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Theoretical Evaluation of Surface Interactions Governing Adsorption in Nanostructured Adsorbents

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Abstract

Adsorption in nanostructured materials plays a crucial role in environmental remediation, gas separation, energy storage, and catalytic applications. The rapid development of nanostructured adsorbents has intensified the need for theoretical approaches capable of elucidating surface interactions and adsorption mechanisms at the atomic and molecular levels. This review presents a comprehensive theoretical evaluation of surface interactions governing adsorption in nanostructured adsorbents, emphasizing quantum mechanical calculations, molecular simulation techniques, and continuum-level models. Density Functional Theory is discussed as a fundamental tool for predicting adsorption energies, electronic structure changes, and preferred binding configurations, while Molecular Dynamics and Monte Carlo simulations provide insights into adsorption dynamics, equilibrium behavior, and thermodynamic properties. The influence of surface chemistry, morphology, and nanoscale confinement on adsorption performance is critically analyzed across a range of nanomaterials, including carbon-based structures, metal oxides, and porous frameworks. By integrating recent advances in computational modeling and data-driven approaches, this review highlights current capabilities, limitations, and future perspectives for theoretical adsorption studies, offering guidance for the rational design of high-performance nanostructured adsorbents.

Keywords: Nanostructured adsorbents; Surface interactions; Density Functional Theory; Molecular Dynamics; Monte Carlo simulations; Theoretical modelling.

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1. Introduction

Adsorption is a fundamental interfacial phenomenon that plays a pivotal role in numerous scientific and technological applications, including environmental remediation, catalysis, gas separation, energy storage, corrosion inhibition, and sensing technologies (Hammouti *et al.*, 2013; Kadda *et al.*, 2023; Husaini *et al.*, 2025a-d; Corrente and Neimark, 2025; Singh *et al.*, 2023). The rapid development of nanostructured adsorbents has significantly enhanced the efficiency and selectivity of adsorption-based processes due to their high surface-to-volume ratios, tunable surface chemistry, and distinct electronic characteristics (Zhang *et al.*, 2024; Lee *et al.*, 2025a). At the nanoscale, adsorption behavior is strongly influenced by atomic-scale surface features such as defects, functional groups, and exposed crystal facets rather than bulk material properties alone.

A comprehensive understanding of adsorption mechanisms in nanostructured materials requires detailed knowledge of surface interactions between adsorbates and adsorbent surfaces. These interactions include van der Waals forces, electrostatic interactions, hydrogen bonding, and chemical bonding, which may coexist or compete depending on surface composition and environmental conditions (Do, 1998; Hansen *et al.*, 2024; Hou *et al.*, 2023). While experimental techniques provide valuable macroscopic information such as adsorption capacity and kinetics, they often lack the resolution needed to elucidate electronic-level interactions and preferred adsorption configurations on complex nanostructured surfaces.

Theoretical and computational approaches have therefore emerged as indispensable tools for investigating adsorption phenomena at the nanoscale. Density functional theory (DFT) has been widely employed to evaluate adsorption energies, charge transfer, and electronic structure modifications induced by adsorption (Kothakonda *et al.*, 2024; Ngana *et al.*, 2025). Molecular dynamics and Monte Carlo simulations further complement these studies by capturing temperature effects, adsorption dynamics, and equilibrium distributions under realistic operating conditions (Hmamou *et al.*, 2013; Ibrahim and Gharbia, 2024; Liu *et al.*, 2025).

Despite considerable progress, challenges remain in accurately describing multiscale surface interactions, incorporating solvent and pressure effects, and bridging the gap between atomistic predictions and experimentally measurable adsorption performance (Ghosh *et al.*, 2024; Hao *et al.*, 2025). Addressing these challenges requires systematic evaluation of theoretical models and critical comparison across different classes of nanostructured adsorbents.

This review therefore focuses on the theoretical evaluation of surface interactions governing adsorption in nanostructured adsorbents. Emphasis is placed on the fundamental interaction mechanisms, the strengths and limitations of commonly used computational approaches, and recent advances that enhance predictive accuracy. By consolidating insights from contemporary theoretical studies, this work aims to support the rational design and optimization of next-generation adsorbent materials for advanced applications (Ma *et al.*, 2025; Lee *et al.*, 2025b).

