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MECHANISTIC INSIGHTS INTO THE CHEMISORPTION OF INDUSTRIAL DYES ON TI_3C_2 MXENE SURFACE FOR WASTE WATER TREATMENT APPLICATION: A THEORETICAL APPROACH

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The discharge of azo dyes from industrial effluents poses serious environmental and health risks due to their persistence and resistance to biodegradation. Hydroxyl-functionalized $Ti_3C_2(OH)_2$ MXenes have emerged as promising adsorbents due to their large surface area, hydrophilicity, and versatile surface chemistry. In this study, we employed Monte Carlo and molecular dynamics simulations to investigate the adsorption behavior of four industrial dyes—Congo Red (CR), Methylene Blue (MB), Direct Black 1 (DBk), and Direct Blue 38 (DBu)—on $Ti_3C_2(OH)_2$ MXene surfaces.

Monte Carlo adsorption locator results showed that CR exhibited the most favorable static adsorption energy (–182.346 kcal/mol), followed by DBu (–46.576 kcal/mol), DBk (–23.994 kcal/mol), and MB (–16.35 kcal/mol). Notably, the deformation energy of CR was –151.353 kcal/mol, indicating strong chemisorption due to significant molecular reorganization. Molecular dynamics simulations in aqueous media further validated these trends, with DBu showing the highest dynamic adsorption energy (–1676.365 kcal/mol), followed by DBk (–1348.604 kcal/mol), CR (–1157.238 kcal/mol), and MB (–895.651 kcal/mol). The binding energies reflected a similar order, confirming that strong π–π stacking, hydrogen bonding, and surface-induced reorientation were dominant interaction mechanisms.

These findings provide molecular-level insight into the structure–function relationship governing dye–MXene adsorption and highlight $Ti_3C_2(OH)_2$ MXene as an effective material for selective and sustainable dye removal in wastewater treatment.

Keywords: Azo dyes, Ti_3C_2 MXene, Adsorption energy, Chemisorption, Molecular dynamics, Wastewater remediation.

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INTRODUCTION

The rampant discharge of synthetic dyes from textile and allied industries poses a serious environmental threat due to their toxicity, persistence, and non-biodegradability. Among various pollutants, azo dyes represent a major class of contaminants that severely degrade water quality and disrupt aquatic ecosystems [1]. The direct discharge of untreated or inadequately treated dye-laden effluents into water bodies leads to reduced light penetration, altered photosynthetic activity, and exerts significant toxicity on aquatic organisms and human health. As traditional wastewater treatment methods often fall short in removing these complex organic molecules effectively, the search for advanced adsorbent materials has become imperative [2].

Adsorption has been widely recognized as one of the most effective techniques for dye removal due to its simplicity, low operational cost, and ability to target a wide range of pollutants without generating secondary waste [3]. However, the success of this method largely depends on the nature of the adsorbent material. Traditional adsorbents such as activated carbon, clays, and zeolites, while effective to some extent, often face limitations such as low selectivity, poor regeneration capability, and high production costs. These shortcomings have spurred the search for next-generation adsorbent materials with superior performance characteristics [4,5].

Recently, MXenes, a family of two-dimensional transition metal carbides and nitrides, have attracted immense attention as novel nanomaterials for environmental remediation applications. Owing to their exceptional surface area, hydrophilic nature, layered structure, and tunable surface chemistry, MXenes exhibit strong potential for the adsorption and removal of various pollutants, including dyes, from aqueous environments [6]. Particularly, Ti_3C_2-based MXenes, functionalized with surface hydroxyl, oxygen, or fluorine groups, offer reactive sites capable of engaging in strong electrostatic, hydrogen bonding, and π–π interactions with organic pollutants. Their lamellar structure and exposed functional groups make them promising candidates for the selective and high-capacity adsorption of dye molecules [7,8].

Despite encouraging experimental findings, a fundamental understanding of the molecular-level interactions between MXenes and complex dye molecules remains limited. To bridge this knowledge gap, computational modeling techniques provide an invaluable tool. By simulating the adsorption process under controlled conditions, computational methods can offer detailed insights into adsorption energies, binding configurations, charge distributions, and the influence of molecular structure on adsorption efficiency [9,10].

