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Historical Perspective

Molecular simulation-based insights into dye pollutant adsorption: A perspective review

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ABSTRACT

Growing concerns about environmental pollution have highlighted the need for efficient and sustainable methods to remove dye contamination from various ecosystems. In this context, computational methods such as molecular dynamics (MD), Monte Carlo (MC) simulations, quantum mechanics (QM) calculations, and machine learning (ML) methods are powerful tools used to study and predict the adsorption processes of dyes on various adsorbents. These methods provide detailed insights into the molecular interactions and mechanisms involved, which can be crucial for designing efficient adsorption systems. MD simulations, detailing molecular arrangements, predict dyes' adsorption behaviour and interaction energies with adsorbents. They simulate the entire adsorption process, including surface diffusion, solvent layer penetration, and physisorption. QM calculations, especially density functional theory (DFT), determine molecular structures and reactivity descriptors, aiding in understanding adsorption mechanisms. They identify stable adsorption configurations and interactions like hydrogen bonding and electrostatic forces. MC simulations predict equilibrium properties and adsorption energies by sampling molecular configurations. ML methods have proven highly effective in predicting and optimizing dye adsorption processes. These models offer significant advantages over traditional methods, including higher accuracy and the ability to handle complex datasets. These methods optimize adsorption conditions, clarify adsorbent functionalization roles, and predict dye removal efficiency under various conditions. This research explores MD, MC, QM, and ML approaches to connect molecular interactions with macroscopic adsorption phenomena. Probing these techniques provides insights into the dynamics and energetics of dye pollutants on adsorption surfaces. The findings will aid in developing and optimizing new materials for dye removal. This review has significant implications for environmental remediation, offering a comprehensive understanding of adsorption at various scales. Merging microscopic data with macroscopic observations enhances knowledge of dye pollutant adsorption, laying the groundwork for efficient, sustainable removal technologies. Addressing the growing challenges of ecosystem protection, this study contributes to a cleaner, more sustainable future.

1. Introduction

A significant source of water contamination is dye pollution, which originates from various industries like textiles, leather, food, and cosmetics [1,2]. Environmental and health hazards associated with dye pollutants include reduced light penetration, photosynthesis disruption, oxygen transfer inhibition, carcinogenicity, and mutagenesis [3]. Additionally, they contain toxic compounds, including carcinogens and mutagens, endangering organisms and causing genetic damage [4]. Dye pollutants must be appropriately treated before being disposed of in

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Table 1
The advantages and challenges of a suitable adsorbent to achieve the best performance in the adsorption of dye pollutants.

Aspect	Description
Attributes for Efficacy	• **High Adsorption Capacity:** • An adsorbent effectiveness lies in its capacity to efficiently remove significant dye amounts from wastewater, with its efficiency directly linked to adsorption capacity. • **Appropriate Functional Groups and Surface Charge:** • Matching surface groups and charges governing dye binding is essential in adsorbent-dye interaction. Success depends on precise chemical alignment, which is crucial when dyes carry charges. Thus, the adsorbent requires proper attributes for compelling dye attraction and interaction. • **Accessibility and Cost-Effectiveness:** • An adsorbent's usefulness hinges on accessibility and affordability. It must be readily available and cost-effective for integration into wastewater treatment, as high cost or scarcity may hinder broad adoption and impact. • **Environmental Compatibility:** • Crucial in adsorbent selection is environmental harmony. It must follow sustainability principles, avoiding harm to nature or health. This means no toxicity, corrosion, or flammability. Plus, it should be biodegradable or recyclable to reduce waste and pollution.
Challenges and Limitations	• **Diversity of Dyes**: • Diverse dyes vary in structure, colour, solubility, and stability. Some are tough to remove due to strong interactions or resistance to degradation. Thus, one adsorbent may not effectively handle the wide range of dye types. • **Competition and Interference**: • Complex wastewater contains dyes, salts, metals, organics, and chemicals. These can compete or interfere with adsorption, altering pH, temperature, or strength. This dynamic affects dye removal efficiency, requiring a selective adsorbent to prioritize dye removal within this intricate mix. • **Regeneration and Reuse**: • As adsorption continues, the adsorbent saturates with dye, prompting capacity restoration. Regeneration recovers dye and functionality, while reusing the adsorbent cuts costs and waste. Feasibility depends on stability and performance across cycles; some adsorbents may degrade after regeneration, necessitating strict measures for capacity recovery.

water bodies to minimize serious health and environmental risks. Consequently, wastewater dye pollution must be removed resourcefully and efficiently [5].

Adsorption stands as one of the extensively employed strategies for removing contaminants, whereby dye molecules are affixed onto the exteriors of solid substances recognized as adsorbents. This process is acknowledged for its economical nature, straightforward operability, and remarkable efficacy in dye removal [6]. However, the choice of adsorbents is crucial for the performance and sustainability of this method [7]. Various adsorbents have been studied for dye removal, such as commercial polymer-based adsorbents [8,9], metal-organic framework [10–12], carbon-based [13,14], metal oxide-based [15], and activated carbon [16]. These adsorbents can remove dye pollutants from wastewater through various mechanisms, such as π–π interactions, surface complexation, ion exchange and electrostatic attraction [17].

Experimental adsorption studies are pivotal for grasping adsorbent-adsorbate interactions, yielding insights into water purification and pollutant removal, but they face significant challenges and limitations. These include high costs, time-consuming procedures, and a lack of detailed mechanistic insights. This limitation restricts the comprehensive understanding needed to optimize adsorption processes or design more efficient adsorbents. As a result, researchers often need to supplement experimental findings with theoretical models and computational simulations to achieve a more holistic comprehension of adsorption mechanisms [18,19].

The role of computational methods in comprehending and enhancing adsorption is paramount. These methods employ advanced computer simulations and theoretical models to delve into the intricate interactions between adsorbents and adsorbates, offering valuable insights and optimization avenues [20,21]. Computational approaches enable the exploration of adsorption mechanisms at a molecular level, providing a profound insight into the fundamental processes involved [22,23]. By simulating the adsorption behaviour of various molecules on different adsorbent surfaces, these methods elucidate the binding energies, adsorption kinetics, and thermodynamic properties governing the system [24]. This information aids in identifying optimal conditions for efficient adsorption, leading to the design of high-performance adsorbents tailored for specific applications [25]. Furthermore, computational methods facilitate predicting adsorption behaviour under diverse conditions, including temperature, pressure, and solution composition variations. This predictive capability expedites the screening of potential adsorbent materials and operational parameters, saving time and resources in experimental trials [26]. The synergy between computational and experimental studies is pivotal. Computational insights guide experimental efforts, leading to more informed design choices and focused investigations. Conversely, experimental data validate and refine computational models, ensuring their accuracy and applicability.

This comprehensive review article explores adsorption processes for dye pollutants removal, focusing on adsorbent materials and computational methodologies. It systematically evaluates key adsorbent types used in wastewater treatment, including activated carbon, zeolites, clays, metal-organic frameworks, and biomass-derived materials. Simultaneously, the review delves into computational methods like molecular dynamics (MD), Monte Carlo (MC) simulations, quantum mechanics (QM), and machine learning (ML) methods, elucidating their role in enhancing dye pollutants adsorption understanding. Comparative assessments of method strengths and limitations regarding accuracy, efficiency, scalability, and practicality are provided, with illustrative examples of their contributions. A meticulous analysis of outcomes from diverse computational approaches, encompassing metrics like adsorption energies, capacities, mechanisms, and selectivities, is undertaken. Furthermore, the article identifies current gaps, challenges, and future directions in computational studies on dye pollutant adsorption, envisioning innovative adsorbent design, hybrid computational frameworks, machine learning, and collaborative endeavours. Culminating in a concise summary, the review underscores the transformative potential of computational methods, offering practical recommendations for researchers, practitioners, policymakers, and stakeholders engaged in the field.

2. Adsorbents for dye pollutants removal

Adsorbents are materials with suitable surface characteristics that facilitate the removal of dye pollutants from wastewater through adsorption. They provide active sites for dye molecules to adhere to, effectively reducing the concentration of dyes in the water and helping mitigate environmental pollution [27]. Table 1 summarizes the advantages and challenges of a suitable adsorbent to achieve the best performance in the adsorption of dye pollutants. Adsorbents can be classified into different types based on their origin, composition, structure, and properties. An extensive array of adsorbents finds application in adsorption processes, depending on the type and properties of the molecules to be adsorbed. Consequently, the ongoing challenge has revolved around identifying novel adsorbents and adapting current adsorbents to attain heightened adsorption capacities and establish more advantageous adsorption conditions. Table 2 displays frequently utilized adsorbents and their strengths and weaknesses in dye adsorption. Some common types of adsorbents used for dye removal are

Table 2
Recent scholarly inquiries into the application of distinct absorbent categories in the context of dye adsorption processes have yielded significant findings of relevance.

Adsorbent	Dye	Aims	Outcome results	Ref.
Carbon-based	Eosin yellow (EY) and methylene blue (MB)	The removal of EY and MB dyes consuming an innovative adsorptive based on activated carbon derived from eucalyptus-derived nanotubes	EY and MB removal were 49.1 5 mg/g and 49.61 mg/g using adsorbent. Pseudo-second-order model explained kinetics. CNT-based carbon adsorbent is extremely capable of water treatment.	[75]
	Methylene Blue	Methylene blue removal from aqueous solutions using sulfonated magnetic graphene-based cation exchangers	MGO effectively removed cationic pollutants and sustained >80% performance over seven cycles for wastewater treatment.	[76]
	Congo red (CR)	CR dye and antibiotic removal using various carbon-based adsorbents	Optimal conditions determined (mCarbon: mMAO = 2.5–10%). Effective adsorption via multiple interactions, pH 7.8 yielded 89.7% CR removal. BP neural network predicted adsorption well.	[77]
Commercial activated carbon (CAC)	Methylene blue (MB)	Date seed physicochemical evaluation	Results varied in moisture content, ash, and seed-to-fruit weight percentage among seed classes. Khalas seeds showed the highest MB adsorption (16 5 mg/g ADS), 71% of CAC.	[78]
		MB adsorptive removal in batch reactors	The utmost MB adsorption capability onto commercial activated carbon (CAC) was recorded at 224 mg/g.	[79]
	Congo red, Methyl orange, Rhodamine B and Methylene blue	anionic and cationic dye adsorption performance using CAC	Enhanced comprehension of dye adsorption onto CAC is facilitated by the utilization of pseudo-second-order kinetic models and Langmuir isotherms. Methylene blue exhibits exceptionally high adsorption capacities on CAC.	[80]
	Reactive Black 5	Wastewater treatment for the removal of azo dyes	This exhibits remarkable adsorption capabilities toward RB5 by utilizing the hierarchically porous carbons derived from lotus pollen.	[81]
	Rhodamine B (RhB)	Dyes wastewater treatment with highly efficient activated carbon derived from algal blooms with wide pH/temperature range adaptability	The adsorbent exhibited superior RhB adsorption compared to other adsorbents; linked to this occurrence is its generous interfacial region and presence of mesopores.	[82]
Metal oxide-based	Congo Red and Titan Yellow	Evaluation of an iron-oxide-based and zinc-doped nanoparticle system for the Titan Yellow and Congo Red adsorption	Magnetic nanoparticles with zinc dopant effectively removed Titan yellow from water through physical adsorption. Redlich-Peterson and Langmuir's models matched adsorption isotherms. These nanoparticles provide rapid, low-cost water purification and easy magnetic separation.	[83]
	Methyl green (MG)	Study of the thermodynamics and kinetics of methyl green adsorption on titanium dioxide (TiO_2)	Four kinetic models discussed MG adsorption. Pseudo-second-order equation ($R^2 = 0.999$) describes MG well. Langmuir and Temkin's models fit isotherm. Batch experiments optimize parameters, removing 384.61 5 mg/g at 2 5 °C.	[84]
	Malachite green	Application of mesoporous chitosan-zinc oxide composite materials for malachite green adsorption	Elemental analysis showed high Zn in comparison to P and Fe. Batch adsorption on chitosan–ZnO composite achieved 98.5% removal with pH 8, dye strength 2.3 mg/L, 0.6 g dosage in 180 min. Langmuir model fit well ($R^2 = 0.998$, capacity 11 mg/g). Favourable MG dye removal (RL = 0.49) followed pseudo-second-order kinetics, making it a rapid, promising wastewater treatment option.	[85]
Metal-organic frameworks (MOFs)	Basic Red 46 (BR46), Basic Blue 41 (BB41), Methylene Blue (MB)	An ultrasound-based dye adsorption experiment using MIL-Ti MOF	Pseudo-second order kinetics drove dye removal (0.000 51, 0.00481, and 0.20833 mg/g min for MB, BB41, and BR46). Langmuir isotherm fit (862, 12 57, 1296 mg/g for MB, BB41, BR46). MIL showed reusability/stability over three cycles. Dye removal was spontaneous, endothermic (308 K) with Gibbs energy −19.424, −1 5.721, −17.413 kJ/mol for BR46, BB41, and MB.	[86]
	Malachite green (MG), methyl red (MR)	A practical method to remove dye pollutants with poly-L-dopa-loaded MIL-101(Fe) MOF particles	High adsorption capacities (12 50 mg/g for MR, 833.33 mg/g for MG) were accomplished. Pseudo-second-order kinetics and Langmuir isotherm applied. Successful removal of textile dyes in real wastewater. Recyclable MIL-101(Fe) @PDopa@Fe_3O_4 for MR, MG removal.	[87]
Polymer-based	Methyl orange (MO), methylene blue (MB)	Improved wastewater treatment via polypyrrole-sodium alginate	Under optimal conditions (pH 6.1, 50 mL volume, 80 mg mass, room temp.), (Ppy-SA) showed high dye adsorption (MB: 196.08 mg/g, MO: 222.22 mg/g), surpassing other polymers. Promising for heavy metals and dye removal from wastewater.	[88]
	Methylene blue	Methylene blue removal using a polymer-magnetic-algae	PPy-Fe_3O_4-SW nano-composite sorbs up to 666.66 mg/g. Negative standard free energy affirms thermodynamic feasibility.	[89]
Biomass-derived materials	Acid Blue 93 (AB), Congo Red (CR), Crystal Violet (CV), Malachite green (MG)	Simultaneous removal of anionic and cationic dyes and Utilizing a hybrid composite derived from *Saccharum munja* biomass	Langmuir isotherm: AB (23 5.29 mg/g), CR (193.42 mg/g), CV (180.51 mg/g), MG (177.62 mg/g), adsorption. Pseudo-second-order kinetics, spontaneous adsorption. Synergistic hybrid biosorbent increased multi-component dye removal—efficient treatment of dye-contaminated effluents.	[90]
	Aniline green (AG)	Aniline Green Adsorption Using Algal Waste Biochar	Optimal conditions for aniline green (AG) adsorption: pH 7.0, 1 g L − 1 adsorbent, 40 min equilibrium, 50 mg L − 1 concentration. AG removal: 99.9%. Pseudo-second-order kinetics and Freundlich isotherm fit. BCH's AG uptake reusability: 88.3% (50 mg/L), 71.6% (100 mg/L) after three cycles. Economically viable for large-scale use.	[91]

Table 3
The predominant functional groups found on the surfaces of adsorbents and dyes and their roles in the dye adsorption process.

Functional Group	Impact on Dye Adsorption
Hydroxyl (-OH) Groups	• Common on adsorbents and dye molecules. • Participate in hydrogen bonding with polar groups in dye molecules. • Enhance adsorption by forming strong and reversible bonds.
Amine (−NH_2) Groups	• Form hydrogen bonds and attractive interactions with various dye groups. • Contribute to effective dye adsorption. • Interact with carbonyl (-C=O) and sulfonyl (-SO_3H) groups.
Carboxyl (-COOH) Groups	• Facilitate electrostatic interactions with cationic dye molecules. • Involve ion exchange or dipole-dipole interactions. • Particularly effective for dye removal from aqueous solutions.
Sulfonic Acid (-SO_3H) Groups	• Negatively charged, interact strongly with cationic dyes. • Electrostatic forces drive adsorption. • Common in adsorbents for cationic dye removal.
Aromatic Rings (π-π Stacking)	• Present in adsorbents and dye molecules. • Undergo π-π stacking interactions. • Electron-rich π-clouds overlap, aiding aromatic dye adsorption.
Thiol (-SH) Groups	• Form covalent bonds with specific dye molecules. • Provide stable and irreversible adsorption. • Valuable for heavy metal ion removal.
Ester (-COO-) Groups	• Participate in hydrogen bonding and other interactions with polar groups in dye molecules. • Contribute to adsorption capacity and selectivity.
Quaternary Ammonium (-N+ $(CH_3)_3$) Groups	• Positively charged, adsorb anionic dyes. • Effective through electrostatic attractions. • Common in cationic surfactants and polymer adsorbents
Phosphonate| (-PO_3H_2) Groups	• Interact with metal ions in dye molecules. • Form chelation complexes. • Contribute to heavy metal ion dye removal.

Table 4
Describing the significance of computational methods in dye adsorption studies.

Role	Description
Molecular Interaction Analysis [118,119]	• Computational methods investigate binding mechanisms and interactions between dyes and adsorbents. Simulations reveal van der Waals forces, electrostatic interactions, hydrogen bonding, and other forces influencing adsorption.
Adsorption Isotherms and Kinetics [120]	• Predict adsorption isotherms (adsorbate concentration vs. adsorbent uptake) and kinetics (adsorption rate). This helps understand factors like concentration and temperature affecting adsorption behaviour.
Surface Characterization [22]	• Computational techniques characterize adsorbent surfaces by calculating surface area, porosity, and structural properties. This information is crucial for understanding the accessibility and availability of adsorption sites for dye molecules.
Adsorption Site Identification [121]	• Computational methods identify favourable adsorption sites on adsorbent surfaces. This knowledge is essential for designing adsorbents with enhanced dye adsorption selectivity and function.
Predicting Adsorption Capacity[122]	• Computational approaches estimate specific dyes' adsorption capacities on adsorbents, aiding in screening and selecting optimal materials for experimental studies.
Comparative Studies Compare	• various adsorbents and their potential for dye removal using computational methods. Identify trends and patterns contributing to effective adsorption by modelling different adsorbents and dyes.
Tailoring Adsorbents	• Design and modify adsorbent materials using computational tools to enhance adsorption capacity and selectivity for specific dye molecules. Contribute to developing efficient and eco-friendly adsorption processes.
Understanding Competitive Adsorption [123]	• Explore scenarios of competitive adsorption where multiple species vie for adsorption sites. This is particularly relevant in real-world contexts with dye mixtures present in wastewater.