2. Overview

2.1. Adsorption and Key Terms

Adsorption is a surface phenomenon where atoms, ions, or molecules from a fluid phase accumulate on a solid surface, forming an interfacial layer. The materials that facilitate this process are known as adsorbents, and the forces binding adsorbates to the surface are collectively referred to as surface interactions (Husaini *et al.*, 2023a-f). These interactions include a combination of physical and chemical forces such as dispersion (van der Waals) forces, electrostatic attraction, hydrogen bonding, and chemical bonding (Chetouani *et al.*, 2003; Singh *et al.*, 2024; Akbari and Morad, 2025).

2.2. Environmental and Industrial Relevance

Adsorption processes play a vital role in addressing environmental challenges by enabling the removal of pollutants such as heavy metals, dyes, volatile organic compounds, and greenhouse gases from air and water (Errich *et al.*, 2021; N'diaye *et al.*, 2022; Rabiu *et al.*, 2023; Hamza *et al.*, 2025, Husaini, 2026;). Industrially, adsorption is crucial for gas purification, catalysis, separation, and energy storage technologies. The efficiency of these applications is highly dependent on the surface characteristics of adsorbent materials (Husaini and Ibrahim, 2025; Li *et al.*, 2024; Mian *et al.*, 2025).

2.3. Importance of Nanostructured Adsorbents

Nanostructured adsorbents exhibit enhanced adsorption performance compared to bulk materials due to their increased surface-to-volume ratio and abundance of active sites. Nanostructuring introduces unique features such as surface defects, edge sites, and customizable functional groups that strongly influence adsorption behavior. Moreover, it enables precise control over pore sizes and surface chemistry, allowing for selective adsorption tailored to target molecules (Lee *et al.*, 2025a; Yuan *et al.*, 2025).

2.4. Limitations of Experimental Approaches

While experimental techniques provide essential macroscopic information such as adsorption capacity and kinetics, they often fall short in elucidating the detailed atomic- and molecular-level mechanisms of adsorption. Complex nanostructured systems involve multiple interaction pathways that are challenging to resolve solely through experimentation, limiting insights into the nature of bonding, charge transfer, and adsorption configurations (Ghosh *et al.*, 2024; Ngana *et al.*, 2025).

2.5. Necessity of Theoretical Evaluation

Theoretical and computational methods serve as indispensable tools to investigate adsorption phenomena in nanostructured adsorbents. These approaches facilitate systematic exploration of surface interactions, adsorption energetics, and the relationship between structure and performance under well-defined conditions. By complementing experimental data, theoretical models provide predictive insights that guide the rational design and optimization of advanced adsorbent materials (Ibrahim and Gharbia, 2024; Lee *et al.*, 2025b).

3.2 Surface Chemistry and Physics

3.2.1 Surface Energy and Defects

Surface atoms or molecules have unsatisfied bonds compared to their bulk counterparts, leading to excess surface energy. This high surface energy drives adsorption as adsorbates tend to minimize the system's total energy by binding to these active sites. Materials with higher surface energy generally exhibit stronger adsorption affinity and reactivity (El Ouafi *et al.*, 2002; Akartasse *et al.*, 2022; Hkiri *et al.*, 2024). Crystallographic defects, such as vacancies (missing atoms), step edges, kinks, and dislocations, alter the local electronic and geometric structure of the surface. These defects act as energetic "hotspots" for adsorption, often possessing higher binding energies and enhanced chemical activity. They can serve as nucleation centers for adsorption and catalysis, influencing overall performance (Kothakonda *et al.*, 2024).

3.2.2 Functional Groups

Surface functionalization introduces chemically active groups like hydroxyl (-OH), carboxyl (-COOH), amine (-NH_2), thiol (-SH), and others. These groups are often introduced intentionally to tailor the adsorbent's surface properties or may arise naturally from precursor materials or processing conditions (Ngana *et al.*, 2025). Functional groups influence adsorption through hydrogen bonding, electrostatic attraction, dipole interactions, and sometimes covalent bonding with target molecules. These interactions enhance selectivity and binding strength for specific adsorbates, especially in aqueous environments where surface charge and polarity are crucial (Husaini *et al.*, 2024a&b; Hou *et al.*, 2023).

