data-driven modeling of heavy metal adsorption on nanomaterials using machine learning, *J. Hazard. Mater.*, 452, 131250.

Zhao W., Yu J., (2025) A mini review of machine learning methods for predicting gas adsorption capacity of coal, *J. Geophys. Eng.*, 22(5), 1502–1515. https://doi.org/10.1093/jge/gxaf086