Carbon-based: Carbon-based materials are promising adsorbents for removing various dyes from wastewater [28]. Some advantages of carbon-based adsorbents are their well-flourished mesopores, cylindrical hollow structure, large surface area, and possible modification to enhance their adsorption capacity [13]. Some common carbon-based adsorbents are biochar [29,30], carbon nanotubes [31,32], graphene [33], activated carbon [34] etc. In these materials, dye adsorption mechanisms include electrostatic interactions, hydrogen bonding, hydrophobic interactions, π–π stacking, and van der Waals forces [35]. However, carbon-based adsorbents may also have high production costs and environmental impacts [36]. **Commercial activated carbon (CAC):** A high adsorption capacity, large surface area, and higher porosity make CAC an ideal dye removal adsorbent [37]. CAC can be produced from various sources, such as coal, wood, coconut shells, and peat [38]. CAC efficiently removes wastewater's acid, primary, and reactive dyes under different conditions [39]. Numerous studies have investigated the use of activated carbon for dye adsorption. Khan et al. found that coconut coir activated carbon had a higher adsorption capacity for Acid Red 18 dye [40]. Parvin [41] and Chinniagounder et al. [42] both investigated the use of activated carbon derived from agricultural waste for dye adsorption, with Parvin focusing on date palm leaf waste and Chinniagounder on cocoa shell. Both studies found these materials to be effective and low-cost adsorbents for dyes. Djilani et al. compared the properties of activated carbon prepared from apricot stones to commercial activated carbon, finding that both were effective for dye adsorption, particularly under acidic conditions [43]. These studies collectively suggest that activated carbon, including CAC, can be a viable and cost-effective option for dye adsorption. However, CAC is also expensive and requires regeneration after saturation. **Metal oxide-based**: A category of metal oxide-based adsorbents has found extensive application in removing diverse dyes and metal ions from wastewater. This application is attributed to their characteristics, including substantial surface area, quantum size effect, porosity, stability, reusability, and a range of pore sizes [15]. Some examples of metal oxide-based adsorbents are manganese dioxide (MnO_2) [44], zinc oxide (ZnO) [45], iron oxide (Fe_3O_4) [46], and titanium dioxide (TiO_2) [47]. The adsorption mechanisms of metal oxide-based adsorbents involve π–π interactions, surface complexation, ion exchange, and electrostatic attraction between dye molecules-adsorbent surfaces. Metal oxide adsorbents and their adsorption performance depend on several factors: contact time, particle size, adsorbent dosage, initial concentration, solution pH, and temperature [48]. Many studies have examined the use of metal oxide-based materials for dye adsorption. Singh et al. synthesized a Fe-Mn-Zr metal oxide nanocomposite with high adsorption capacities for anionic dyes [49], while Li (201 5) demonstrated the super adsorption capability of amorphous transitional metal oxide nanoparticles, particularly NiO, for methyl blue [50]. Kumar (2013) focused on the low-cost synthesis of metal oxide nanoparticles, such as ZnO and SnO_2, and their application in the adsorption of commercial dyes and heavy metal ions, showing promising results [51]. These studies collectively underscore the potential of metal oxide-based materials for dye adsorption, with various approaches and materials showing high adsorption capacities and potential for further development. However, metal oxides may have low solubility and recyclability in aqueous media. **Metal-organic frameworks (MOFs):** Recently, there has been a

Table 5
Compared and contrasted the strengths and limitations of the MD simulations, MC simulations, QM, QM/MM, and ML methods in terms of accuracy, efficiency, scalability, and applicability.

Method	Accuracy	Efficiency	Scalability	Applicability
Molecular Dynamics (MD)	High for classical systems; limited for quantum effects	Moderate to high; depends on system size and time step	Scales linearly with the number of particles, but large systems can be computationally expensive	Studying the time evolution of large biomolecules, materials, and molecular systems
Monte Carlo (MC)	High for equilibrium properties; low for dynamics	Generally high; efficiency depends on sampling strategy	Scales well with system size; often better than MD for large systems	Calculating thermodynamic properties, phase transitions, and statistical mechanics problems
Quantum Mechanics (QM)	Very high; can capture electronic structure accurately	Low; computationally very expensive	Poor scalability; scales poorly with system size (typically polynomial or exponential)	Studying small molecules, reaction mechanisms, electronic properties, and spectroscopy
QM/MM	High for active site; moderate for environment	Moderate; more efficient than full QM for large systems	Better scalability than QM alone; scales well with hybrid systems	Investigating enzymatic reactions, large molecular systems with localized quantum effects
Machine Learning (ML)	Varies; depends on training data quality and model	Very high once trained; training can be expensive	Excellent scalability; can handle very large datasets and systems once trained.	Predicting molecular properties, materials design, wastewater treatments, and accelerating other simulations

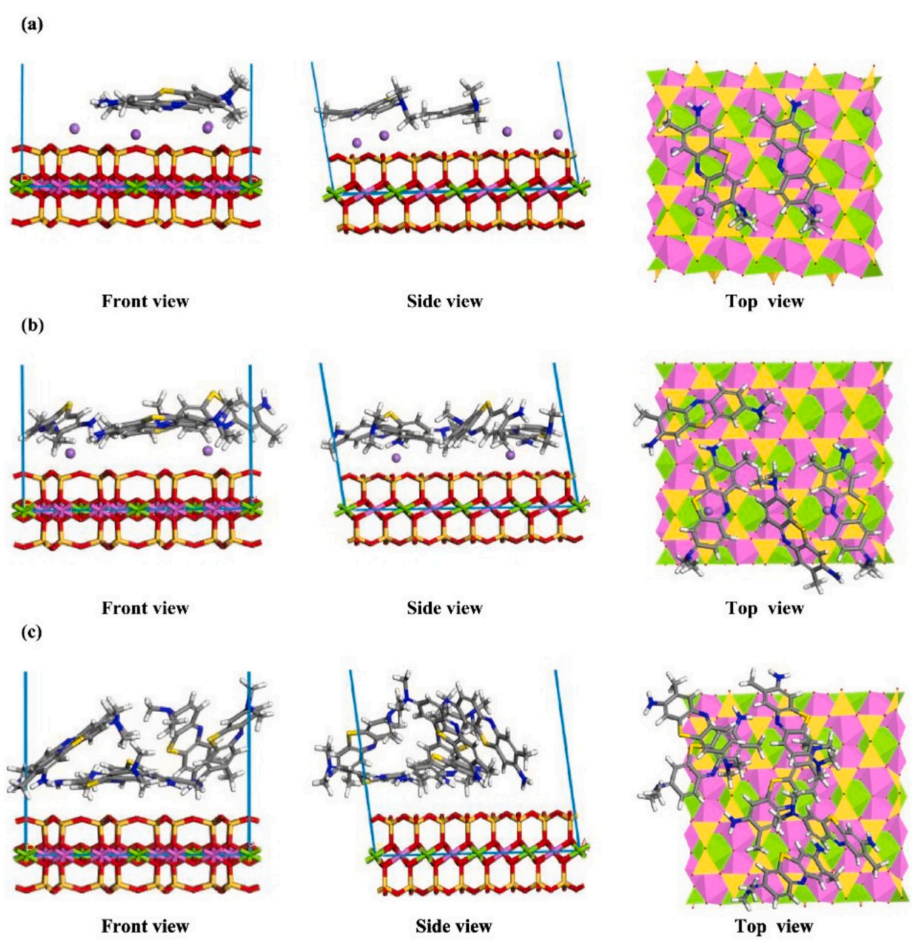

Fig. 1. Equilibrium adsorption configurations of TB in adsorbent were analyzed using NVT ensemble for different surface loading rates: (a) 33%, (b) 66%, and (c) 100% [193].

notable upswing in scientific interest focused on the advancement and application of MOFs within water treatment [52]. This is predominantly attributed to the captivating and distinctive attributes exhibited by MOFs, which encompass the capacity for facile adjustments of porosities, the accommodation of substantial pore volumes, the establishment of intricate hierarchical arrangements, and the manifestation of commendable adsorption and renewal proficiencies. Consequently, MOFs have emerged as a commendable and eco-conscious alternative to conventional adsorbents, mainly showcasing their prowess in effecting the adsorptive decontamination of organic wastes from aqueous solutions [53]. The augmentation of MOFs' functionalities and capabilities has been systematically achieved through strategic interventions incorporating functional groups, magnetic moieties, and selectively chosen extraneous materials into the foundational MOF framework [54]. Overall, MOFs have shown great potential in the adsorption of organic dyes due to their modifiable porous structures [55]. Different types of MOFs, including aluminum carboxylate-based MOFs, have been found to be effective in the removal of toxic dyes from wastewater

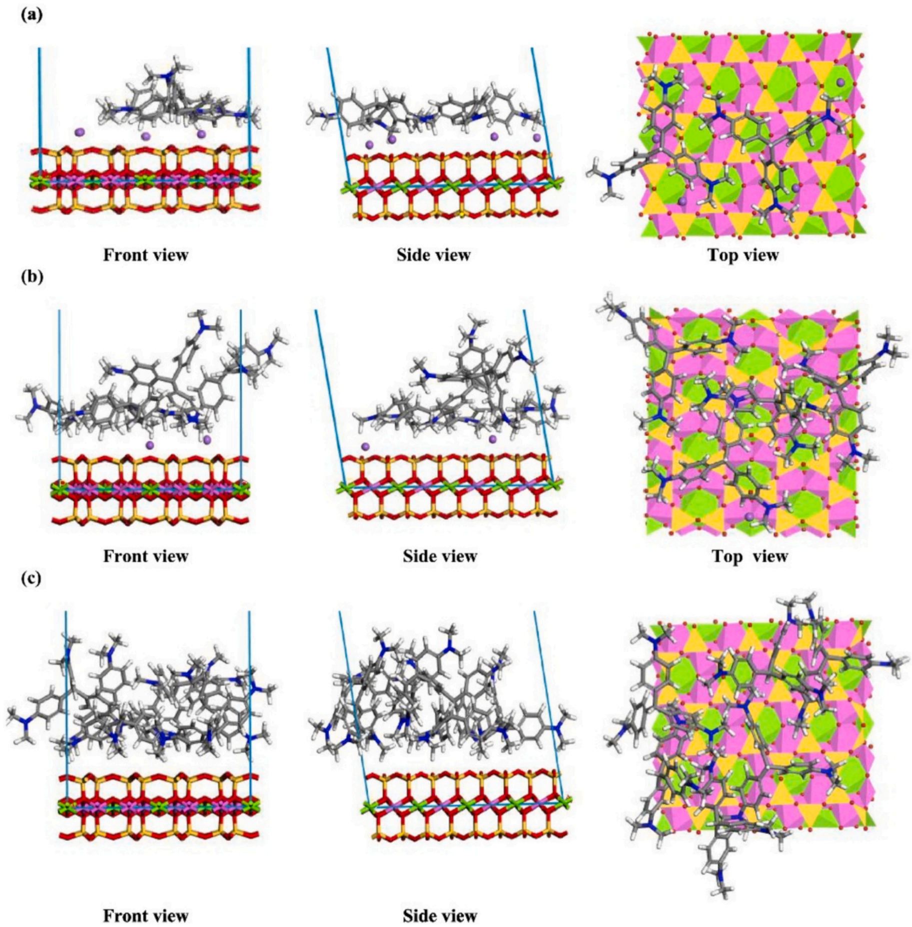

Fig. 2. Using the NVT ensemble, equilibrium adsorption configurations of CV onto MNC were studied for different surface loading rates: (a) 33%, (b) 66%, and (c) 100% [193].

[56,57]. The adsorption process is influenced by factors such as the type of MOF, presence of functional groups, ligands, and pH [58]. These studies collectively highlight the promising role of MOFs in the efficient removal of dyes from wastewater. While this has undeniably contributed to the realization of heightened performance benchmarks for MOFs, it is noteworthy to acknowledge that this deliberate augmentation inevitably accompanies an escalation in the overall manufacturing outlays associated with MOFs. Consequently, this cost-intensive enhancement trajectory introduces a substantial impediment that necessitates meticulous consideration and resolution, especially when contemplating the viable deployment of MOFs within expansive and large-scale operational contexts. **Polymer-based:** Polymer-based adsorbents have advantages over other adsorbents, such as easy functionalization, recyclability, scale-up, easy preparation, simplicity, and a variety of monomers are available for their preparation, as well [59,60]. Different types of polymer-based adsorbents exist, such as natural polymers [61], synthetic polymers [62], and cross-linked polymers [59]. Polymer-based adsorbents have shown promising results for removing different kinds of dyes from wastewater, such as direct dyes [63], basic dyes [64], acid dyes [65], reactive dyes [66], etc. Polymer-based adsorbents, such as PVA and PVA-based composites, have shown promising results in the adsorption of dyes, with high removal efficiency and good agreement with kinetic and equilibrium models [62]. Similarly, a synthetic carboxymethyl cellulose-acrylic acid adsorbent has demonstrated high removal ratios for various dyes, suggesting its universal removal potential [67]. The use of polymeric adsorbents to remove azo dyes has been extensively reviewed, highlighting their potential as cost-effective and efficient alternatives to conventional adsorbents [68]. Furthermore, nanotechnology-based polymer adsorbents, such as nano composite α-Fe_2O_3/graphene oxide and PAN–polyamidoamine nanoparticles, have been identified as highly effective for dye removal from aqueous media [69]. Nonetheless, the employment of polymer-based adsorbents is accompanied by certain hurdles and constraints, such as mechanical stability, swelling tendency, regeneration capacity, and possible leaching of toxic substances. Therefore, further research and development are needed to improve the performance and efficiency of polymer-based adsorbents for dye removal. **Biomass-derived materials:** These adsorbents are natural or waste materials that could be applied as economical and environmentally sound adsorbents for dye adsorption. Biomass-derived materials include algae, yeast, bacteria, fungi, agricultural wastes, industrial wastes, and plant debris. Biomass-derived materials can remove various types of dyes from wastewater through biosorption, bioaccumulation, biodegradation, and biotransformation. However, biomass-derived materials may also have low purity, consistency, and reusability [70–72]. A range of studies have explored the potential of biomass-derived materials as adsorbents for dye removal from wastewater. Ali et al. [72] and Aragaw et al. [70] highlight these materials' cost-effectiveness and environmental benefits. Aragaw specifically discusses the influence of surface chemistry, pH, and other factors on adsorption. Hassan et al. provides a comprehensive review of the potential of biomass-derived porous carbonaceous materials for dye removal, emphasizing their high dye-binding capacity and the influence of preparation conditions on their effectiveness [73]. Bello et al. further underscores the importance of these materials in pollution control and environmental conservation [74]. These studies collectively suggest that biomass-derived materials hold significant promise as economical and

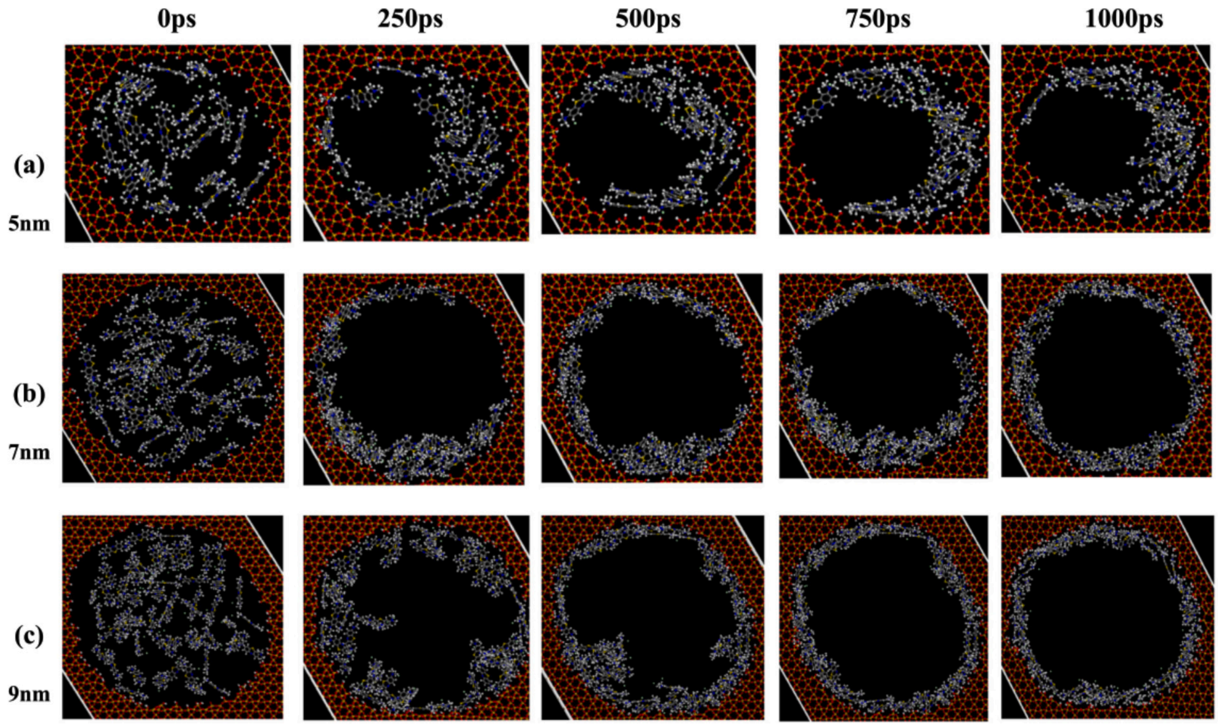

Fig. 3. Visual representations of MB molecule arrangements within mesoporous silica of SBA-1 5, characterized by diverse pore diameters, have been obtained through MD simulations. These snapshots correspond to pore sizes of (a) 5 nm, (b) 7 nm, and (c) 11 nm and have been taken at different instances during the simulation process [194].

environmentally sound adsorbents for dye adsorption. As represented in Table 2, the utilization of the aforementioned types of adsorbents is detailed with respect to their role in the intricate processes of adsorption and subsequent removal of a diverse array of dye pollutants from various aqueous environments.

Various parameters affect the adsorption efficiency of different adsorbents. These parameters include the surface area's size, the pores' dimensions, the surface's composition, functional components, and the presence of metal ions. **Surface area:** An adsorbent's capacity to effectively capture and retain dye molecules from a solution is significantly influenced by its surface area [92]. A larger surface area provides more active sites and interaction points for dye molecules to adhere to the material's surface. This larger interaction area improves the adsorbent's adsorption capability and effectiveness. A larger surface area means more binding sites are available, which results in more dye molecules being captured and retained on the material [93]. Materials with a higher surface area-to-volume ratio, such as porous materials like activated carbon, zeolites, and specific MOFs, exhibit excellent dye adsorption performance. The intricate network of pores and voids in these materials provides a high surface area, making them very effective at removing dyes and other contaminants from the solution. **Pore size:** An adsorbent's pore size is an important factor influencing the dye adsorption capacity. Different pore sizes can affect the accessibility, diffusion, and interaction of dye molecules with the adsorbent surface. The effect of pore size on dye adsorption performance is a complex interplay of factors, including surface area, diffusion kinetics, chemical interactions, and pore accessibility [94]. Anastopoulos et al. [95] and Jiang et al. [56] highlight nanoparticles and MOFs' potential as effective adsorbents for dye removal. These materials offer high porosity and tunable pore size, making them suitable for various dyes. Xin et al. [96] and Parker et al. [97] further explore the role of mesoporous materials in dye adsorption, with Xin demonstrating the efficient adsorption of bulky dye molecules by ordered mesoporous carbons and Parker emphasizing the importance of mesoporosity in polysaccharide-derived materials for enhanced adsorption capacity and speed. These studies underscore the significance of pore structure in dye adsorption, with mesoporous materials balancing adsorption sites and diffusion pathways for various types of dyes. The adsorbent's optimal pore size depends on the dye's characteristics to be removed, such as molecular size, shape, charge, polarity, and solubility.