3.2.3 Morphology

The porous architecture of adsorbents significantly impacts adsorption performance. Micropores (<2 nm) provide large surface areas and strong adsorbate confinement, promoting high adsorption capacity. Mesopores (2–50 nm) enhance molecular diffusion and transport within the material, improving kinetics. Macropores (>50 nm) serve primarily as channels facilitating rapid access to inner adsorption sites, reducing diffusion limitations (Corrente and Neimark, 2025). Nanomaterials exhibit a variety of exposed surface features such as edges, corners, and specific crystal facets that differ from flat surfaces in atomic coordination and electronic structure. These sites often possess unique chemical reactivity and adsorption properties, significantly influencing the overall adsorption energetics and selectivity (Husaini, 2023a). The control of morphology at the nanoscale is therefore a powerful tool in designing effective adsorbents (Shi *et al.*, 2024).

3.3 Nanostructured Adsorbents

3.3.1 Carbon-Based Nanomaterials

Graphene is a two-dimensional allotrope of carbon consisting of a single atomic layer arranged in a hexagonal lattice. It offers exceptional mechanical strength, high electrical and thermal conductivity, and an enormous specific surface area, making it a highly attractive adsorbent. Its surface can be chemically modified to introduce functional groups that enhance adsorption selectivity (Ngana *et al.*, 2025; Husaini, 2023b).

CNTs are cylindrical nanostructures formed by rolling graphene sheets into tubes with diameters in the nanometer range and lengths up to several microns. Their high aspect ratio and unique electronic properties provide adsorption sites on both the outer surface and the hollow interior. CNTs can be functionalized to improve dispersibility and tailor adsorption characteristics (Hou *et al.*, 2023).

Activated carbon is a highly porous carbon material produced by carbonizing organic precursors and activating them physically or chemically. Its large surface area and broad pore size distribution, combined with various oxygen-containing functional groups, enable efficient adsorption of a wide range of contaminants from gases and liquids (Corrente and Neimark, 2025).

3.3.2 Metal Oxides and Composites

Metal oxides such as titanium dioxide (TiO_2), zinc oxide (ZnO), iron oxide (Fe_3O_4), and alumina (Al_2O_3) exhibit versatile surface chemistry, including the presence of hydroxyl groups and redox-active sites. Their variable oxidation states and surface charge properties make them effective for adsorbing gases, heavy metals, and organic pollutants (Ghosh *et al.*, 2024). Combining metal oxides with other materials, including carbon-based nanomaterials or polymers, can enhance adsorption properties through synergistic effects. These composites often improve mechanical stability, surface area, and regeneration potential, addressing some limitations of individual components (Ngana *et al.*, 2025).

3.3.3 Metal-Organic Frameworks (MOFs), Zeolites, and Porous Polymers

MOFs are crystalline porous materials composed of metal ions or clusters coordinated with organic linkers. Their highly tunable pore sizes, shapes, and surface chemistries enable precise control over adsorption selectivity and capacity. MOFs have found applications in gas storage, separation, catalysis, and sensing (Corrente and Neimark, 2025; Chaouiki *et al.*, 2026).

Zeolites are microporous aluminosilicate minerals with a well-ordered crystalline framework. Their uniform pore size distribution and high thermal and chemical stability make them excellent molecular sieves and catalysts. Zeolites are widely used in industrial adsorption and catalysis processes (Hkiri *et al.*, 2024). Porous polymers include a variety of amorphous or semi-crystalline materials designed to have high surface areas and functional group diversity. Their chemical versatility enables selective adsorption of organic pollutants, gases, and biomolecules. Porous polymers can be engineered to provide tailored pore sizes and surface functionalities suitable for specific applications (Liu *et al.*, 2025).

4. Theoretical Methods for Adsorption Evaluation

This section reviews key theoretical and computational approaches utilized to study adsorption phenomena on nanostructured adsorbents. Each methodology offers unique advantages and limitations, enabling complementary insights into adsorption mechanisms across different scales. By combining these approaches, researchers can develop a comprehensive understanding of adsorption processes from the atomic level to macroscopic applications, helping to optimize adsorbent design and predict performance under various conditions.

4.1 Quantum Mechanical Approaches

4.1.1 Density Functional Theory (DFT)

Density Functional Theory forms the cornerstone of quantum mechanical simulations for adsorption studies. It is based on solving the electronic structure of materials by approximating electron density distributions, enabling accurate predictions of adsorption energies, preferred binding sites, and molecular configurations with atomistic detail (Al Hamzi *et al.*, 2013; Husaini, 2024). DFT allows for in-depth analysis of the electronic properties of both adsorbent and adsorbate, including charge transfer, orbital interactions, and chemical bonding, which are crucial for understanding adsorption mechanisms at the fundamental level (Hou *et al.*, 2023; Chikaodili *et al.*, 2024).

4.1.2 Strengths of DFT

DFT accurately captures complex electronic interactions that govern adsorption, providing detailed insights into how adsorbates bind to surfaces and how the electronic environment changes during adsorption. This makes it invaluable for studying catalytic activity, selectivity, surface reactivity, and the effect of defects and dopants on nanostructured adsorbents (Shi *et al.*, 2024; Ahn *et al.*, 2025).

4.1.3 Limitations of DFT

Despite its predictive power, DFT calculations are computationally demanding, especially for large or structurally complex systems such as extended surfaces, large molecules, or nanoporous materials. The computational cost often restricts its application to relatively small model systems or requires simplifications, such as cluster models or periodic boundary conditions, which can introduce approximation errors (Chikaodili *et al.*, 2024).

4.2 Molecular Simulation Techniques

4.2.1 Molecular Dynamics (MD)

Molecular Dynamics simulations provide a time-resolved picture of atomic and molecular motions by numerically integrating Newton's equations of motion. MD is useful for studying dynamic aspects of adsorption, including diffusion of adsorbates on surfaces, conformational changes of molecules, temperature-dependent effects, and interactions within solvent environments. It reveals transient phenomena and kinetic pathways that static methods like DFT cannot capture, offering a more realistic representation of adsorption under operational conditions (Chikaodili *et al.*, 2024).

4.2.2 Dynamic Effects Captured by MD

MD allows observation of adsorption-desorption events, molecular rearrangements, and the influence of thermal fluctuations, which are critical for understanding adsorption kinetics and mechanisms in real time. These insights help predict performance changes due to temperature, pressure, and surface heterogeneity (Chikaodili *et al.*, 2024).

4.2.3 Limitations of MD

MD simulations require accurate force fields or interatomic potentials to realistically model interactions. Additionally, MD is often limited by accessible timescales (typically nanoseconds to microseconds) and system sizes due to computational constraints, which may not be sufficient for slow adsorption processes or very large systems (Chikaodili *et al.*, 2024).

4.2.4 Monte Carlo (MC) Simulations

Monte Carlo simulations employ stochastic sampling techniques to explore configurational space and evaluate thermodynamic properties of adsorption systems at equilibrium. MC is highly efficient in predicting adsorption isotherms, surface coverages, and thermodynamic averages by statistically sampling many possible adsorbate configurations and orientations, especially useful for porous materials and gas adsorption (Ghosh *et al.*, 2024; Liu *et al.*, 2025).

4.2.5 Advantages of MC

Monte Carlo simulations can handle large system sizes and long timescales more efficiently than MD, providing ensemble averages of adsorption behavior without requiring explicit time-dependent trajectories. This makes MC particularly valuable for screening adsorbents and understanding equilibrium adsorption in complex porous materials (Liu *et al.*, 2025).

4.2.6 Limitations of MC

While powerful for equilibrium properties, MC simulations do not inherently provide dynamic information or adsorption kinetics. They complement MD and DFT by focusing on thermodynamics rather than detailed atomic motions (Chikaodili *et al.*, 2024).

4.3 Continuum and Mesoscale Models

4.3.1 Purpose and Scope

Continuum and mesoscale modeling techniques aim to describe adsorption phenomena beyond the molecular scale, linking atomistic adsorption mechanisms to macroscopic experimental observations and practical engineering applications. These models bridge gaps where explicit atomistic simulations become computationally unfeasible (Zhu *et al.*, 2025).

4.3.2 Modeling Approaches

Mean-field theories, coarse-grained models, and other continuum approaches simplify the representation of adsorbate molecules and porous media by averaging molecular details. These models capture large-scale phenomena such as adsorbate diffusion through complex pore networks, phase behavior, and mass transport, enabling the study of adsorption kinetics, capacity, and breakthrough behavior at practical scales (Zhu *et al.*, 2025).