Surface chemistry: An adsorbent's surface chemistry affects the nature and strength of the interactions in the adsorbent-dye interaction. The surface chemistry could be modified by adding functional groups, including carboxyl, hydroxyl, amino, sulfonic acid groups, etc., or metal ions, such as iron, copper, zinc, etc., to the surface of the adsorbent. These modifications can enhance the electrostatic attraction, hydrogen bonding, coordination bonding or complex formation between the adsorbent and the dye molecules [70,98,99]. Polymer-based adsorbents, for example, can be modified with various functional groups to increase their selectivity and affinity for different dyes [100]. **Functional groups:** The presence of specific functional groups in both the dye molecules and adsorbent significantly affects the dye adsorption performance. These functional groups contribute significantly to determining the adsorbent-dye interaction and affect the adsorption function, kinetics and overall efficiency. These functional groups' specific chemistry and compatibility with the targeted dye molecules are critical factors in developing effective dye removal and purification adsorbents [101]. The functional groups in the dye molecules also affect their adsorption behaviour on different adsorbents. The functional groups determine the dye molecules' charge, polarity, solubility and molecular structure [102]. These factors influence dye molecules' interaction with adsorbent surfaces. For example, acidic dyes with sulfone or carboxyl groups are more soluble and negatively charged in aqueous solutions. Therefore, positively charged or hydrophobic adsorbents tend to capture them more readily. Basic dyes with amino or imino groups tend to be less soluble and positively charged in aqueous solutions. Therefore, they are more likely to be adsorbed by negatively charged or hydrophilic adsorbents. Overall, the presence of specific functional groups significantly influences dye adsorption, as demonstrated by various studies. Jiang et al. highlight MOFs' roles in dye removal, emphasizing their diverse

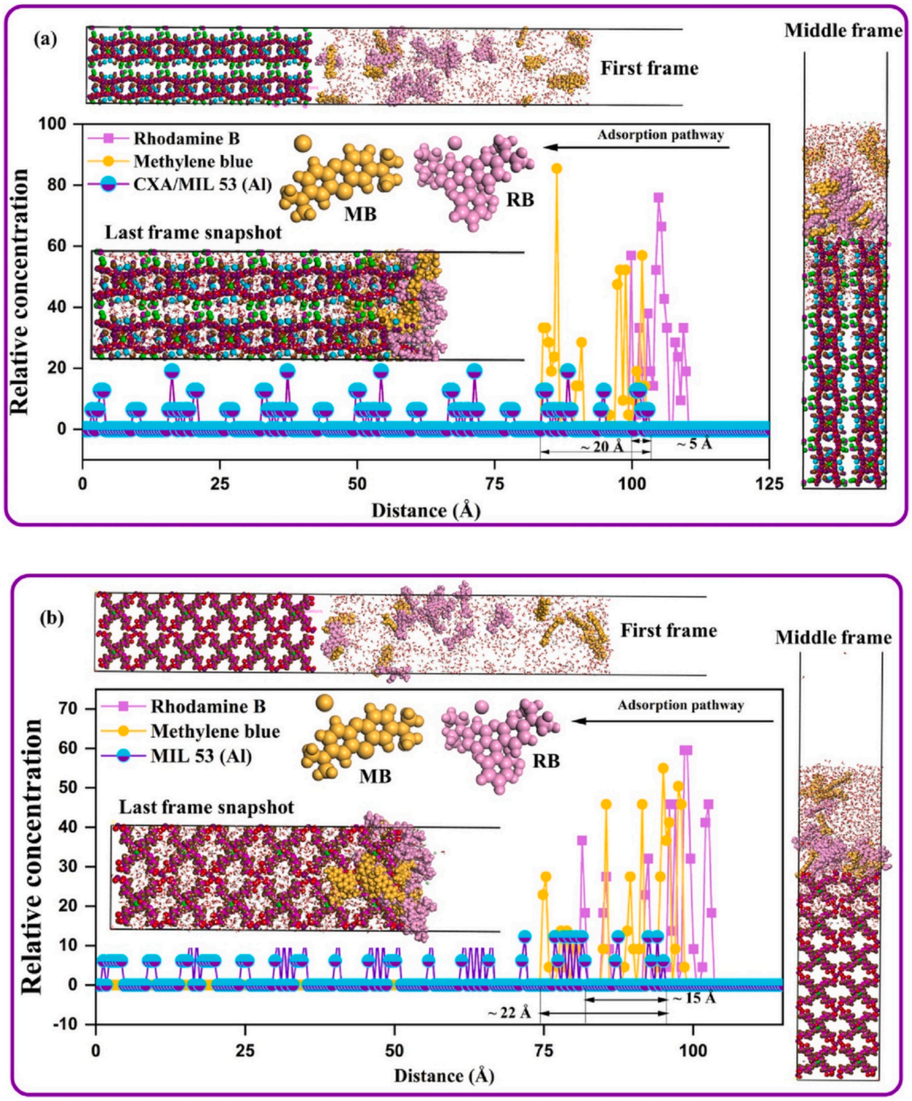

Fig. 4. Illustrations portraying the primary, transitional, and conclusive frames, complemented by the corresponding concentration patterns, are showcased for both a) the dyes-water-functionalized MIL and b) the dyes-water-neat MIL compositions [123].

structures and surface functionalities [56]. Rajabi et al. further explore this, noting the enhanced sorption capacity of functionalized carbon nanotubes (CNTs) compared to as-grown CNTs [31]. Razi et al. [103] underscore the importance of operational parameters in textile dye removal using activated carbon, while Liu et al. [104] review the adsorption properties of clays, including their modification for enhanced dye removal. These studies underscore the critical role of specific functional groups in dye molecules and adsorbents in determining dye adsorption performance. Table 3 presents the prevailing functional groups detected on both adsorbent and dye surfaces, along with their respective functions in the dye adsorption process. Moreover, several factors, including dye structure, solution pH, temperature, and pressure, influence a material's adsorption performance.

1. **Dye Structure:** The structure of the dye molecules significantly influences their adsorption behaviour. Factors such as the dye molecules' size, shape, and functional groups determine how effectively they can interact with the adsorbent material. Dyes with larger molecular sizes might have reduced access to adsorption sites on the material's surface. Dye molecules with functional groups that can form hydrogen bonds, electrostatic interactions, or other chemical interactions with the adsorbent tend to have higher adsorption capacities.
2. **Solution pH:** The pH of the solution impacts the adsorbent substance and dye particle surface charges. The pH influences the degree of ionization of the dye and adsorbent functional groups, affecting their electrostatic interactions. An optimal pH range exists for the adsorption of a specific dye onto a particular adsorbent. This is often related to the adsorbent's point of zero charges (pHpzc), where the surface charge is neutral. At pH values away from the pHpzc, electrostatic attractions or repulsions between the adsorbent and dye can significantly impact adsorption efficiency [105,106].
3. **Temperature:** Temperature affects the kinetic energy of the molecules in solution and the adsorbent's surface, influencing the rate and extent of adsorption. Generally, higher temperatures enhance the mobility of molecules in solution, which can promote diffusion and increase the rate of adsorption [99,107]. However, the impact of temperature can be complex and is also linked to adsorption thermodynamics. In some cases, higher temperatures might lead to decreased adsorption due to increased desorption rates or changes in surface chemistry.
4. **Pressure:** Studies have shown that high pressure can affect dyes' adsorption efficiency and characteristics on various surfaces

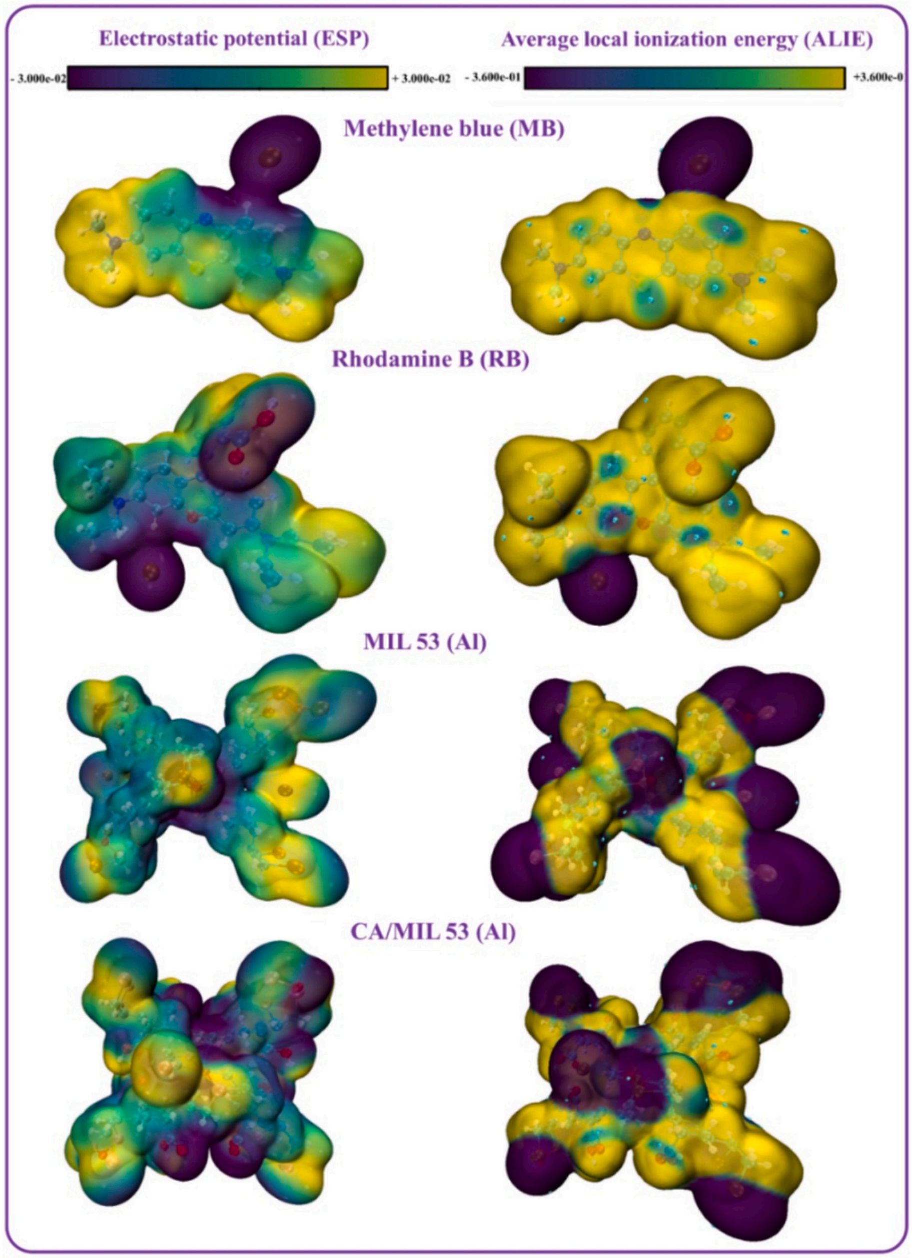

Fig. 5. Visual ESP and ALIE analysis representation for a single dye and adsorbent structure [123].

[108,109]. For instance, in the case of crystal violet dye, pressure up to 10 kbar led to redshifts in the peak locations of monomeric isomers and dimers, impacting their equilibrium characteristics [110]. Additionally, high hydrostatic pressures up to 600 MPa influenced the affinities of direct dyes for cellophane, with discussions revolving around the change in the substrate volume available for dye adsorption [111]. These findings highlight the intricate relationship between pressure and dye adsorption behaviour, showcasing the importance of pressure conditions in controlling and optimizing dye adsorption processes.

It is crucial to highlight that the interaction between these factors is often complex, and their effects on adsorption performance can be interrelated. The choice of adsorbent material, the type of dye, and the specific conditions of the adsorption process will determine how these factors collectively influence the overall performance. Experimental studies and modelling approaches are often employed to better understand and optimize adsorption processes for various applications, such as wastewater treatment, purification, and separation.

3. Computational methods for dye adsorption studies

The complexity of dye impurity adsorption onto adsorbents arises from the intricate dye molecules/adsorbent surface physicochemical interactions. The computational prediction of dye adsorption behaviour and its congruence to experimental findings hold noteworthy significance, mainly due to laboratory techniques' time and cost constraints [112,113]. Computational methods serve a vital role in unveiling fundamental adsorption mechanisms, encompassing aspects like binding sites and interaction types, including van der Waals forces and hydrogen bonding [114]. Furthermore, computational techniques enable the calculation of thermodynamic parameters like binding energies [115], enthalpies, and entropy changes, glimpses into the adsorption process' energy dynamics and can be subsequently validated

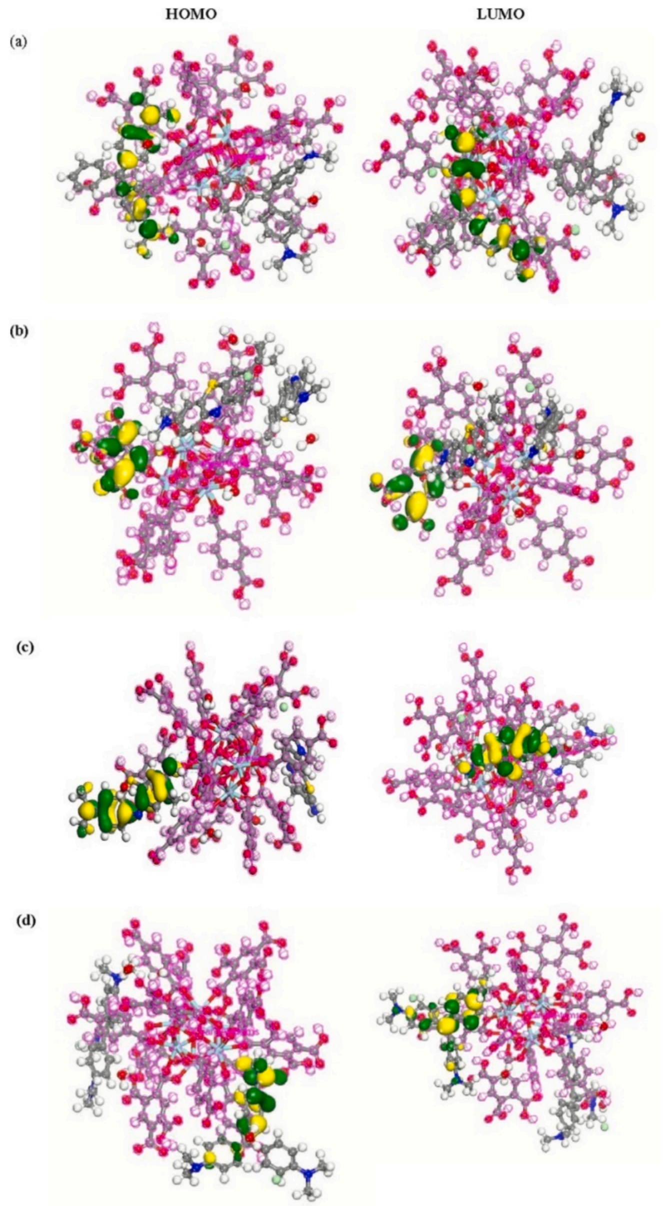

Fig. 6. The HOMO-LUMO patterns of (a) functionalized/MOF-MG-water, (b) functionalized/MOF-MB-water, (c) functionalized/MOF-TB-water, and (d) functionalized/MOF-CV-water structures [195].

against empirical data [116,117]. These methodologies extend to comparing simulated adsorption isotherms, kinetics, and thermodynamic parameters with experimental outcomes. Using computational approaches further encompasses investigating and predicting influential factors affecting dye adsorption, including initial dye concentration, temperature, pressure, pH, and contact time. Diverse computation methods, varying in precision and granularity, facilitate an in-depth analysis of the adsorption process. Fundamental techniques encompass MD, MC simulations, QM calculations, and ML. Table 4 interprets some key roles that computational methods play in dye adsorption studies.

3.1. Fundamental molecular modelling approaches for dye pollutant adsorption

3.1.1. Molecular dynamics (MD) simulations

In recent years, MD simulations have gained significant attention in pollution control and environmental monitoring. These simulations, known for their ability to simulate the complex behaviour of particles at the atomic level, have found a niche in contaminant adsorption [124,125]. They offer a comprehensive and detailed representation of interactions between adsorbents and various contaminants, including dyes, contaminants, and impurities. These simulations provide insights with high temporal precision, capturing particles' dynamic changes and intricate motions with exceptional accuracy. Recent advances in computational technology have made MD simulations more accessible and practical for researchers. The availability of experimental data on the structural properties of materials has complemented computational advances, enabling a synergistic approach that leverages both computational and experimental findings. These simulations are valuable tools for deciphering the functional intricacies of various adsorbents and contaminant molecules, contributing to the fundamental understanding of adsorption processes [126]. MD simulations also serve as a creative platform for discovering and designing efficient adsorbents and membranes. The knowledge gained from these simulations can guide the formulation of materials with optimized properties and improve their effectiveness in pollution control and environmental remediation strategies [127]. In summary, MD simulations represent a synergy between computational advances and experimental findings, providing the opportunity to explore the intricacies of adsorbent-pollutant interactions at the atomic level, decipher adsorption processes, and develop effective materials for pollutant control. A substantial body of investigation has been carried out by employing the MD simulation technique to explore the efficacy of different adsorbents in prognosticating their conduct during the adsorption of pollutants exhibiting assorted hues during the adsorption process [128–131].

3.1.2. Monte Carlo (MC) simulations

MC simulations are a valuable tool for estimating and studying the adsorption performance of dyes on surfaces. They provide detailed insights at the molecular level, help understand the underlying mechanisms, and allow exploring a wide range of conditions and scenarios to aid in experimental design and optimization. Employing stochastic sampling, this methodology traverses the configuration space of a given system, enabling the computation of its thermodynamic attributes [132]. MC simulations allow us to model the dye-adsorbent interactions at the molecular level. By incorporating information about the molecular structure of both the dye and the surface, we can simulate how these molecules interact and arrange on the surface. Dye adsorption is often an energy-driven process. MC simulations can be used to calculate the energy changes associated with different dye-surface configurations. This analysis helps to understand the preferred orientation, binding sites, and stability of adsorbed dye molecules [133]. MC simulations can help predict the most favourable binding sites for dye molecules on the surface. This information is critical for understanding the adsorption mechanism and developing materials with improved adsorption capacity for dyes.

3.1.3. Quantum mechanics (QM)

QM calculation plays a significant role in understanding and describing dye adsorption behaviour, particularly at the atomic and molecular levels [134,135]. This method uses various approximations and techniques to solve the Schrödinger equation for the electrons and nuclei in a system [136,137]. QM can provide detailed information about the electronic structure, bonding, charge distribution, and reactivity of the dye and adsorbent molecules [138,139]. QM can also predict different dye-adsorbent systems' adsorption energies, geometries, and mechanisms. However, QM is computationally demanding and can only handle small systems with a few hundred atoms. Here is how QM is relevant to dye adsorption behaviour:

1. **Electronic Structure and Binding Energies:** QM is essential for understanding the electronic structure of the substrate surface and dye structure to which they are adsorbed. It provides insights into the

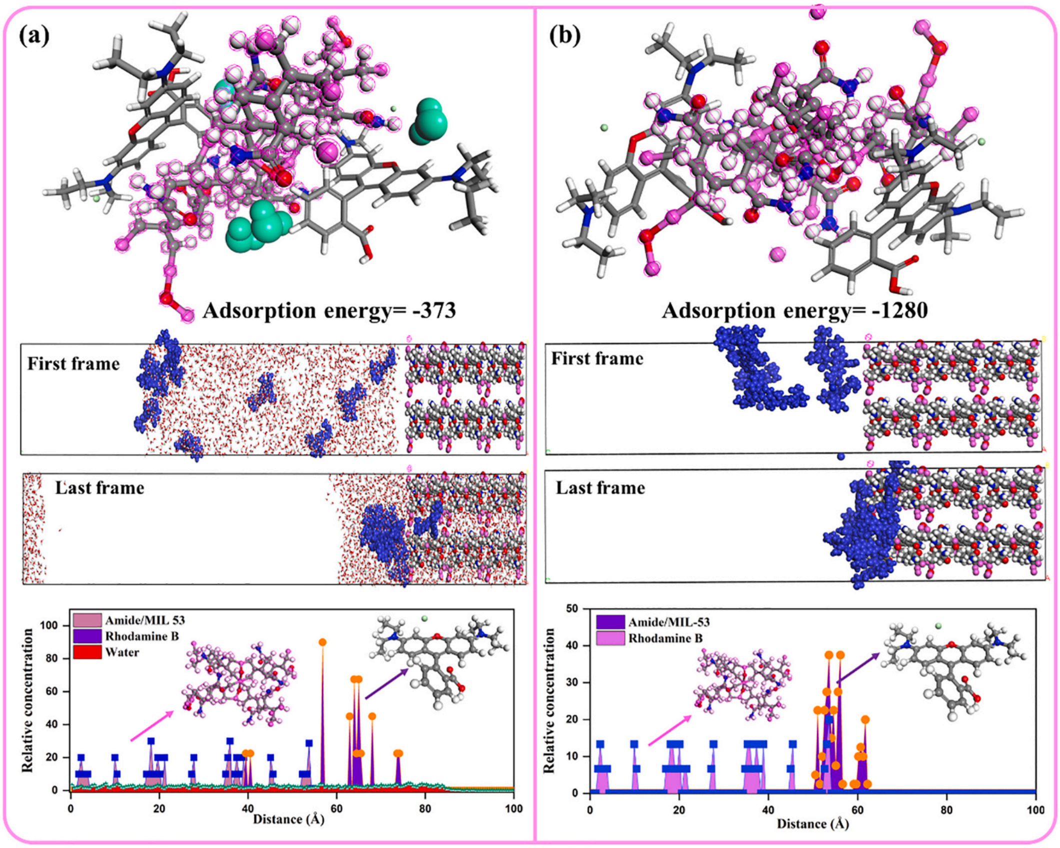

Fig. 7. Snapshot assessment contrasts RHB adsorption conduct on functionalized MOF adsorbent via paired MD and MC simulations, elucidating non-aqueous and aqueous scenarios [147].

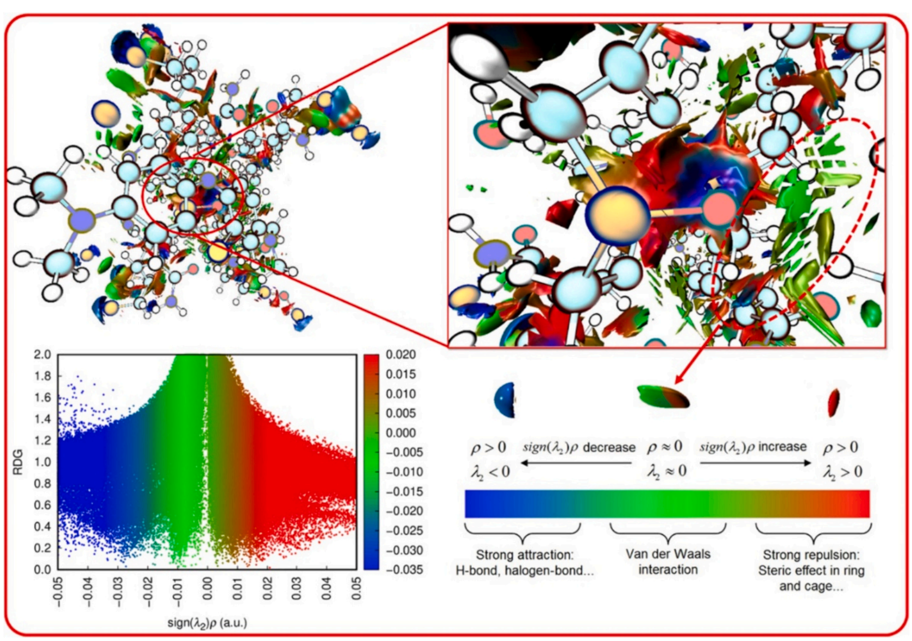

Fig. 8. Comprehensive insights into the blending of RHB, water, and functionalized-MIL-53 are garnered through an analytical exploration encompassing scatter graphs RDG and isosurfaces graphs [147].

interacting molecules' energy levels and electronic configurations. The adsorption process involves interactions and chemical bond formation in the dye-substrate surface. QM calculations can help determine the binding energies, which reflect the strength of these interactions [140–143].

2. **Molecular Orbitals and Charge Transfer:** QM allows us to inspect the substrate and dye structure's molecular orbitals. Charge transfer

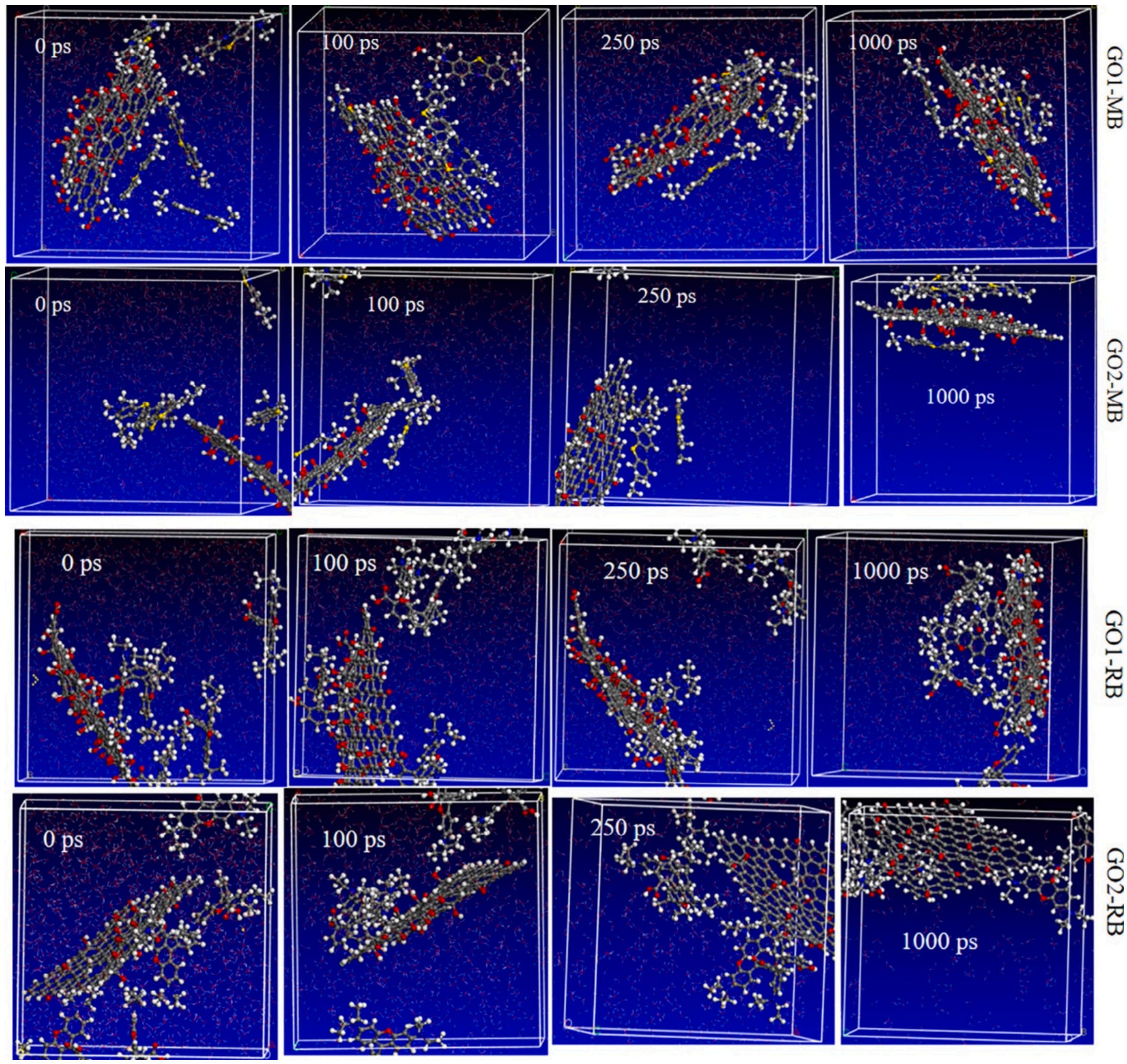

Fig. 9. Instances captured from MD simulations portraying the MB/GO1, MB/GO2, RB/GO1, and RB/GO2 systems [197].

between the dye and the substrate is often a key aspect of adsorption behaviour. QM calculations can provide information about the extent of charge transfer, which can influence the colour and stability of the dye [123,144–146].

3. **Geometric Structure and Adsorption Sites:** The geometric structure of the pollutant fragments and the adsorbent surface influence adsorption behaviour. QM can predict the optimal adsorption sites and configurations for these molecules on the substrate. Accurate modelling of these geometries is crucial for understanding how the adsorption process occurs and how it affects the properties of the adsorbed system. In the context of this specific goal, a range of techniques have demonstrated significant practicality and gained widespread adoption. Notably, Average Local Ionization Energy (ALIE), Mulliken Population, The Reduced Density Gradient (RDG), Hirshfeld Surfaces (HS), and Electrostatic Potential (ESP) collectively serve as valuable tools in this pursuit. Their broad utilization underscores their importance in achieving the intended outcome [18,114,147–149].
4. **Vibrational Modes and Spectroscopy:** QM also plays a role in understanding the vibrational modes of the adsorbed system. These vibrational modes can be probed through various spectroscopic techniques, such as infrared spectroscopy [150,151]. The vibrational modes provide information about the interactions between the dye and the substrate and the adsorbed complex's overall stability.
5. **Quantum Confinement Effects:** In some cases, dye molecules adsorbed onto nanoscale substrates exhibit quantum confinement effects. These effects arise due to the spatial confinement of electrons within the nanoscale dimensions. QM helps to explain how these effects influence the electronic and optical properties of the adsorbed dye molecules [152,153].
6. **Density Functional Theory (DFT) Calculations:** DFT is a widely used QM method for calculating the electronic structure and properties of molecules and materials. DFT can be employed to predict adsorption energies, electronic structures, and vibrational frequencies, providing valuable information about the adsorption behaviour of dye molecules [154–180].

3.1.4. Quantum mechanics/molecular mechanics (QM/MM)

QM/MM is a hybrid computational method that combines the accuracy of quantum mechanics (QM) with the efficiency of molecular mechanics (MM) [181]. This approach is advantageous in studying complex systems like dye adsorption, where both electronic interactions and large-scale molecular behaviour play significant roles [182]. This hybrid approach ensures accurate and consistent results by carefully

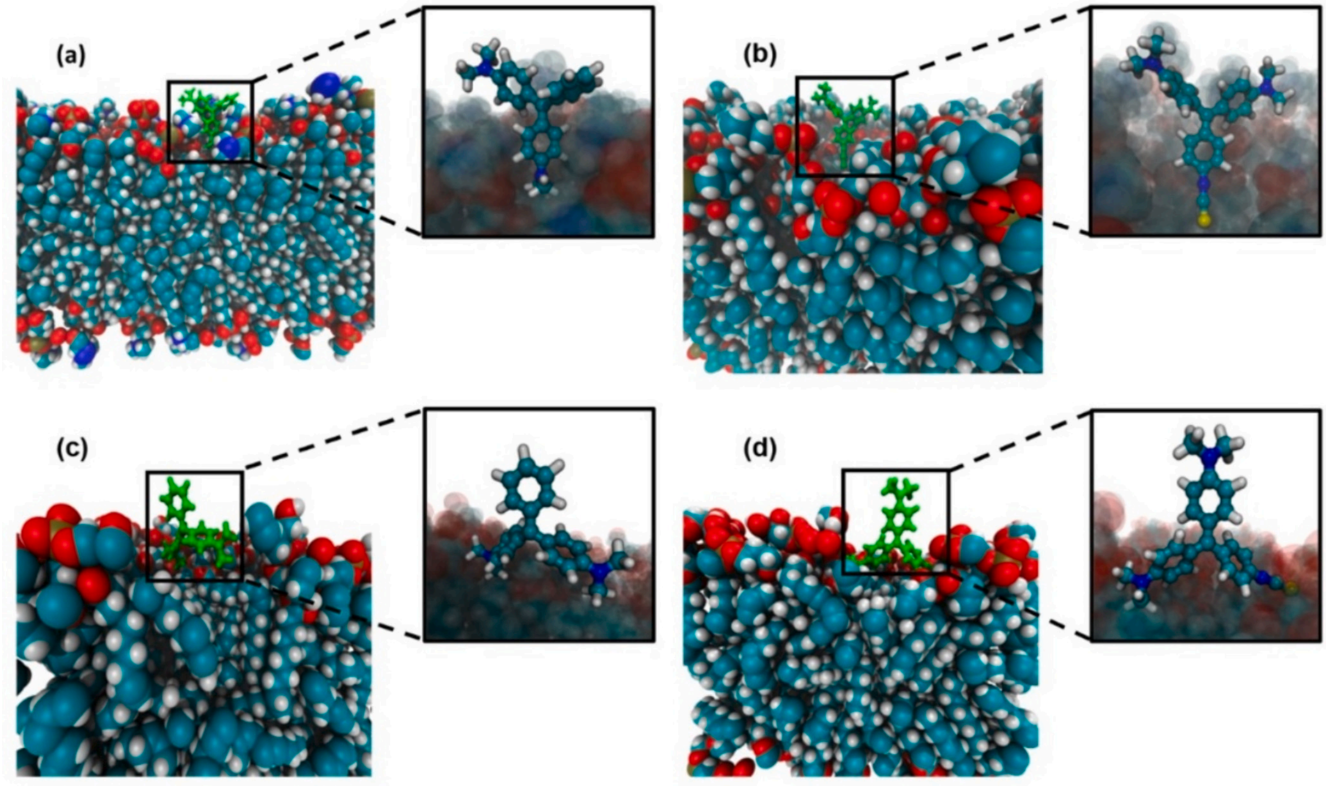

Fig. 10. Illustrative images portraying the alignment of the dye molecules at the lipid bilayer's interface, accompanied by magnified close-ups for (a) MG within DOPC, (b) MGITC within DOPC, (c) MG within DOPG, and (d) MGITC within DOPG, are showcased. The visualization employs distinct colour schemes, wherein carbon atoms are rendered in cyan, oxygen in red, sulfur in yellow, nitrogen in blue, and hydrogen in white [198]. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

managing the interaction between the QM and MM regions, often through electrostatic interactions or boundary conditions.

In pollutant adsorption, QM/MM offers several significant advantages. This hybrid approach divides the system into two regions: the active site, where the pollutant interacts with the substrate, is modelled using QM to capture detailed electronic behaviour, and the surrounding environment is treated with MM to handle larger-scale interactions efficiently. The fundamental concept involves defining a QM region for the pollutant and nearby substrate atoms, performing complex QM calculations to describe electronic interactions, and using MM for the rest of the system with predefined force fields. Information is exchanged between the QM and MM regions to maintain consistency. QM/MM applications in pollutant adsorption include elucidating pollutant-substrate interactions, predicting adsorption mechanisms, designing new adsorbents, and investigating environmental effects. Despite its computational cost and the challenge of selecting appropriate methods, QM/MM is a powerful tool that balances accuracy and computational efficiency, and it is invaluable for designing and optimizing materials for applications like wastewater treatment and environmental remediation.

3.1.5. Machine learning (ML)

Dye adsorption is a widely used process with applications in wastewater treatment, textile dyeing, and sensor development. Traditionally, optimizing these processes relied on extensive experimentation, which is time-consuming and resource-intensive. ML offers a powerful alternative for predicting and optimizing dye adsorption, enabling more efficient and cost-effective solutions [183]. ML algorithms operate on a data-driven approach, learning from existing experimental data to make predictions. This data typically includes input variables such as dye concentration, pH, temperature, and adsorbent properties like surface area and pore size. The output variable is usually the quantity of dye adsorbed or the removal efficiency. ML algorithms identify patterns and relationships between these input and output variables, allowing the model to accurately predict adsorption behaviour for new, unseen data points [184].

Several ML techniques are particularly effective in the context of dye adsorption. Support Vector Regression (SVR) excels at modelling non-linear relationships by finding hyperplanes that best separate data points in high-dimensional space [185,186]. Random Forest, an ensemble method, combines multiple decision trees to make predictions based on random subsets of input variables, reducing the risk of overfitting [187,188]. Artificial Neural Networks (ANNs) mimic the brain's structure, consisting of interconnected layers of neurons that learn complex, non-linear relationships through a training process that adjusts the connections between neurons [189].

ML models have various applications in dye adsorption. They can predict the adsorption capacity of an adsorbent under specific conditions, significantly reducing the need for extensive laboratory experiments. Researchers can optimize process parameters such as pH and temperature by analyzing model predictions to maximize dye removal efficiency. Additionally, ML models can virtually screen an extensive library of potential adsorbent materials, prioritizing the most promising candidates for further experimental evaluation. Furthermore, by examining the internal structure of the models, researchers can gain insights into the most critical factors influencing dye adsorption for specific systems [190].

The primary benefits of ML in dye adsorption include reduced experimentation, saving time and resources, and faster design cycles for developing new and improved adsorbent materials. ML can also identify complex, non-linear relationships between variables that traditional methods might miss. However, the accuracy of ML models depends heavily on the quality and quantity of training data; insufficient or noisy

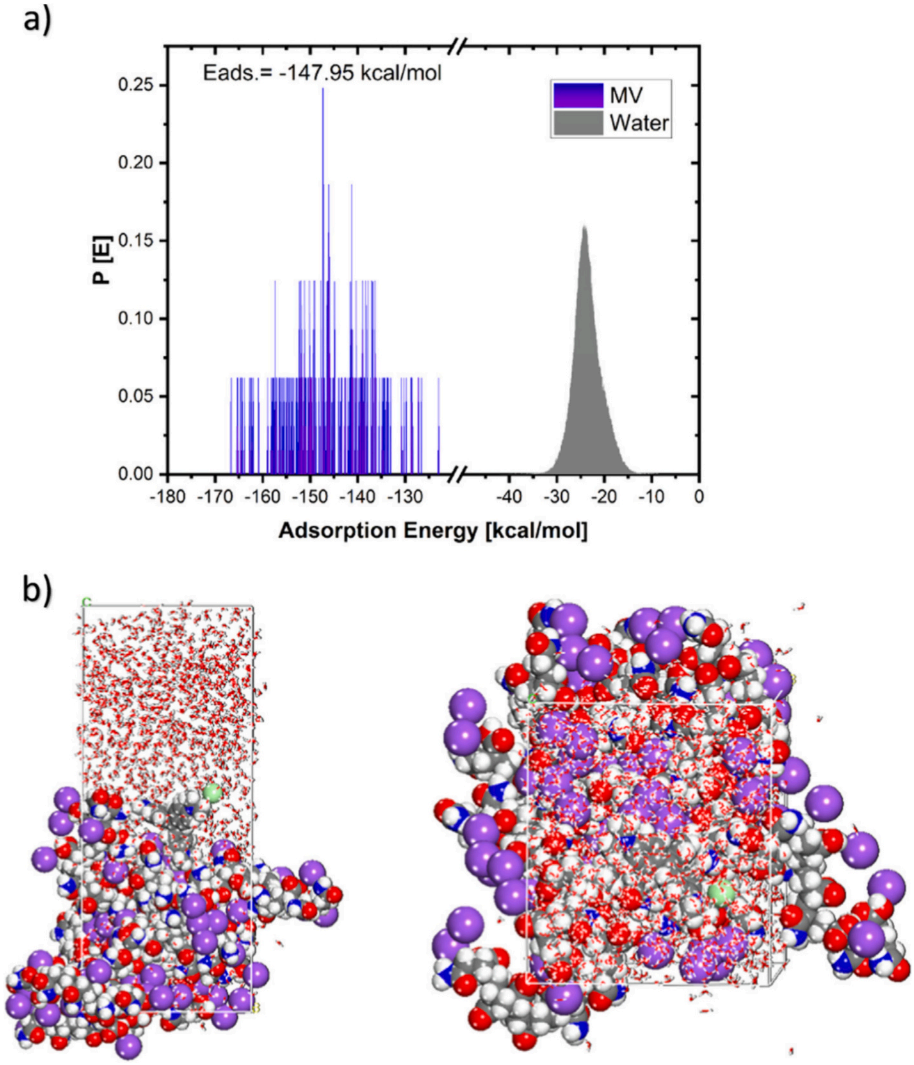

Fig. 11. A) During the MC simulations, analysis was carried out to decipher the probability distribution of adsorption energies for CV molecules onto the APAM surface. B) the configuration characterized by the lowest energy state within the simulation box was also ascertained through MC simulations [199].

data can lead to unreliable predictions. Additionally, some ML models, particularly complex ones like ANNs, can be challenging to interpret, making it difficult to understand the model's reasoning behind its predictions. Lastly, models trained on limited data may overfit, performing well on training data but failing to generalize to unseen data, necessitating careful selection and validation techniques. In conclusion, machine learning offers a valuable tool for researchers and engineers working on dye adsorption. By leveraging the power of data and pattern recognition, ML can streamline the development of efficient and sustainable dye adsorption processes, leading to significant advancements in wastewater treatment, textile dyeing, and sensor development.

3.2. Strengths and limitations overview

MD simulations capture atomic motions and interactions, allowing the study of dynamic properties like diffusion and phase transitions. They are versatile and can handle various systems and phenomena. However, MD simulations are computationally expensive for large systems or long timescales and rely on accurate force fields, which may not perfectly represent all interactions. MC simulations efficiently sample various system configurations and are useful for studying equilibrium properties like free energy calculations. Their limitations include not directly providing information about dynamics and requiring careful design of the moves used to sample the system. QM methods offer the most accurate description by considering the electronic structure for detailed chemical reactions and bonding, but they are extremely computationally expensive for large systems and often require approximations that can introduce errors. QM/MM combines QM for a specific region with MM for the rest, balancing accuracy and efficiency, and is useful for studying systems where a specific region needs high-level treatment. However, QM/MM can be complex to set up, requires defining the QM/MM boundary, and inherits limitations of both QM and MM methods. ML methods can learn complex relationships from data and potentially accelerate simulations, promising to reduce computational cost while maintaining accuracy. Their limitations include reliance on large data for training, which can be expensive to generate, a potential lack of generalizability outside the training data, and the difficulty of interpreting the learned model as it can be a "black box." In conclusion, each method has its own strengths and weaknesses, and the choice of method depends on the specific question being asked the size and complexity of the system, and the available computational resources. Machine learning is a growing field that holds promise for improving the efficiency and accuracy of simulations in the future. Table 5 compares MD simulations, MC simulations, QM, QM/MM, and ML methods regarding accuracy, efficiency, scalability, and applicability.