4.3.3 Applications and Limitations

These methods are essential for investigating large-scale systems, such as industrial adsorbents or environmental materials, where molecular simulations alone are impractical. Although continuum models sacrifice molecular detail, they integrate theoretical insights into practical adsorbent design and process optimization, supporting scale-up and commercialization (Zhu *et al.*, 2025).

5. Surface Interaction Mechanisms

5.1 Origin and Significance of van der Waals and Dispersion Forces

van der Waals forces arise from transient fluctuations in the electron clouds of atoms or molecules, creating temporary dipoles that induce weak, non-specific attractions. These interactions are fundamental in physisorption, where adsorbates attach to surfaces without forming chemical bonds. Nanostructured materials, due to their high surface area and curved surfaces, enhance van der Waals forces by increasing the number of contact points with adsorbates. This enhancement is particularly important for adsorption of nonpolar gases and molecules. Computationally, dispersion-corrected density functional theory (DFT-D) and Lennard-Jones potentials are widely used to model these forces. Key calculated properties typically include adsorption energies, equilibrium distances between adsorbates and surfaces, and molecular orientation preferences (Medel and Vargas, 2025; Akbari and Morad, 2025).

5.2 Electrostatic Forces and Their Environmental Modulation

Electrostatic interactions result from the attraction or repulsion between charged or polar adsorbates and charged or polarized surface sites. The magnitude of these forces depends on surface charge density, adsorbate polarity, and the ionic makeup of the surrounding environment. In ionic or aqueous media, dissolved ions screen electrostatic forces, modifying the electrical double layer structure and influencing adsorption equilibrium and kinetics. Modeling approaches range from continuum-level descriptions like the Poisson-Boltzmann equation to atomistic simulations that incorporate explicit charges and polarizability. Typical computed outcomes include electrostatic potential profiles, interaction energies, and charge density distributions near surfaces (Yao *et al.*, 2025; Wang and Chen, 2024).

5.3 Chemisorption: Mechanistic Insights and Electronic Structure Changes

Chemisorption is characterized by the formation of strong, specific covalent or coordination bonds between adsorbates and surface atoms. This interaction often causes significant changes in the electronic and geometric structures of both adsorbate and substrate. It plays a critical role in selective adsorption and catalysis by enabling molecular activation and surface reactions. Quantum mechanical methods, especially density functional theory (DFT), provide detailed insights into bond formation, charge transfer, and reaction pathways. Important calculated metrics include bond dissociation energies, alterations in bond lengths and angles, and electron density redistribution (Sun and Wu, 2025; Zhang *et al.*, 2025).

5.4 Role of Hydrogen Bonding in Directional and Selective Adsorption

Hydrogen bonding occurs when a hydrogen atom covalently bonded to an electronegative donor atom interacts with an electronegative acceptor atom. This interaction is directional and stronger than van der Waals forces but weaker than covalent bonds. Hydrogen bonding plays a crucial role in the adsorption of water, biomolecules, and other polar compounds, influencing molecular orientation, structure, and stability on surfaces. Computational studies use high-level quantum chemical calculations and parameterized classical force fields to describe hydrogen bond energetics and geometry, while molecular dynamics simulations capture their dynamic and cooperative nature. Typical calculated properties include bond energies, donor-acceptor distances, and bond angles (Medel and Vargas, 2025; Yao *et al.*, 2025).

6. Comparative Analysis of Materials

6.1 Interaction Mechanisms in Graphene Derivatives

Graphene derivatives primarily exhibit adsorption dominated by π–π stacking and dispersion forces. These weak, non-covalent interactions result in strong physisorption that is highly sensitive to surface modifications. Functionalization of graphene surfaces with various chemical groups can significantly tune the adsorption selectivity and capacity. Computational techniques such as density functional theory (DFT) and molecular dynamics (MD) simulations are extensively used to investigate how these interactions govern the adsorption process on graphene-based materials (Smith and Lee, 2024).

6.2 Surface Chemistry and Adsorption on Metal Oxides

Metal oxides rely predominantly on electrostatic interactions and coordination bonds for adsorption. Their surfaces often possess charged or polar sites, as well as variable oxidation states, which provide specific binding environments for targeted adsorbates like heavy metals or gases. Modeling these materials typically involves a combination of DFT and MD methods to capture both the electronic and dynamic aspects of adsorption. The presence of surface defects further enhances their adsorption performance by acting as active sites for chemisorption (Patel and Kumar, 2025; Liu and Chen, 2024).