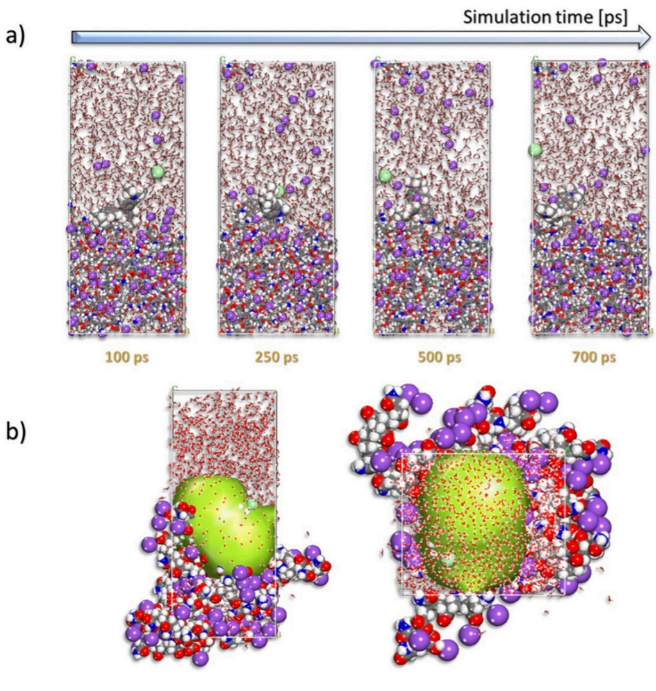

Fig. 12. A) Examining the lowest adsorption energy configurations achieved through MD, the morphological transformations of adsorbate molecules onto the APAM surface were elucidated. B) Further, a significant representation was embodied by the isosurface (depicted in yellow), which encapsulated the average volume occupied by the CV molecule throughout the entirety of the MD trajectory. (For clarification regarding the colour references in this legend, readers are encouraged to refer to the online version of this article.) [199] (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

4. Case studies of computational methods in dye adsorption

4.1. Cationic dyes

Cationic dyes, used in textile, paper, and plastic industries, pose a significant environmental concern due to their discharge into water bodies as industrial effluents. These dyes, characterized by their positive charge, bond with negatively charged surfaces, complicate aquatic contamination and are toxic to aquatic life and humans [191]. The release of cationic dyes into water ecosystems leads to water contamination, disruption of aquatic ecosystems, bioaccumulation within organisms, and alteration of water bodies' aesthetic appeal, potentially impacting tourism and local economies [192]. Exposure to these dyes also poses significant health risks, including carcinogenicity, mutagenicity, and allergic reactions. Therefore, removing cationic dyes from water solutions is crucial to protect environmental integrity, public health, regulatory compliance, and water bodies' aesthetic and economic value. Computational methods can speed up material discovery for cationic dye adsorption by simulating interactions between materials. Understanding the molecular process of adsorption is crucial for optimizing the process. Computational dynamics simulations provide detailed insights into bond types, pH, and temperature factors. This knowledge can be used to design better adsorbents, such as modifying existing materials' surface properties. This section references recent research applied in cationic dye adsorption processes through computational methods simulations.

The investigation carried out by El Haouti et al. focused on the uptake of positively charged dyes, toluidine Blue (TB) and crystal violet (CV), onto Na-Montmorillonite Nano Clay as efficient adsorbent via MD simulations and QM calculations. To elucidate the spatial arrangement of these investigated positively charged dyes near the adsorbent surface, they conducted NVT simulations at a temperature of 298 K. Equilibrated CV and TB structures on dry adsorbent (Figs. 1 and 2) displayed diverse orientations. At 33% loads, a monolayer formed with TB's rings parallel and CV's moieties oriented for optimal interaction (Fig. 1a, 2a). Higher loads (66%, 100%) led to various orientations (Fig. 1b-c, 2b-c), including flat and tilted arrangements, confirming the complex adsorption process. Moreover, interaction energies between adsorbed dyes and Na-MNC were explored to determine the optimal orientation.

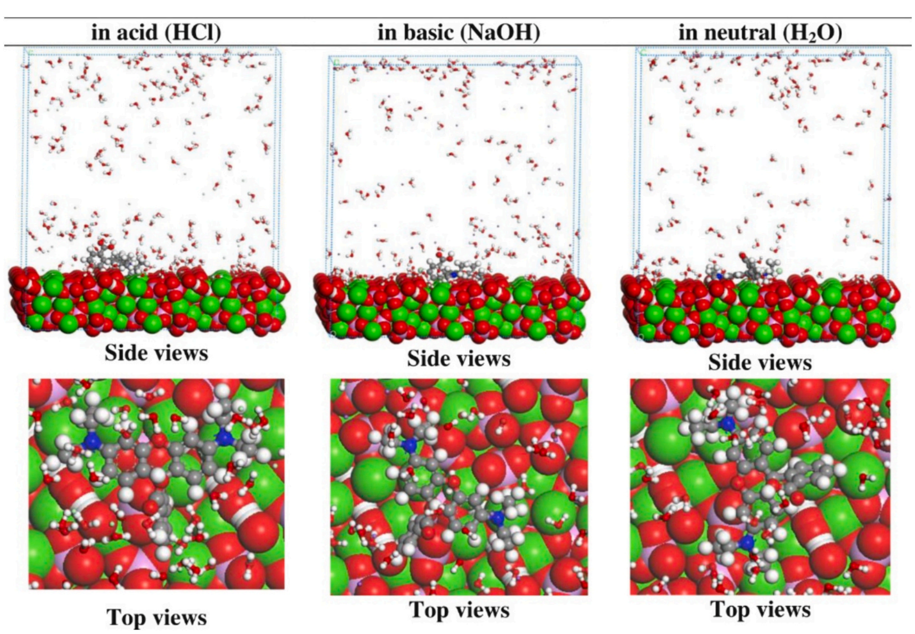

Fig. 13. Different media (acidic, basic, and neutral) are explored to observe the most stable low-energy configuration of the RhB molecule's adsorption onto the hydroxyapatite (211) surface, as depicted in both side and top views [200].

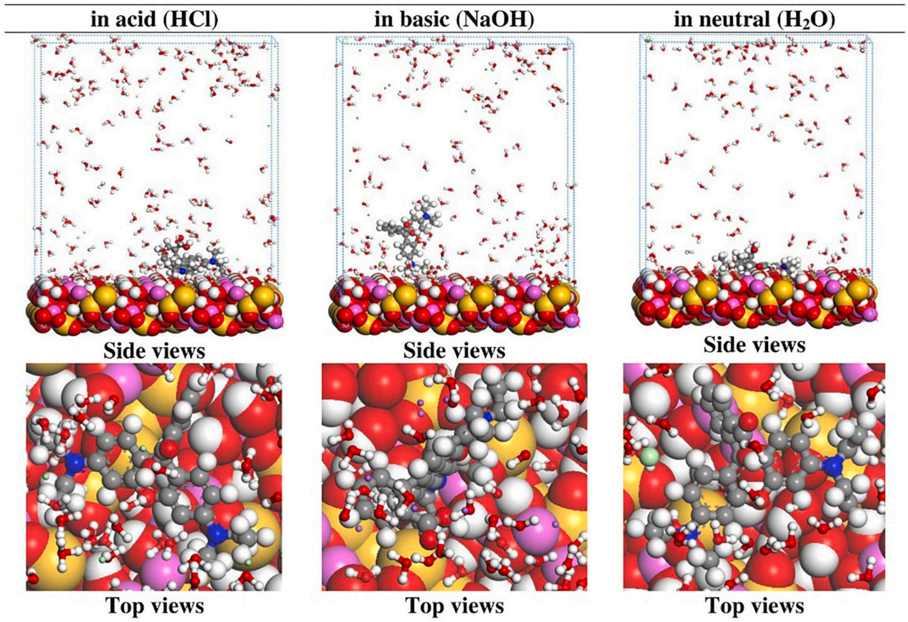

Fig. 14. Varied chemical environments (acidic, alkaline, and neutral) are investigated to unveil the preferred low-energy arrangement of RhB molecule adsorption onto the kaolinite (211) surface. Comprehensive insights are presented through both lateral and overhead perspectives [200].

The rising surface charge led to stronger interactions in both dyes at full surface loads. TB exhibited more favourable interactions than CV, affirming its greater adsorption capacity, which is consistent with experimental findings. Furthermore, The study used DFT parameters to study organic molecules' reactivity and interactions with solid surfaces. It compared the reactivity of two dye molecules, CV and TB, using the Becke3-Lee-Yang-Parr functional and 6-31G(d) basis set. The solvation effects approach was used to simulate solvent effects. Chemical hardness and electrophilicity power are crucial indicators of a dye's chemical reactivity. They reported that the TB dye has a higher electron-accepting ability than the CV dye. TB dye's slightly lower chemical hardness value suggests similar reactions and its higher electrophilic character indicates stronger interactions with surface sites [193].

In another investigation, Boukoussa et al. performed MD simulations on Models with different pore diameters based on pure SBA-1 5 configuration types. The objective was to gain insight into the dynamic behaviour of methylene blue (MB) molecules when adsorbed onto the mesoporous substance. Fig. 3 illustrates the dynamic conditions of the MB molecules in varying silica pore configurations observed at different temporal gaps. The simulations' snapshots show that the MB molecules migrate through pores of different sizes to the vicinity of the pore walls. This migration culminates in achieving stable arrangements within a 7 50 ps timescale, perhaps owing to the resilient interplay between the hydroxyl (OH) moieties present on the silica surface and the molecules of MB as guests. The MD simulations provided snapshots confirming the MB molecules' interaction with the pore walls' boundaries. These visual testimonies irrefutably confirm the compelling and reciprocal interplay that characterizes the host-guest interaction between MB molecules and the inviting boundaries of the mesoporous pore landscape [194].

Salahshoori et al. recently used MD, MC and QM simulation to comprehensively analyze the interaction between dyes and their cationic dye's adsorption behaviour in mixing mode (methylene blue and rhodamine B) on the adsorbent. MD simulation method investigated the mutual influence of dyes on their adsorption properties throughout the mixing form. The selectivity ratio and dye rejection rate were quantified using eqs. (1) and (2), respectively. These mathematical expressions served as tools to measure the dye removal efficiency and evaluate the discrimination properties of the system.

$$\text{Selectivtiy ratio} = \frac{\text{Dye Rejection Rate}_{RB}}{\text{Dye Rejection Rate}_{MB}} \tag{1}$$

$$\text{Dye Rejection Rate\%} = \left(1 - \frac{D_{adsorbed}}{D_{feed}}\right) \times 100 \tag{2}$$

Within Fig. 4 (a-b), the progression of events from initial to intermediate and finally to concluding frames is depicted. Additionally, the associated concentration profiles are presented, showcasing the adsorption processes occurring over the period of 0–5 ns for both dyes-water-functionalized MIL and dyes-water-neat MIL mixtures. These visuals depict adsorption evolution. Fig. 4 (a-b) defines dye rejection: MB at 20%, RB at 80% for dyes-water-functionalized MIL; MB at 30%, RB at 60% for dyes-water-neat MIL Selectivity ratio (RB/MB) determines affinity, indicating 4 for dyes-water-functionalized MIL and 1.5 for dyes-water-neat MIL. Competitive, electrostatic, and dye-dye interactions control cationic dye adsorption onto mixed adsorbents. RB's augmented rejection is due to size hindrance, electrostatic attraction with adsorbent, and CXA group interactions, enhancing its adsorption propensity [123].

QM calculations, including Electrostatic Potential (ESP) and Average Local Ionization Energy (ALIE), were used to analyze the structures of adsorbent and cationic dyes (Fig. 5). Methylene Blue (MB), a pollutant dye, showed electron-rich areas near nitrogen, chlorine, and carbon atoms, enhancing solubility in water. Oxygen and chlorine atoms had low ESP, while hydrogen atoms had positive ESP. ALIE analysis indicated regions conducive to nucleophilic interactions near chlorine, nitrogen, carbon, and oxygen atoms, facilitating electron lone pair donation [123].

According to their MC simulation results, dye molecules spontaneously adsorb on MOF and MOF/functionalized surfaces. MIL-53 (Al) shows efficient dye adsorption due to aromatic rings forming π-π bonds. CXA-functionalized MIL-53 (Al) enhances adsorption via increased surface area, improved charge distribution, and selective binding. RB dye exhibits higher adsorption energy and stability than MB dye [123].

Feng et al. utilized QM calculations and MD simulations to investigate the adsorption mechanisms of four toxic cationic dyes—malachite green (MG), methylene blue (MB), toluidine blue (TB), and crystal violet (CV)—on MOF/$(COOH)_2$ in the presence of water molecules. Their MD

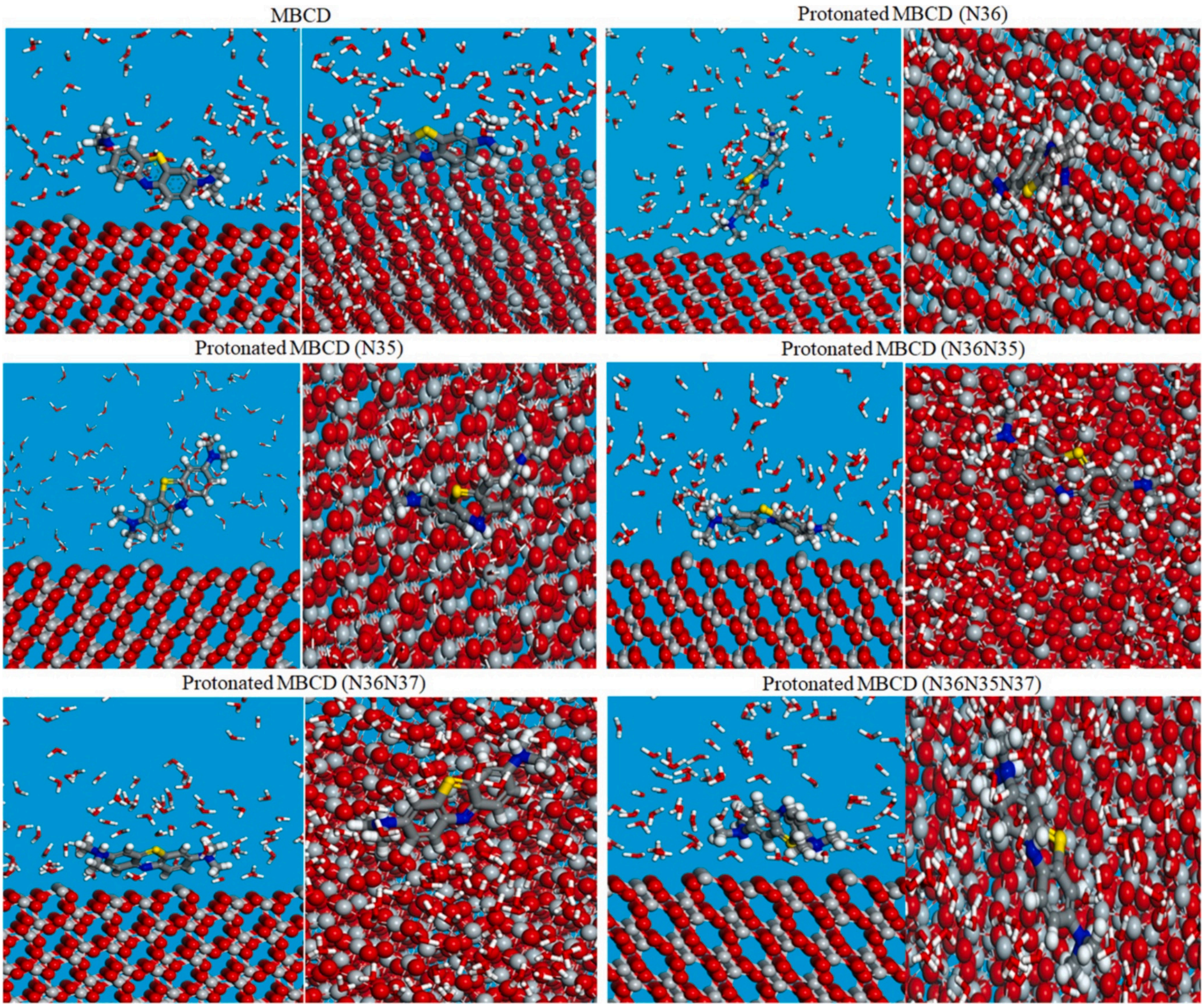

Fig. 15. The utilization of the adsorption locator module led to the determination of the most stable adsorption configurations for the (MBCD/400 H_2O/Brookite (110)) complexes, as observed from both the superior and lateral perspectives [201].

simulation results indicated that MOF/$(COOH)_2$ surfaces can form π-π stack bonds, facilitating dye adsorption. The aromatic rings of MOF/$(COOH)_2$ enable sulfur, nitrogen, and oxygen in dye structures to conduct chemical adsorption. CV and MG dyes interact more readily with the MOF/$(COOH)_2$ surface due to these π-π stack bonds. Adsorption analysis revealed that the energy for CV and MG dye adsorption on MOF/$(COOH)_2$ in an aqueous solution is higher than that for MB and TB dyes, leading to a more stable configuration. Organic molecules, including dyes and drugs, exhibit van der Waals forces due to interactions between the molecules and adsorbents. In their study, Feng et al. exploited the power of QM by employing the HOMO-LUMO (Fig. 6) to demonstrate the reactivity inherent in the structures of adsorbent-dye-water mixtures. The analysis of adsorption ability unveiled that the functionalized/MOF-water-crystal violet configuration exhibited the most elevated adsorption values, surpassing the other examined arrangements. Consequently, crystal violet dye manifested a notably favourable propensity for adsorption onto the functionalized/MOF surface within the dyes under consideration [195].

In a recent scientific investigation, Salahshoori et al. devoted themselves to deciphering the complicated adsorption properties of widely known cationic dye impurities. In particular, they focused on studying their interaction through the employment of amide/ MIL-53 (Al). The discourse included a comprehensive investigation of the adsorption dynamics of the functionalized MOF adsorbent with an emphasis on dye hydration. A SENSIBLE INQUIRY WAS CONDUCTED using MC and MD simulations to analyze the dye Rhodamine B (RHB) adsorption characteristics. This investigation spanned several areas, including non-aqueous and aqueous environments, focusing on deciphering the complicated interplay between hydration and adsorption rate (see Fig. 7). The figure shows notable non-aqueous RHB absorption rise (−1280 vs. -373 aqueous). Concentration profiles and snapshots reveal divergent adsorption in both environments. Hydration's impact on rate arises from water-dye interactions hindering functionalized MOF interactions in water, reducing adsorption. RHB's cationic charge drives favourable electrostatic interactions with negatively charged sites on functionalized MOF surfaces in non-aqueous environments, enhancing absorption [147].

Moreover, they used QM tools to account for reduced density gradient (RDG) analysis comprehensively. This strategic endeavour targeted to accurately illuminate the panorama of intermolecular and intramolecular associations embedded in the complex fusion of adsorbent, water, and dye. Fig. 8 provides a visual chronicle of the RDG analysis, revealing the intricate choreography of the amalgamated dye, water, and adsorbent landscape. The analysis shows that the interactions

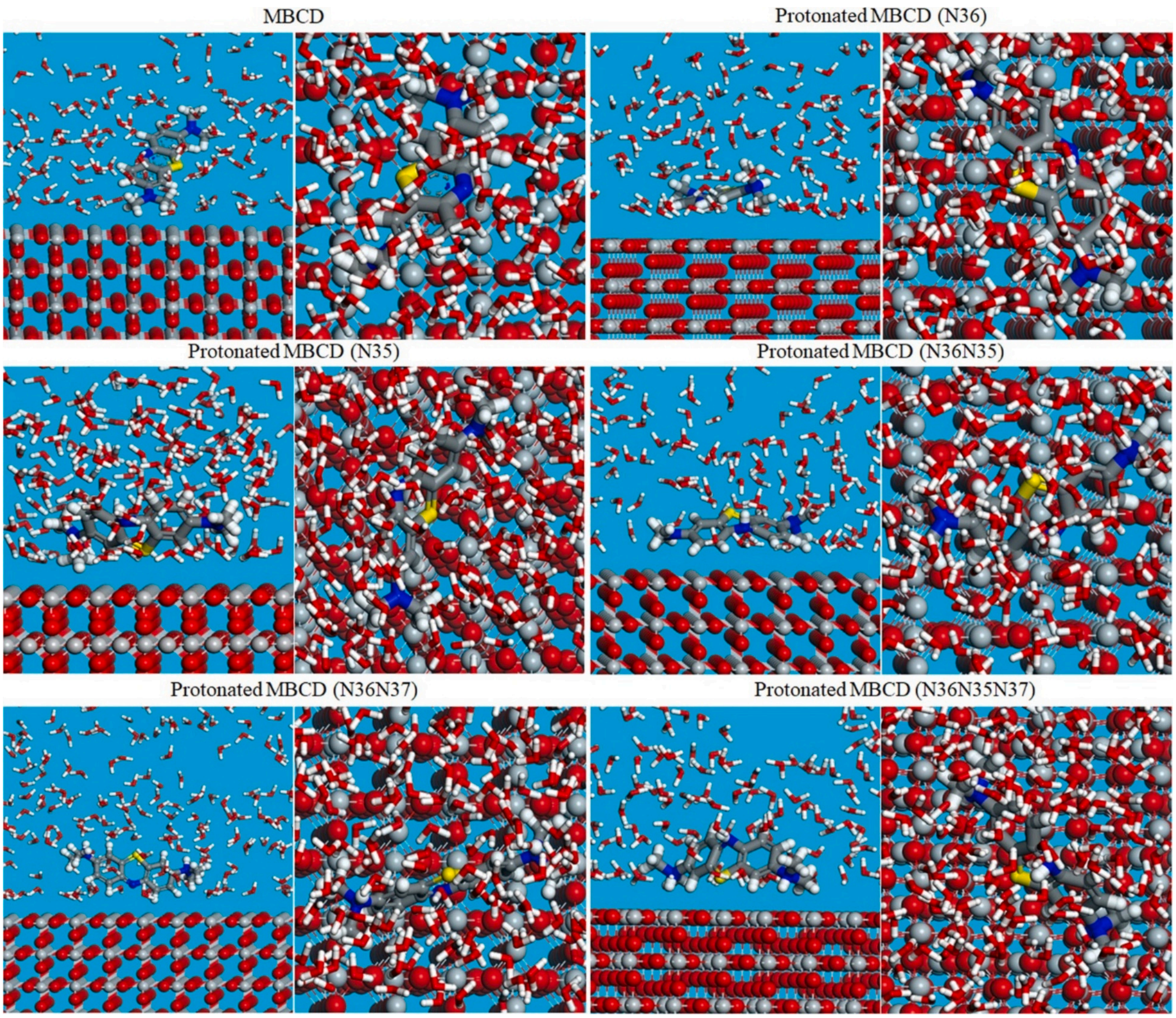

Fig. 16. The adsorption locator module facilitated the acquisition of top and lateral perspectives depicting the utmost stable adsorption arrangements for the (MBCD/400 H_2O/rutile (1 1 0)) complexes [201].

between adsorbent and RHB during adsorption at the surface are predominantly due to van der Waals forces. These general non-covalent interactions depend on distance and orientation and arise from fluctuations in electron density. Although weak, they gain importance in multi-species scenarios and crucially stabilize the adsorbed molecules. MIL -the flexible structure of 53 (Al), due to the movement of the organic linkers, accommodates adsorbed molecules by changing the pore size and shape [147].

Pedebos et al. conducted a study aiming to synthesise and characterize a zeolite doped with cobalt (ZO-Co) sourced from materials like rice husk, residual sludge, and pumice stone. The goal was to utilize this material to remove RhB dye through adsorption. They employed both experimental design and machine learning to identify the optimal conditions for RhB adsorption. According to the machine learning results, the ideal conditions for RhB adsorption were determined to be [RhB] = 130 mg/L, [ZO-Co] = 0.6 g/L, pH around 7, and temperature of approximately 298.1 5 ± 2 K. Thus, cobalt-doped ZO emerges as a promising candidate for efficiently adsorbing organic pollutant RhB, bridging the realms of environmental concerns and nanotechnology [196].

The exploration of molecular simulation concerning the adsorption behaviour of methylene blue and rhodamine B was undertaken by Narayanaswamy et al. on graphene-based substrates to advance water decontamination techniques. Fig. 9 depicts the progression of the cationic dye's adsorption characteristics onto the adsorbent structures across various simulation durations. Evidently, this observation highlights the direct correlation between the adsorption propensity and the density of oxygen within the structures of graphene oxide. The augmented interaction between the p electron cloud of methylene blue and the graphene framework, attributable to the planar geometry of methylene blue, stands in contrast to rhodamine B [197].

Hamal et al. leveraged the capabilities of MD simulations to probe into the intricate intricacies of adsorption and transport characteristics. Within the confines of DOPC and DOPG liposomes, their exploration extended to malachite green and its isothiocyanate variant (MGITC). Guided by the methodology of umbrella sampling, the investigation unveiled the tapestry of free energy profiles and the orientations exhibited by molecules interfacing at the interfaces. Fig. 10a,b provides a visual exposition of characteristic snapshots that artistically capture the spatial arrangement of both the MGITC and MG dyes as they find themselves confined within the intricate matrix of the DOPC membrane. Specifically, the NCS moiety of the MGITC molecule exhibits a distinct orientation, favouring alignment toward the DOPC membrane. MG probably aligns itself in a manner where both of its amine groups are directed toward the DOPG membrane. Conversely, MGITC exhibits a configuration wherein one amine and the NCS group are oriented

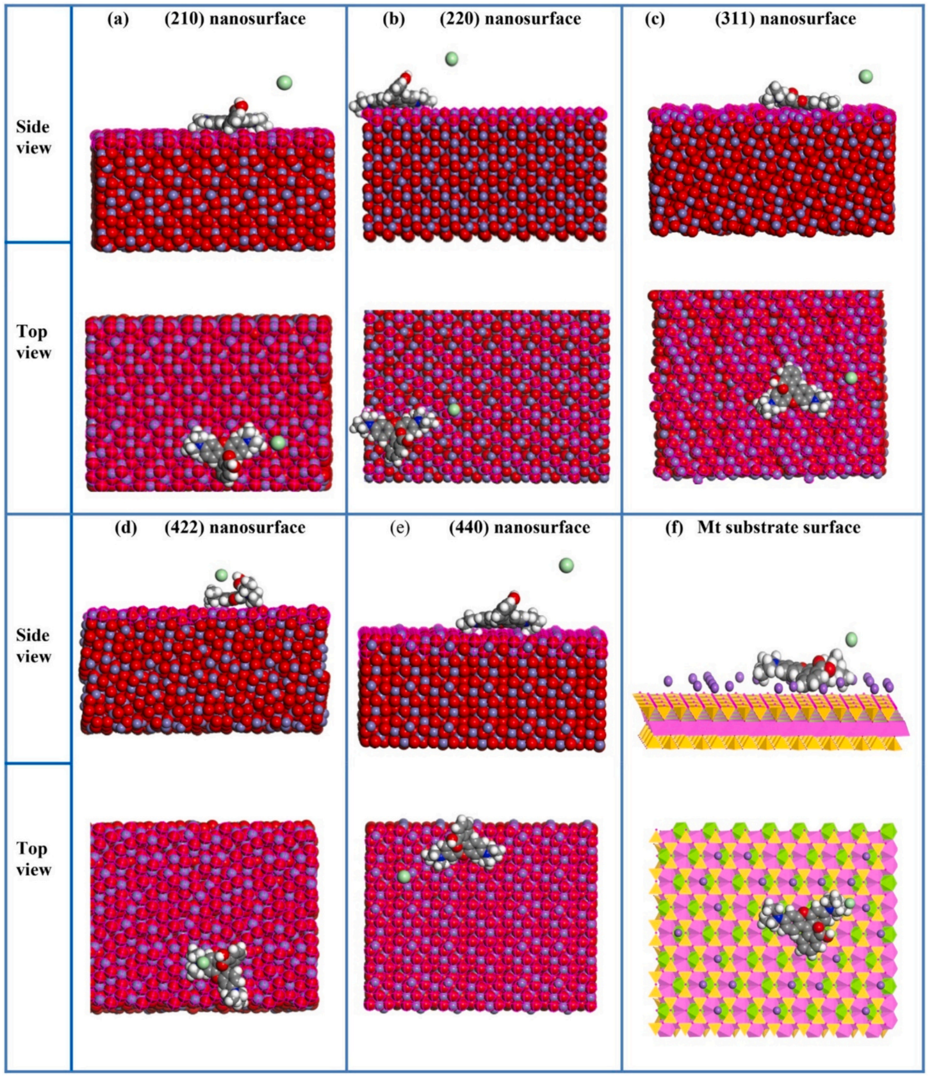

Fig. 17. Illustrated in CPK style are the lowest RhB molecule adsorption configurations on different maghemite surfaces, denoted as (210), (220), (311), (422), and (440), along with the Mt. substrate (displayed as polyhedra), in both side and top views. The visual representation assigns distinct colours: blue for nitrogen, dark grey for carbon, white for hydrogen, pale green for chlorine, red for oxygen, light blue for iron, pink for aluminum, light green for magnesium, and golden for silicon. Additionally, a violet hue on the Mt. surface signifies the presence of sodium [202]. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

toward the membrane, as depicted in Fig. 10c,d. MG's charge disperses, yet it binds stronger to charged DOPG than weak DOPC dipole interaction. Positively charged amine groups in MG interact favourably with negatively charged DOPG, promoting adsorption via charge−charge interactions over weak dipole−charge interactions with neutral DOPC [198].

In a remarkable convergence of experimental testing and computational finesse, Lebkiri et al. conducted a comprehensive investigation encompassing both empirical and theoretical dimensions. MC and MD simulations, conducted in parallel with their practical investigations, were at the forefront of their methodology. This multi-faceted approach was orchestrated with a single goal: to provide a solid foundation for evaluating an innovative application using anionic polyacrylamide hydrogels to separate the cationic dye crystal violet from aqueous solutions. The synergy of empirical and computational findings has enhanced the understanding of this application and underscored the inherent value of coupling experiments with sophisticated simulations for versatile scientific exploration. A versatile methodology has bridged the gap between empirical observation and computational exploration. The discovered correspondence between experimental data and theoretical predictions was illuminated through the strategic implementation of MC and MD simulations. This integrated analysis supported the credibility of the empirical results and provided a tangible rationale for the claim that CV molecules maintain proximity to the APAM surface. This molecular proximity is vividly illustrated in the visual representations in Figs. 11 and 12, where the intricate dynamics of molecular interactions are vividly depicted [199].

El Hassani et al. have studied the Rhodamine B dye adsorption in water solutions on kaolinite and hydroxyapatite substrates. This investigation involved a synergistic integration of molecular simulations and experimental analyses. In addition, MC was performed to investigate the possible interactions between adsorbate and adsorbent. Fig. 13 and Fig. 14 illustrate the predominant conformations adopted by the RhB dye and the respective surfaces of two different materials: Hydroxyapatite (211) and Kaolinite (211). Fig. 13 visually shows the pronounced RhB molecule's adsorption performance on the metallic surface. Of significance is the sustained parallel orientation exhibited by the RhB molecule on the hydroxyapatite surface across distinct media conditions, including neutral, alkaline, acidic and environments. The interplay among the atoms constituting RhB and the atoms residing on the

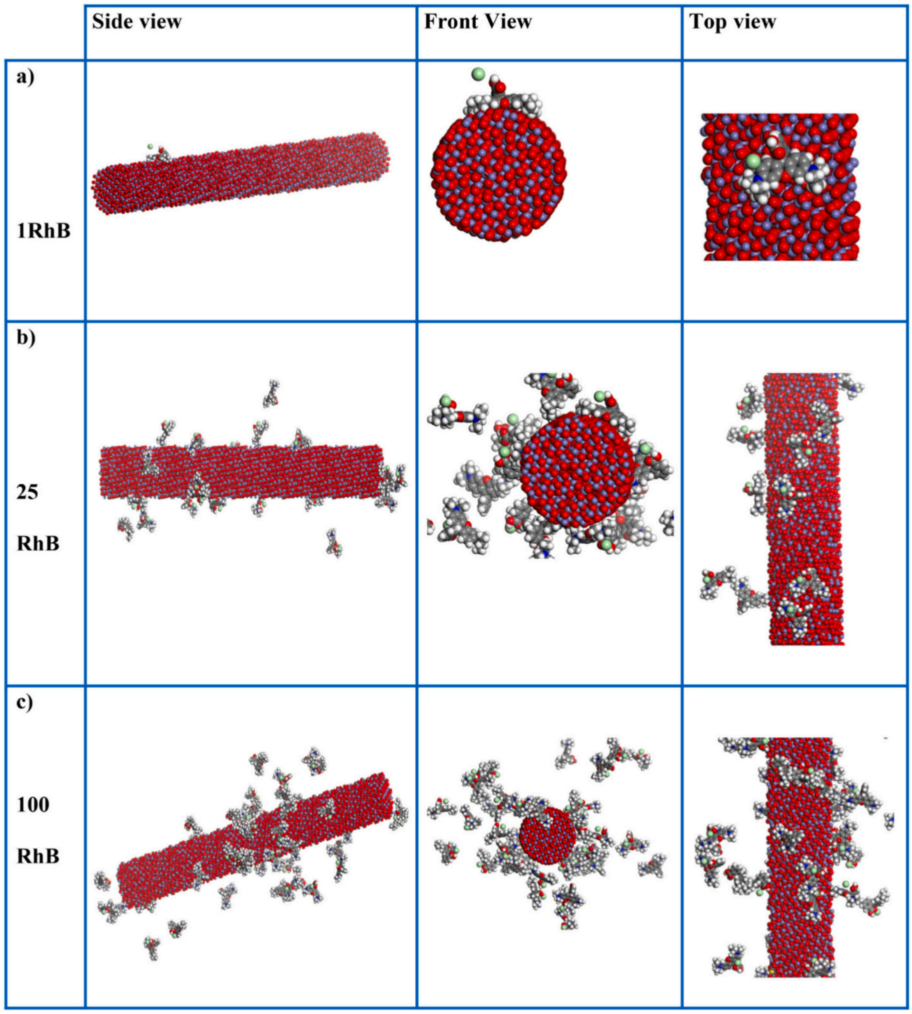

Fig. 18. The adsorption scenarios of (a) one RhB molecule, (b) twenty-five RhB molecules, and (c) one hundred RhB molecules onto the maghemite cylindrical nanoparticle are illustrated through side, front, and top views, employing NVT molecular dynamics. Key elements are colour-coded: nitrogen in blue, carbon in dark grey, hydrogen in white, chlorine in pale green, oxygen in red, and iron is visually represented by a light blue shade [202]. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

surface of hydroxyapatite engenders an interaction of interest. In contrast, analysis of the RhB molecules' adsorption configurations on kaolinite (211) yields quite different findings, as shown in Fig. 14. The RhB molecule in the basic medium occupies a perpendicular position relative to the diethylammonium group on Kaolinite's metal surface. Conversely, a notable distinction emerges as the orientation of the RhB molecule on the kaolinite surface is explored within both acidic and neutral media—a parallel arrangement prevails. This consistent parallel alignment was prevalent in different media, implying that the parallel interaction mode between the kaolinite (211) surface and the RhB molecule persists [200].

M. Khnifira et al. used molecular simulation to investigate the cationic dye methylene blue's adsorption performance on the rutile and brookite phases of TiO_2. Figs. 15 and 16 show the vertical and horizontal perspectives of the most stable adsorption arrangements obtained for the (rutile (110) and brookite (1 1 0) surface) systems by applying MC simulation. The methylene blue molecule aligns parallel to both surfaces at the equilibrium point within the system under study, as shown in Figs. 15 and 16. The findings revealed that the active zones are predominantly located along the molecular framework of the dye, which adopts a flat orientation on the TiO_2 surface, with interactions mediated mainly by aromatic rings. In addition, the methyl substitutions (–CH_3) on the thioninium units orient toward the uppermost facet of the adsorbent surface. Examination of the adsorption arrangements within the aqueous environment from both top and side perspectives reveals robust interactions between the protonated variants and the surfaces. This phenomenon is mainly attributed to resonance interactions indicative of chemical adsorption and the influential van der Waals forces contributing to the adsorption process [201].

Ouachtak et al. computationally investigated RhB dye interaction with γ-Fe2O3@Mt. composite through adsorption, encompassing initial MC exploration and MD simulations. Fig. 17 illustrates equilibrated RhB adsorption on various maghemite nanosurfaces and Mt., demonstrating interactions involving nitrogen atoms and benzene rings. This results in a planar orientation of the interconnected entities, though the third ring exhibits a tilted disposition. Fig. 18 presents the lowest RhB adsorption conformations in cylindrical maghemite nanoparticles. For single RhB molecules (Fig. 18(a)), interactions are via nitrogen atoms and benzene rings; introducing multiple RhB molecules (2 5, 100) yields flat, tilted, and random pile orientations (Fig. 18(b) and (c)), indicating diverse binding affinities. Notably, these configurations exhibit varying proximity to the cylindrical nanoparticle, implying differing binding affinities of adsorbed RhB molecules to the γ Fe_2O_3 iron oxide cylindrical nanoparticle [202].