6.3 Multifunctional Adsorption in Metal-Organic Frameworks (MOFs)

Metal-organic frameworks are distinguished by their diverse adsorption mechanisms, which include hydrogen bonding, coordination interactions, and van der Waals forces. MOFs feature highly tunable porous structures that allow precise control over pore size, shape, and surface chemistry. This structural flexibility results in high adsorption capacity and selectivity for a variety of adsorbates. Computationally, DFT combined with Monte Carlo simulations are powerful tools to explore adsorption within MOF pores and guide the design of materials optimized for specific applications (Chen *et al.*, 2025).

6.4 Influence of Structural Factors on Adsorption Efficiency

The efficiency of adsorption in all these materials is heavily influenced by structural characteristics such as pore size, surface functional groups, and defects. Micropores provide strong adsorbate confinement and large surface areas, boosting adsorption capacity. Functional groups modulate chemical affinity through hydrogen bonding, electrostatic attraction, or covalent interactions, thus enhancing selectivity. Surface defects, including vacancies and dislocations, act as energetically favorable sites that increase adsorption strength and catalytic activity. Understanding and tailoring these structural features are essential for optimizing adsorption performance, kinetics, and the recyclability of adsorbents (Garcia and Lopez, 2023).

7. Key Challenges in Theoretical Evaluation

7.1 Bridging Quantum-Scale Models to Realistic Systems

One of the major challenges in theoretical adsorption studies is the difficulty of extending quantum mechanical predictions, often limited to small systems due to computational cost, to realistic, larger-scale materials and operational environments. Quantum-level methods such as density functional theory (DFT) provide detailed insights into atomic-level interactions but struggle to capture the complexity of real adsorbents that feature large surface areas, structural heterogeneity, and diverse active sites. Developing scalable approaches that maintain quantum accuracy while addressing the size and complexity of practical materials remains a pressing need (Darwish and Eapen, 2025; Sun and Wu, 2025).

7.2 Accurate Representation of Solvent and Temperature Effects

Most quantum mechanical calculations are performed under idealized, vacuum conditions, which neglect the influence of solvents and temperature. However, in many practical applications, adsorption occurs in liquid or humid environments where solvent molecules significantly alter surface energetics and adsorption dynamics. Incorporating solvent effects and temperature-dependent behavior into theoretical models poses a substantial challenge, requiring either explicit solvent modeling—often computationally expensive—or implicit solvent approaches that may lack detailed accuracy (Ta *et al.*, 2024). Addressing this gap is critical for realistic predictions of adsorption thermodynamics and kinetics.

7.3 Integrating Multiscale Modeling Approaches

Adsorption phenomena inherently span multiple length and time scales, ranging from electronic interactions at the atomic scale to mass transport and surface coverage at the mesoscale and system levels. Capturing this breadth requires integrated multiscale modeling frameworks that link quantum mechanical simulations with mesoscale techniques like kinetic Monte Carlo or molecular dynamics, and system-level continuum models. Achieving seamless communication between these scales, with consistent transfer of information such as energies, rates, and structural changes, remains a significant theoretical challenge (Park *et al.*, 2025; Wang and Zhou, 2025).

7.4 Accounting for Dynamic and Operating Conditions

Real-world adsorption processes occur under dynamic conditions involving fluctuating temperature, pressure, and chemical environments. Static calculations often fail to capture time-dependent phenomena such as surface restructuring, adsorbate diffusion, competitive adsorption, and catalyst deactivation. Incorporating dynamic effects through time-resolved simulations, reactive molecular dynamics, or ab initio molecular dynamics is computationally demanding but necessary to realistically model adsorption under operational conditions. Enhancing the capability to simulate these effects will improve the predictive power of theoretical models (Sankaranarayanan, 2024; Swenson and Stadie, 2019).

8. Future Directions

8.1 Machine Learning-Assisted Potential Energy Surfaces

Advancements in machine learning (ML) techniques offer promising opportunities to accelerate and enhance theoretical adsorption studies. ML-assisted potential energy surfaces can efficiently approximate complex quantum mechanical calculations, significantly reducing computational costs while maintaining accuracy. These surrogate models enable exploration of larger configurational spaces and dynamic adsorption processes that are otherwise computationally prohibitive with traditional methods. Incorporating ML into adsorption simulations holds the potential to revolutionize material discovery and optimization by rapidly predicting adsorption energetics and mechanisms (Zhang *et al.*, 2024).

8.2 High-Throughput Computational Screening

High-throughput computational screening methods are increasingly being adopted to identify promising adsorbent materials from vast chemical and structural spaces. By automating the evaluation of adsorption properties across large libraries of candidates using efficient computational workflows, researchers can accelerate the discovery of materials with optimal performance. This approach facilitates rapid narrowing down of viable adsorbents before experimental validation, significantly reducing development time and costs (Garcia and Kim, 2023).

8.3 Integration of Experimental and Theoretical Approaches

Coupling theoretical simulations with experimental investigations is crucial for accurate model validation and comprehensive understanding of adsorption phenomena. Advances in in situ characterization techniques, combined with real-time data integration into computational models, enable simultaneous observation and prediction of adsorption behavior under relevant conditions. This synergy enhances the reliability of theoretical predictions and guides the design of experiments, fostering more efficient development of adsorbent materials (Lee *et al.*, 2025a).

8.4 Real-Time Dynamic Simulations under Reactive Environments

Future theoretical frameworks aim to simulate adsorption processes dynamically in real-time under realistic flow conditions and reactive environments. Incorporating the effects of temperature fluctuations, pressure variations, and chemical reactions within simulation environments will provide deeper insight into adsorption kinetics, surface restructuring, and catalyst stability. Developing computational methods capable of capturing these complex dynamic interactions will significantly advance the predictive accuracy and practical relevance of adsorption models (Singh and Patel, 2024).

Table 1: Reviewed Literature on Theoretical Evaluation of Adsorption in Nanostructured Adsorbents

Study Area	**Method Used**	**Highlights**	**References**
Introduction and Background	Review of molecular simulation approaches	Highlights the role of simulations in adsorbent design and adsorption analysis.	Zhu *et al.,* 2025
	Integrated DFT, MD, and MC simulations	Distinguishes physisorption and chemisorption on MOF surfaces.	Chikaodili *et al.,* 2024
Adsorption Fundamentals	DFT with kinetic Monte Carlo	Explains N_2 adsorption pathways on ZnO monolayers.	Ghosh *et al.,* 2024
	Lattice grand canonical Monte Carlo	Predicts water adsorption isotherms in porous materials.	Liu *et al.,* 2025
Surface Chemistry and Physics	Density Functional Theory Highlights(DFT)Highlights	Reveals surface chemistry effects on sulfide adsorption.	Hou *et al.,* 2023
Nanostructured Adsorbents	Computational screening and modeling	Identifies efficient molecular adsorbents for CO_2/CH_4 separation.	Yang *et al.,* 2025
	DFT and machine learning comparison	Demonstrates rapid adsorption prediction using hybrid models.	Aljamal and Wang, 2025
Theoretical Methods	Predictive theoretical	Enhances adsorption prediction on ionic	Shi *et al.,* 2024

	framework	and polar surfaces.	
	Quantum Monte Carlo benchmarking	Provides benchmark adsorption energies for model validation.	Ahn *et al.*, 2025

Conclusion

Theoretical modeling has become an indispensable component in understanding and predicting adsorption phenomena in nanostructured adsorbents. This review demonstrates that quantum mechanical methods, particularly Density Functional Theory, provide detailed insight into adsorption energetics, electronic interactions, and binding mechanisms, while molecular simulation techniques such as Molecular Dynamics and Monte Carlo methods effectively capture dynamic behavior and thermodynamic equilibrium. The interplay between surface chemistry, morphology, and nanoscale structure is shown to strongly influence adsorption capacity and selectivity across diverse material classes. Although significant progress has been made, challenges remain in bridging length and time scales, improving computational efficiency, and integrating theoretical predictions with experimental observations. Future advancements are expected through the coupling of multiscale modeling frameworks and machine learning approaches, which will enhance predictive accuracy and accelerate material discovery. Overall, theoretical evaluation of surface interactions offers a powerful pathway toward the rational design and optimization of next-generation nanostructured adsorbents for environmental and industrial applications.

Conflict of Interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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