Abedini et al. conducted a study on the adsorption of aniline onto single-walled carbon nanotubes (SWCNT) using QM/MM methodology. They used three models: open-ended, cap-ended, and 1-cap-ended SWCNT. Model 2 showed the most favourable adsorption kinetics,

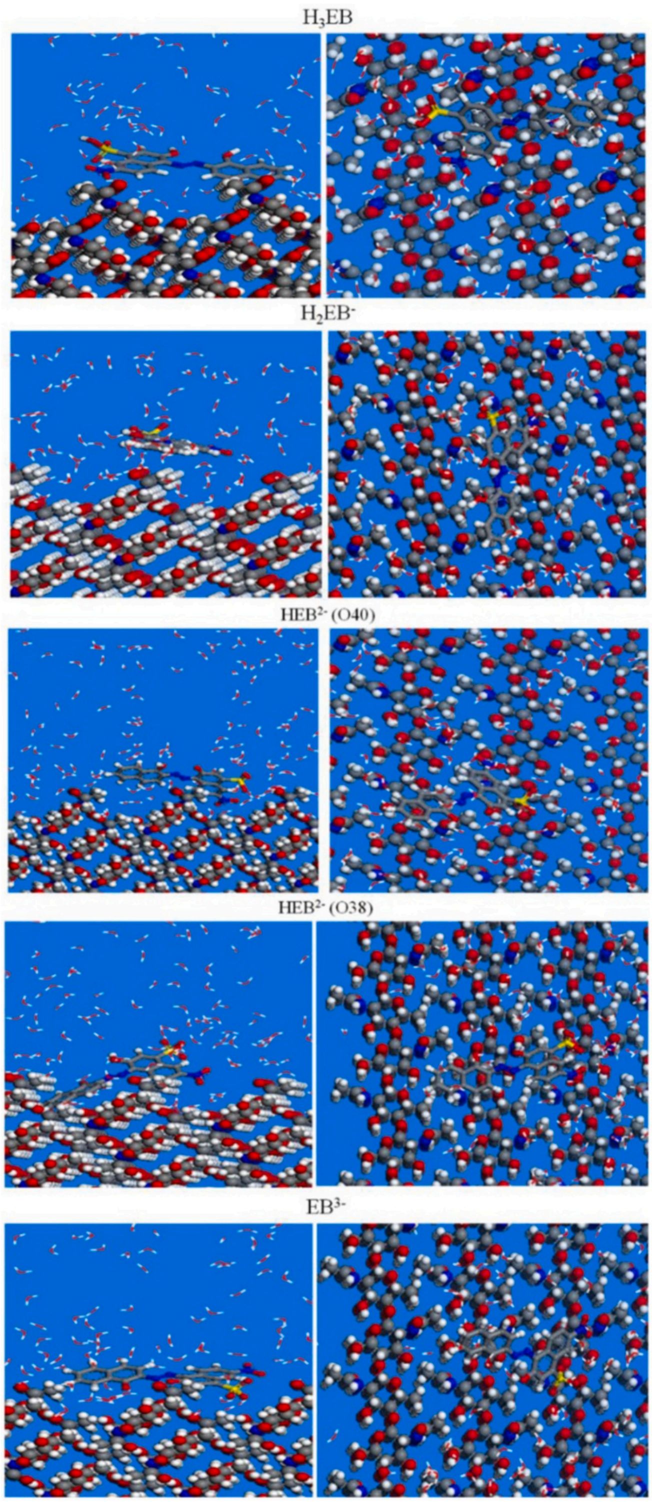

Fig. 19. The optimal adsorption arrangements for complexes acquired via the adsorption Locator module are depicted from aerial and lateral vantage points [218].

with an activation energy of 40.8 kcal/mol. The study also found a charge transfer from aniline to SWCNT and a shift in the Fermi level post-adsorption. Quantum reactivity indices revealed new linear correlations linking chemical hardness, charge transfer, and activation energy and an inverse relationship between electrophilic property and chemical electronic potential [203]. Petrone and colleagues investigated the absorption and emission electronic spectra of *N*-methyl-6-oxyquinolinium

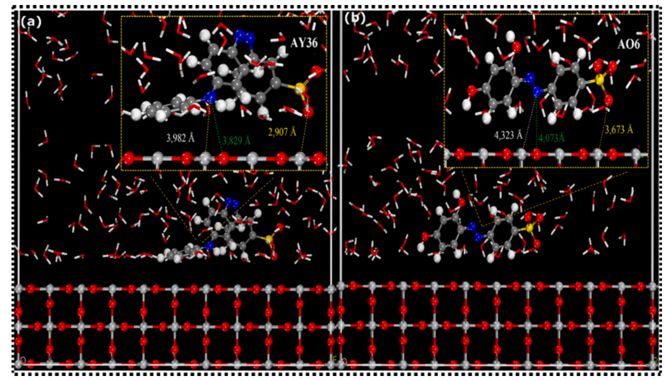

Fig. 20. MC simulation results of the most stable configurations for the adsorption of AY36 on rutile TiO_2 in aqueous medium [219].

betaine (MQ) in water, noting a change in polarity and hydrogen bond capability between its ground and excited states. They compared two methods: one employing explicit solvent models and DFT/molecular mechanics calculations and the other utilizing DFT calculations on cluster models within a polarizable continuum (PCM). Both techniques provided absorption and emission spectra that matched well with experimental data. However, Qst calculations accurately reproduced the Stokes shift and offered a better fit to the experimental line shape, particularly in absorption. The researchers observed that solvent effects on spectral width are complex, with broadening from solute-solvent interactions partially offset by narrowing due to solute vibrational modes [204].

4.2. *Azo dyes*

Azo dyes, characterized by one or more azo groups (-N=N-) attached to aromatic rings, are synthetic organic compounds extensively used in industries like textiles, leather, cosmetics, food, and pharmaceuticals due to their vibrant colours and stability. However, their environmental persistence leads to long-term contamination, and their toxicity, including mutagenic and carcinogenic effects, poses significant risks to aquatic life and human health. Azo dyes contribute to eutrophication by disrupting photosynthesis in aquatic plants and algae, causing dye pollution and making the water unsuitable [205–207]. Therefore, removing azo dyes from water solutions is crucial to protect ecosystems, ensure human health, comply with regulations, and facilitate water reuse in industrial processes. Researchers are using molecular simulation and machine learning to predict the effectiveness of adsorbent materials in capturing azo dyes [208–213]. Simulations can model the effects of pH and temperature on dye breakdown, optimizing degradation processes for faster removal. ML algorithms can analyze large datasets of dye-adsorbent interactions to identify patterns and predict optimal properties. This can accelerate the development of new adsorbent materials and optimize operating conditions in wastewater treatment plants. This approach can lead to more efficient resource use and reduced treatment costs.

Sudarshan Sahu and his team researched to evaluate the effectiveness of algae and algae-bacteria symbiosis (ABS) in decolorizing Remazol Red 5B, a common dye pollutant. The study found a significant interaction between the dye and the biosorbent, with the Temkin model showing the best fit for the experimental data. The Langmuir model indicated a high biosorption capacity, emphasizing the potential of the algae-bacteria composite as an effective adsorbent. Various machine learning algorithms were evaluated for their ability to predict dye removal efficiency. The Random Forest model emerged as the most accurate, boasting an R^2 value of 0.98. Support Vector Regression and Artificial Neural Networks also demonstrated robust predictive capabilities. This study contributes to advancing sustainable dye removal

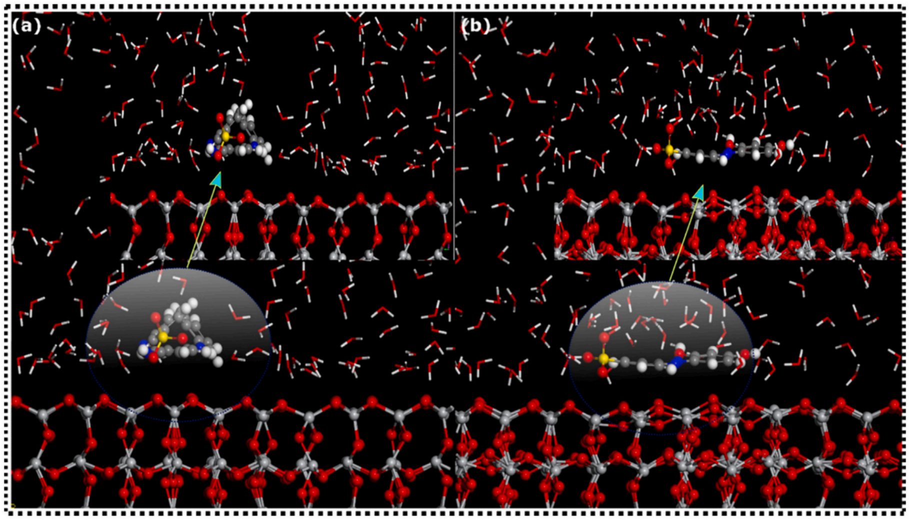

Fig. 21. MD simulation results of the most stable adsorption configurations for AY36 and AO6 on rutile TiO_2 (1110) surfaces [219].

strategies and advocates for further exploration of hybrid approaches to enhance predictive accuracy and efficiency in wastewater treatment processes [214].

Mandal et al. investigated QM, MD and MC simulations to comprehend the adsorption behaviour and configurational aspects of three specific selective dye molecules classified as organic azo-dyes. The focus of this study involved the interaction of these dye molecules with TiO_2 and ZnO surfaces, which were meticulously tailored to emulate authentic adsorption processes and surface protection phenomena. To evaluate the strength of the interactions among the three dye molecules after adsorbing onto the metal oxide substrate, calculations were conducted to ascertain the binding energy ($E_{binding}$) and the energy of interaction ($E_{interaction}$) under equilibrium conditions. Ultimately, it becomes apparent that the dye molecules assume a nearly planar configuration upon both the ZnO(110) and rutile TiO_2(110) surfaces. The findings obtained through MD simulations underscore its efficacy as a potent analytical instrument in prognosticating adsorption tendencies and, crucially, corrosion inhibition attributes. This becomes particularly salient in scenarios where the steadfastness of inhibitor assimilation onto the target metal oxide surface emerges as a pivotal influence factor [157].

The study by Zhao et al. used molecular DFT calculations and machine learning to investigate the impact of multivalent background ions (Ca^{2+}, K^+, Na^+, Mg^{2+}) on the adsorption of azo dye molecules. It was found that mixed background ions significantly affect adsorption capacity more than individual ions, with the inhibitory strength ranked as $Mg^{2+} > Ca^{2+} > K^+ > Na^+$. This indicates that these ions can hinder azo dye adsorption, with Mg^{2+} having the most pronounced inhibitory effect. DFT calculations revealed that the adsorption process is primarily driven by hydrogen bonding (C-H…O) and van der Waals forces (Si-H…C), contributing to high adsorption efficiency. Background ions can alter electron transfer pathways and reduce complex stability, thus decreasing the number of available adsorption sites. However, azo dye molecules can counteract this by adhering to adsorbed background ions through cation-π interactions, mitigating the inhibitory effect. The study also employed machine learning, particularly the gradient-boosting decision tree model, which proved effective in predicting adsorption, underscoring the role of machine learning in optimizing adsorption processes. Overall, the research highlights the importance of considering environmental factors like background ions in designing adsorption processes for azo dye removal and demonstrates the potential of machine learning to enhance these processes [215].

Understanding the maximum absorption wavelength (λ_{max}) is crucial when working with azo dyes, as it helps in the swift development of new molecules. In a study by Mai et al., they employed the XGBoost machine learning algorithm to construct a model capable of predicting the λ_{max} of azo dyes. The model demonstrated impressive coefficients of determination (R^2) of 0.87 during leave-one-out cross-validation (LOOCV) and 0.73 for the test set. An analysis using SHapley Additive exPlanations (SHAP) revealed a significant positive correlation between the number of sulfur atoms in the R_2 group and the λ_{max}. Furthermore, a higher count of C—N pairs with a topological distance of 4 in the R_1 group increased the probability of a red shift in the λ_{max}. The study successfully pinpointed 26 azo molecules with larger λmax from a pool of nearly 20,000 virtual samples by employing a high-throughput screening strategy. These predictions indicated a red shift from the 610 nm observed in the dataset. This research introduces an efficient approach for identifying azo dyes with higher λ_{max} values [216].

In another study conducted by Gamboa et al., the focus was on understanding how Congo red (CR) binds to activated biochar material derived from *Haematoxylum campechianum* (ABHC) waste. They utilized advanced ML techniques to refine a chemical removal process. By tapping into a rich dataset, they developed a gradient-boosting regression model honed to precision through Bayesian optimization within a Python programming framework. This optimization algorithm adeptly explored the input space to maximize the removal percentage. As a result, it predicted an efficiency of around 90.47% under optimal conditions. These findings present promising prospects for improving the efficiency of similar removal processes. They underscore the potential of ML in optimizing processes and addressing environmental concerns [217].

The investigation of Eriochrome Black T adsorption onto the chitin surface was conducted by Boumya et al. through a combined approach involving experimental study and molecular simulation. In this study, MC simulations were executed to decipher plausible interactions between EB molecules and the chitin (110) surface. The visual representation of this analysis is depicted in Fig. 19. Through examination, the sites of heightened adsorption sensitivity for EB molecules on the chitin (110) surface were discerned to be the hydroxyl (O\H) group and the oxygen atoms within the sulfonic moiety. Additionally, the alignment of EB dye species in a parallel configuration along the chitin (110) surface indicates a potent interplay between EB and the surface atoms of chitin (110), thereby implying a mechanism of chemical adsorption [218].

The adsorption behaviour of anionic dyes, namely acid orange 6 (AO6) and acid yellow 36 (AY36), on the absorbent surface of rutile TiO_2 was scrutinized by Amrhar et al., employing MD and MC techniques. The preeminent adsorption arrangements of AO6 and AY36 molecules onto the Ti oxide adsorbent, post-Monte Carlo optimization, are visually

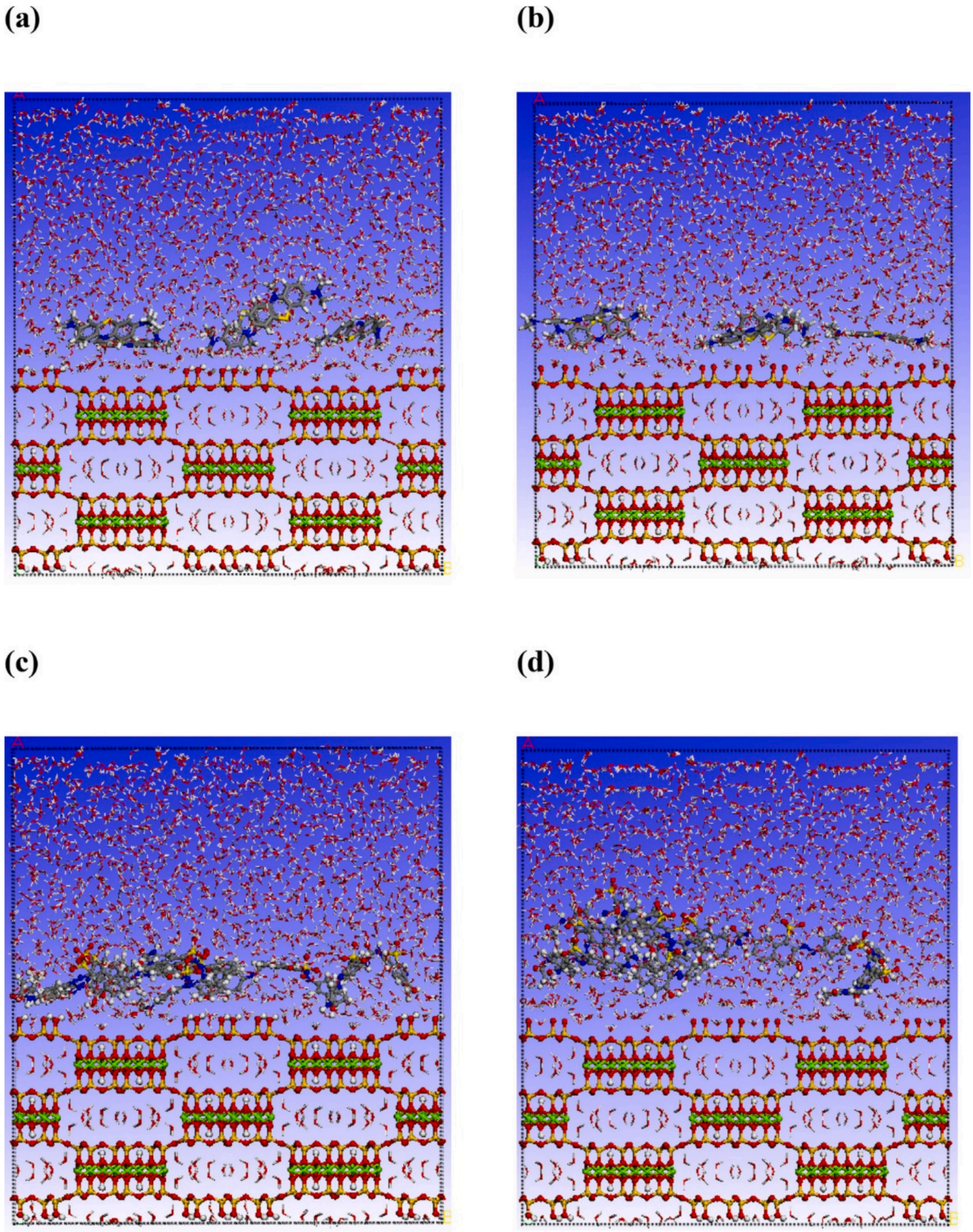

Fig. 22. The adsorption configurations at equilibrium for MB (depicted in panels a and b) and DR-23 (shown in panels c and d) molecules onto the adsorbent surface have been ascertained within both acidic and alkaline solutions [222].

represented in Fig. 20. The discernible shift of the dye molecules toward proximity with the adsorbent surface, as juxtaposed with their initial configurations (not depicted here), serves as a compelling indicator of the inherent predilection of AO6 and AY36 molecules for binding onto the aqueous facet of TiO_2. Remarkably, the rutile surface showcases an elevated degree of responsiveness throughout the adsorption involving the AY36 molecule, a contrast to the behaviour exhibited by the AO6 molecule. In Fig. 21, the most favourable adsorption conformations following MD optimization for AY36@TiO_2 and AO6@TiO_2 are vividly portrayed. Detailed scrutiny of the MD-driven adsorption arrangements

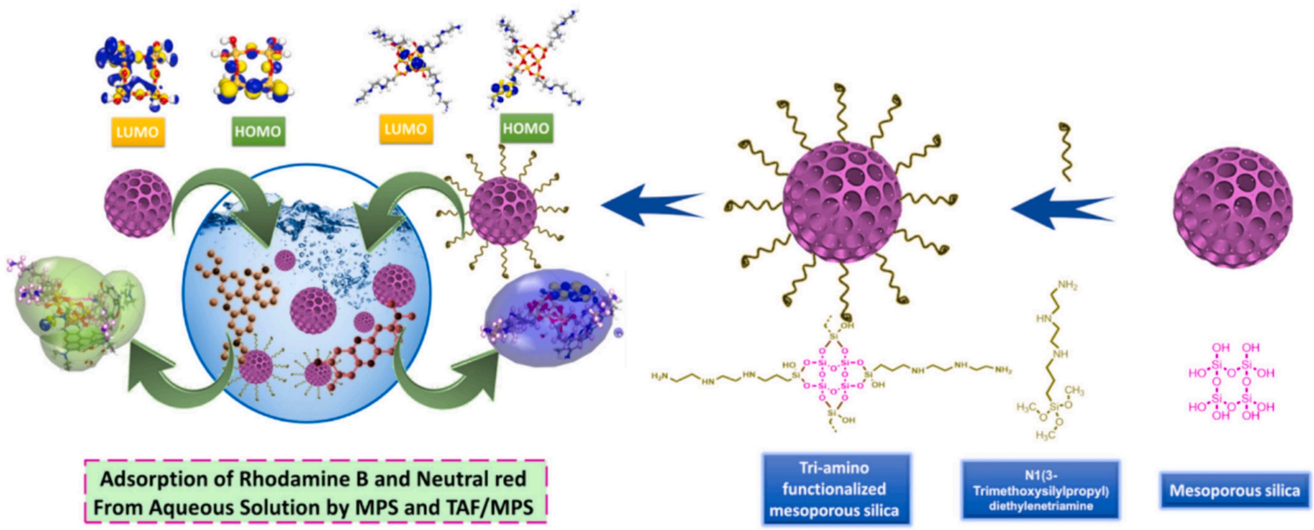

Fig. 23. The schematic representation of the formation of ATP/MPS and analysis using QM calculations [134].

reveals substantial alterations in the molecular architecture, a direct outcome of the comprehensive MD simulations. The dye molecules exhibit a noteworthy migration toward proximity with the rutile surface, adopting a parallel alignment that emerges as the optimal orientation for organic moieties interacting with solid substrates. Within this parallel adsorption arrangement, a robust potential for chemicophysical interactions between the active sites of the dyes and the rutile atoms is inherently established [219].

4.3. Mixing dyes

Various studies have explored the adsorption of cationic and anionic dyes using molecular simulations [220]. Chanajaree et al. investigated the removal of cationic (Malachite Green) and anionic (Indigo Carmine) dyes using cross-linked chitosan (CSglu) beads through both experimental and computational methods. Their experiments on adsorption isotherms, kinetics, and thermodynamics showed a strong correlation with computational studies regarding structures and binding energies (ΔE_B). MD simulations were conducted to understand the interaction between the dyes and CSglu at the atomic level. These simulations revealed that Malachite Green binds more favourably to CSglu than Indigo Carmine due to Malachite Green's complementary molecular electrostatic potential (MEP) with the CSglu surface. QM calculations using DFT with various levels and basis set superposition error (BSSE) corrections were employed to calculate ΔE_B. These calculations effectively predicted the adsorption capabilities of both cationic and anionic dyes on cross-linked chitosan, reinforcing the experimental findings [221].

Largo et al. scrutinized the adsorptive elimination of dyes, encompassing both cationic and anionic varieties. This exploration employed an adsorbent based on sepiolite clay and was approached through experimental analysis and MD simulation studies. Fig. 22 visually presents the definitive equilibrium adsorption configurations of both DR-23 and MB entities at the adsorbent's surface under both acidity and alkalinity conditions. Upon analyzing the completed adsorption configurations, it becomes evident that the investigated dye molecules are situated close to the surface of sepiolite, underscoring their propensity for adsorption across both acidic and alkaline environments [222].

A study by V.E. Sathishkumar et al. used machine learning techniques to assess the effectiveness of a catalyst PdO-NiO in reducing harmful nitrophenols and azo dyes from drinking water. The catalyst was used to purify water from contaminants like 4-nitrophenol, 2,4-dinitrophenol, 2,4,6-trinitrophenol, methylene blue, Rhodamine B, and Methyl Orange. The effectiveness of these algorithms was evaluated using RMSE, MAE, and MAGE. The XGB algorithm outperformed others in predicting catalytic activity for NP and DNP, while RF excelled with TNP, MB, and RHB, and SVM demonstrated superior performance with MO. The PdO-NiO bimetallic catalyst showed a remarkable 98% reduction efficiency of the azo compounds mixture within 8 min, making it a highly efficient catalyst suitable for real-site applications [223].

In an investigation, Rajjak Shaikh et al. simulated methylene blue, methyl orange, and bromophenol blue adsorption performances using asphaltene and its modified form. The QM computations were performed to comprehend the characteristics and potency of the interactions between the dyes and asphaltene. This exploration also encompassed the assessment of binding energy, electrostatic potential, frontiers of molecular orbitals, and noncovalent interactions. The DFT analyses validated the experimental discovery that the functionalized version of asphaltene (FASP) is a more effective adsorbent for the dyes than the unmodified asphaltene [224].

M. BinMakhashen et al. devised a highly promising adsorbent by combining polyethyleneimine, graphene oxide, bentonite, and MgFeAl-layered triple hydroxide (MgFeAl-LTH). They evaluated its ability to adsorb methyl orange (MO) and crystal violet (CV) through both experimental testing and machine learning analyses. The nanocomposite surpassed its individual components, achieving maximum adsorption capacities of 1666.7 mg/g for MO and 12 50.0 mg/g for CV. Furthermore, it demonstrated excellent reusability, maintaining high performance even after multiple uses. The gathered data served as the foundation for developing ensemble meta-machine learning techniques aimed at cost-effective simulation and prediction of the adsorption process. Among these techniques, the Extra Trees model stood out, boasting a remarkable 99% correlation coefficient along with low computed RMSE and MAE errors. These findings underscore the robust capability of the Extra Trees model in accurately simulating and predicting the adsorption process, highlighting its potential for practical applications [225].

In the investigative work led by Yan Cao et al., the central thrust was directed toward an in-depth exploration of the adsorption tendencies exhibited by a pair of cationic dyes, specifically rhodamine B (RB) and neutral red (NR), upon both neat and amino-functionalized mesoporous silica. This study's analytical foundation rests upon applying QM calculations, vividly illustrated in Fig. 23. Distinct interactions during adsorption were discerned through quantum calculations. Theoretical investigations yielded valuable insights into the particular significance of amino functionalization. A comparison of quantum molecular

Table 6
The research conducted in the field of dye adsorption using computational approaches such as MD, MC and QM.

Adsorbent	Dye	Sofware	Properties	Ref
Molecular dynamics (MD)				
Neat and functionalized asphaltene	Methyl orange, methylene blue, bromophenol blue	GROMACS 2018	The interaction energy between dye and adsorbent	[224]
Aerated NaOH and HNO_3 corrosion of iron	Bis–azo dye derivatives	Materials Studio		[229]
Silk fibroin-g- Chitosan	Laccaic acids A and B	GROMACs V5.1.4	Binding energies	[230]
Superb organo-montmorillonite	Orange G	Materials Studio 6.0		[231]
graphene nanosheet	Azo Dye	DL_POLY 2.17	Structural and Transport Properties	[232]
Synthesized GO-Cu-MOF	Methylene blue	Materials Studio 6.0	The intermolecular interaction,	[233]
Cellulose's hydrophobic surface	Congo red	Materials Studio 5.5	Gas-phase and aqueous adsorption processes	[234]
$CoFe_2O_4$/graphene oxide	Methyl orange, rhodamine B, methylene blue	Materials Studio	Adsorption mechanism	[235]
Activated carbon/montmorillonite	Crystal violet, methylene blue	Materials Studio 6.0	Adsorption process, Radial distribution function (RDF)	[126]
Organo-bentonite	Methylene blue	Materials Studio 2017	Adsorption geometry and interaction energies	[236]
Metal fluorides	Malachite green	Materials Studio 8.0	Interfacial adsorption	[237]
sodium dodecyl sulfate micelles.	Sulforhodamine B	GROMACS 4.0		[238]
Agricultural Algerian olive cake waste	Acid Blue 80	Materials Studio 2017	Adsorption dynamics	[239]
polyaniline	Mordant Black 11	Materials Studio		[240]
Graphene oxide	Methyl blue	GROMACS		[241]
Mesoporous carbon	Methyl orange, methylene blue	Materials Studio	Adsorption behaviour	[242]
Cadmium(II) and Zinc(II) coordination polymers	Methylene blue	Materials Studio 8.0	The interaction energy between dye and adsorbent	[243]
Functionalized Au Nanoparticle	dye anions	NAMD 2.12	The radial distributions, Adsorption behaviour	[244]
Graphene oxide	Methylene blue	Material Studio	The interaction energy between dye and adsorbent	[245]
Polysulfone/polyetherimide	Basic Red 1, reactive blue 171		Fractional free volume (FFV), Dyes diffusion	[246]
TiO_2 hydroxylated	Rhodamine laser	GULP code	Adsorption dynamics	[247]
Liposome Surfaces	malachite green	GROMACS	Molecular orientation distributions	[248]
Bituminous Coal	Methylene blue	Materials Studio 8.0	Interaction Energies, Water Molecule's Mobility	[249]
Cross-linked chitosan	Indigo carmine, Malachite Green	DLPOLY 4.08	The adsorption and structural properties	[221]
Nanocellulose	Victoria Blue B	Amsterdam Density Functional (ADF)/ReaxFF	Adsorption characteristics	[250]
Graphitic carbon nitride (g-C3N4)	Methyl orange, methylene blue		The adsorption mechanism	[19]
chitosan/polyvinyl alcohol/ functionalized ZIF-8	Reactive green 19	Materials Studio	Binding energies	[251]
g-C3N4 Surface	Rhodamine B		The adsorption and structural properties	[252]
Micelles	Reichardt's dye	GROMACS 5	Adsorption characteristics	[253]
H-PVDF@ZnO/Ag	Methylene blue	Materials Studio 8.0	MB adsorption behaviour	[254]
Cetyltrimethylammonium bromide	reactive red	YASARA dynamics	The interaction energy between dye and adsorbent	[255]
Au/Cu_2O	Rhodamine B, Methyl blue, Methyl orange, Congo red	Materials Studio	Dye adsorption behaviour	[256]
Pepsin	Naphthol Yellow S	Gromacs 5.7.1	Stability, flexibility, conformational changes, structural properties	[257]
PES/SPSf	methyl red, acid blue 25, methyl orange	GROMACS	Dye hydration radius	[258]
Carboxymethyl-chitosan-montmorillonite	Congo red	Materials Studio	Dye adsorption behaviour	[259]
Graphene oxide/methylene blue	rhodamine B, disperse black 9, methyl orange	GROMACS	Interfacial behaviours	[260]
Monte Carlo (MC)				
Chitosan	Eriochrome Black T		Energy adsorption configuration, Chitosan-dye interaction mechanism	[261]
Neat and amino-functionalized silica	Rhodamine B, Neutral Red		The different configuration's adsorption energy	[134]
synthesized GO-Cu-MOF	Methylene blu			[233]
Diamino-functionalized hollow mesosilica	Crystal Violet, Neutral Red		Energy adsorption configuration	[262]
graphene and graphene oxide	Rhodamine B, Methylene blue	Adsorption Locator modules of Materials Studio		[197]
GO-Fe3O4				[263]
Polymeric[Pb4(Ben)2(H_2O)]	Methyl red			[264]
bismuth oxy-bromide kaolinite BiOBr@Kaol	Rhodamine B dye		Adsorption Energy	[265]
Carbonized activated bagasse	Crystal-violet			[266]
Zeolite 4 A	Methylene blue			[267]
Quantum mechanics (QM)				
Chitosan	Eriochrome Black T	Gaussian 09	Frontier molecular orbitals (FMO), dipole moment (μ), Mulliken charges, the fraction of electrons transferred (ΔN), Natural bond orbital (NBO), Fukui functions	[261]
ZnO and TiO_2 surfaces	Organic azo dyes	Material Studio	Fukui indices analysis, Frontier molecular orbitals (FMO)	[157]
Aerated NaOH and HNO_3 corrosion of iron	Bis–azo dye derivatives	Gaussian 09, Gauss View 5.0.8,	the dipole moment (μ), Frontier molecular orbitals (FMO), electrons transferred (ΔN)	[229]

(*continued on next page*)

Table 6 (*continued*)

Adsorbent	Dye	Sofware	Properties	Ref
Chitin surface	Eriochrome Black T	Gaussian 09	ΔNmax (charge transfer capability), FMO (frontier molecular orbital)	[218]
Neat and carboxylic acid-MIL-53 (Al)	rhodamine B (RB) and methylene blue (MB)	Multiwfn_3.8, Avogadro, Gaussian 16, GaussView 6	FMO (frontier molecular orbital), Sigma profiles (COSMO analysis)	[123]
Amide-MIL-53 (Al)	Six cationic dyes			[147]
TiO_2 in two forms, brookite and rutile	Methylene blue	Gaussian 09 W	Natural bond orbital, FMO (frontier molecular orbital)	[201]
TiO_2	A-D(π)-A organic dye		Frontier molecular orbitals, an Absorption spectrum, Dye aggregation	[268]
diamino-functionalized hollow mesosilica	Crystal Violet, Neutral Red	Materials Studio	FMO (frontier molecular orbital), Sigma profiles (COSMO analysis)	[262]
Metal fluorides	Malachite green	Gaussian 09 W	Natural bond orbital, FMO (frontier molecular orbital)	[237]
Surfactants: nonionic Tx 100, cationic CTAB, anionic SDS	rhodamine 6G		Surfactant interactions at low concentrations (premicellar)	[269]
Agricultural Algerian olive cake waste	Acid Blue 80	Materials studio	FMO (frontier molecular orbital)	[239]
polyaniline	Mordant Black 11	Gaussian 09 W	Fukui indices analysis, Frontier molecular orbitals (FMO)	[240]
Polymeric[$Pb_4(Ben)_2(H_2O)$]	Methyl red	Gaussian16, Gauss View 6.0	the frontier molecular orbital (FMO), quantum chemical descriptors	[264]
sludge derived activated carbon	Methyl Violet, Food Red 17	Materials studio	chemical reactivity descriptors, interaction parameters	[228]
Cross-linked chitosan	Indigo carmine, Malachite Green	ORCA	Binding energies	[221]
Fe (110)	Mono-azo dye derivatives	Gaussian 9.0, Gauss View 5.0.8	The frontier molecular orbital (FMO), quantum chemical descriptors	[270]
TiO_2 anatase (101)	D102 Indoline Dye	Amsterdam Density Functional (ADF)	dye-dye interactions	[271]
Zeolite 4 A	Methylene blue	Gaussian	The frontier molecular orbital (FMO), quantum chemical descriptors	[267]
Anthocyanins from blueberry waste	Natural dyes	Gaussian16	dye-adsorbent interactions	[272]
Fly ash/inorganic polymer	Rhodamine B	Gaussian 09	Natural bond orbital, FMO (frontier molecular orbital)	[273]

descriptors revealed the heightened reactivity of the functionalized adsorbent conformation when contrasted with neat adsorbent [134].

M. Khnifira et al. conducted a study on the adsorption interaction of synthetic dyes, methyl blue (MeB) and methyl orange (MeO), with commercial activated carbon (CAC) surfaces in various mediums. They used molecular dynamic simulations and density functional theory (DFT) calculations to investigate the adsorption mechanisms of these dyes. The results showed that the adsorption of both dyes followed the Langmuir isotherm, with maximum adsorption capacities of 229.89 mg/g and 312.39 mg/g, respectively. The study also revealed that the molecular structure's influence on electron donating/accepting ability determines adsorption potential trends. MD simulations identified the most suitable adsorption configurations of MeB and MeO molecules. The study can serve as a reference for researchers investigating using CAC adsorbent in water contamination treatment [226].

Various studies have explored the adsorption of cationic and anionic dyes using molecular simulations. Aguiar et al. found that anionic dyes were more effectively adsorbed than cationic dyes on non-calcined Mg—Al layered double hydroxide (LDH). This study synthesized Mg—Al LDH and investigated its sorption capabilities for both types of dyes, showing different behaviours based on pH and dye type, with anionic dyes being more effectively adsorbed. The Langmuir-Freundlich model described the equilibrium data well, and the adsorption mechanism was evaluated using the Monte Carlo approach [227].

Benabid et al. used molecular simulations to demonstrate that Methyl Violet (MV) was more efficiently adsorbed than Food Red 17 (FR17) on sludge-derived activated carbon (SDAC). The study examined the adsorption of both dyes onto SDAC, with experimental and molecular simulation analyses revealing that MV was more efficiently adsorbed on SDAC despite FR17 showing better affinity. These studies collectively highlight the potential of molecular simulations in understanding and predicting the adsorption behaviour of cationic and anionic dyes [228]. These studies collectively highlight the potential of molecular simulations in understanding and predicting the adsorption behaviour of cationic and anionic dyes.

Table 6 serves as a visual representation showing a compendium of scientific activities in the vast landscape of dye adsorption research. In particular, these efforts are supported by the strategic use of computational methods, including the intricate realms of MD simulation, MC simulations, and the complicated principles of QM.

5. Future perspectives and challenges

5.1. Current gaps and challenges

Researchers face several gaps and challenges in the field of computational studies of dye pollutant adsorption. These challenges can affect computational models' accuracy, reliability, and applicability. The lack of comprehensive and high-quality experimental data on the adsorption of various dye pollutants can hinder the development and validation of computational models. Accurate experimental data are essential for parameterization and validation of these models. Validation and verification of computational models for dye adsorption can be challenging due to the complexity of real systems. Adequate experimental validation is often difficult, especially considering the variety of dye structures, solution conditions, and adsorbents. Quantifying uncertainties associated with computational predictions is essential for evaluating the reliability of results. However, robust methods for quantifying uncertainties in adsorption simulations, including uncertainties in force fields, parameter selection, and simulation conditions, are still under development. Adsorption processes occur on multiple length and time scales, from atomic interactions to macroscopic behaviour. Integrating information and modelling techniques across these scales (multiscale modelling) to capture the entire adsorption process is challenging and requires careful balancing of accuracy and computational efficiency. Many adsorbents used for dye adsorption, such as porous materials, exhibit heterogeneous structures at different scales. Accurately capturing this heterogeneity in computational models is complex and often requires specialised techniques, such as advanced sampling techniques and coarse-grained modelling. In many adsorption scenarios, multiple dye molecules may interact on the surface of the adsorbent. Accurate modelling of these interactions requires special treatment beyond standard single-molecule adsorption models, especially for dye-solid interactions. Adsorbents, especially porous materials, can exhibit flexibility and structural changes upon adsorption. Accurate modelling of such structural changes requires advanced techniques that capture both the dynamics of the interactions between adsorbate and adsorbent and the changes in the structure of the adsorbent. Realistic simulations can be very computationally intensive, especially when considering realistic system sizes and time scales. Balancing accuracy and computational efficiency is challenging, especially for large-scale and long-term simulations. The chemical composition of the solution, including pH, ionic strength, and other solutes, can significantly affect adsorption behaviour. Integrating realistic solution conditions into computational models increases complexity and requires an accurate description of solvent-solute interactions. A wide range of adsorbent materials can be used for dye adsorption, each with its own characteristics. Developing generalised models that accurately predict the adsorption behaviour of different materials is challenging and requires an understanding of material-specific properties.

Addressing these gaps and challenges requires interdisciplinary collaboration among chemistry, materials science, physics, computer science, and engineering researchers. Advances in experimental techniques and computational methods can help overcome these challenges and produce more accurate and reliable computational studies of dye pollutant adsorption.

5.2. Suggest possible directions and strategies for future research and development

Several exciting directions and strategies may guide future research and development in computational studies of dye pollutant adsorption. Researchers can explore the design of novel adsorbent materials with tailored properties for efficient dye adsorption. This includes designing materials with increased surface area, specific functional groups, and adjustable pore sizes to optimize adsorption performance. The development of advanced multiscale modelling techniques can bridge the gap between molecular-level interactions and macroscopic adsorption behaviour. This involves the integration of molecular dynamics, continuum models, and other methods to capture the full range of adsorption phenomena. Considering the role of solvents and solvent conditions in computational models can lead to a more realistic representation of the adsorption process. This includes consideration of solvent-solution interactions, ionic strength, and pH effects. The study of novel adsorption materials, such as metal-organic frameworks (MOFs), covalent organic frameworks (COFs), and nanomaterials, holds potential for high-performance adsorption due to their unique properties and tunability. Collaborations between experimentalists and computational researchers can provide a holistic approach to understanding dye adsorption. Experimental data can guide and validate computational models, while computational insights can help interpret experimental results. Developing environmentally friendly adsorption processes that minimize energy consumption and waste generation is critical. Computational tools can support the design of sustainable adsorption systems and materials. Advances in modelling adsorbate-adsorbate interactions, such as dye-dye interactions, can accurately represent adsorption behaviour in complex systems. Exploring improved sampling methods, such as metadynamics and replica exchange, can help overcome energy barriers and accelerate the exploration of different adsorption configurations. Establishing iterative workflows that combine computational predictions and experimental testing can lead to rapid development and optimization of adsorption processes. By following these directions and strategies, researchers can improve our understanding of dye pollutant adsorption, design more effective adsorption materials, and contribute to sustainable solutions for water treatment and environmental remediation.

6. Conclusions

This review article explores the removal of dye impurities through adsorption processes, focusing on various adsorbents used in wastewater treatment. It evaluates key factors affecting adsorption performance, such as surface properties, pore characteristics, chemical composition, functional groups, and metal ions. The advantages and disadvantages of each adsorption type are considered, considering factors like availability, cost, stability, reusability, and environmental impact. The article also discusses the role of computational methods such as molecular dynamics (MD) simulations, Monte Carlo (MC) simulations, quantum mechanics (QM) calculations, and machine learning (ML) methods in improving the understanding of dye pollutant adsorption. It provides comparative assessments of these methods regarding accuracy, efficiency, scalability, and practicality. The review includes a detailed analysis of the results of various computational methods, including adsorption energies, capacities, mechanisms, and selectivities. The article identifies gaps, challenges, and future directions in the computational study of dye pollutant adsorption, looking at innovative adsorbents, hybrid computational systems, machine learning, and collaborative efforts as possible ways to advance the field. The transformative potential of computational methods is highlighted, providing practical recommendations for researchers, practitioners, policymakers, and stakeholders involved in removing dye pollutants through adsorption processes. These methods provide valuable insights into the complex interactions between dye molecules and adsorbent materials, aiding in developing efficient and sustainable adsorption processes.

CRediT authorship contribution statement

Iman Salahshoori: Conceptualization, Formal analysis, Investigation, Methodology, Supervision, Writing – original draft. **Qilin Wang:** Writing – review & editing. **Marcos A.L. Nobre:** Formal analysis, Investigation, Methodology. **Amir H. Mohammadi:** Formal analysis, Supervision, Writing – review & editing. **Elmuez A. Dawi:** Writing – review & editing. **Hossein Ali Khonakdar:** Writing – review & editing.

Declaration of generative AI and AI-assisted technologies in the writing process

During the preparation of this work, the author(s) used [ChatGPT/OpenAI, Elicit, ConnectedPapers, MicrosoftBeing, GoogleBard] to optimize, integrate, and summarise the text. After using this tool/service, the author(s) reviewed and edited the content as needed and take(s) full responsibility for the publication's content.

Declaration of competing interest

All authors state that there is no conflict of interest.

Data availability

Data will be made available on request.

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