In this study, we conduct a theoretical investigation of the interaction mechanisms between $T_{i3}C_2OH)_2$ MXene and four representative industrial azo dyes: Congo Red (CR), Methylene Blue (MB), Direct Black 1 (DBk), and Direct Blue 38 (DBu). These dyes were selected based on their widespread industrial usage and varying structural, electronic, and functional characteristics. By using Monte Carlo-based adsorption locator simulations and molecular dynamics (MD) modeling, we analyze key parameters such as adsorption energy, deformation energy, and binding configurations to evaluate the strength and spontaneity of dye adsorption on the MXene surface. Additionally, solvent effects are considered through the inclusion of water molecules in the simulation box to mimic realistic aqueous conditions.

The results not only provide comparative insights into the adsorption potential of various dye molecules but also reveal the role of functional groups, molecular geometry, and electronic structure in determining adsorption efficiency. This study contributes to the rational design and optimization of MXene-based materials for sustainable wastewater treatment technologies.

COMPUTATIONAL METHOD

To investigate the adsorption behavior of industrial azo dyes on the $Ti_3C_2(OH)_2$ MXene surface, a series of computational simulations was performed using BIOVIA Materials Studio (Versions 7.0 and 8.0) [11]. The crystal structure of Ti_3C_2 MXene (100 surface orientation) was obtained from the Materials Project database and processed using the Materials Studio interface. Similarly, molecular structures of the selected dyes—Congo Red, Methylene Blue, Direct Blue 38, and Direct Black 1—were downloaded from the Materials Explorer database and geometry-optimized using the Universal Force Field (UFF) [12,13]. The structures of MXene (Fig. 1) and the four industrial dyes are shown in Fig. 2. Initial geometry optimization was conducted to minimize the total energy of each system and ensure a stable configuration. During this process, atomic positions were iteratively adjusted until the system reached a local minimum on the potential energy surface. Following successful optimization, a simulation box was constructed containing the MXene (100) slab, individual dye molecules, and water molecules to mimic aqueous environmental conditions [14].

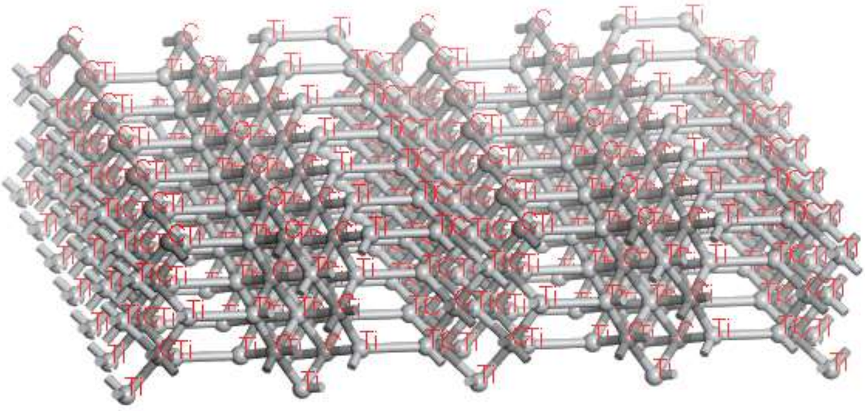
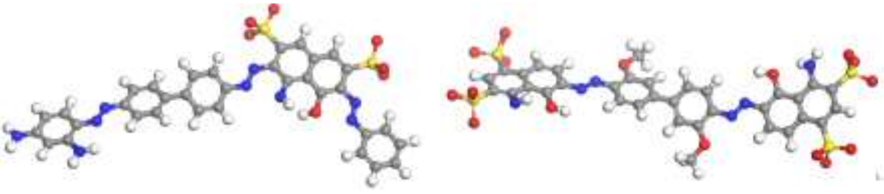


Figure 1. 3D structure of Ti3C2-based MXene

Methylene Blue
(MB)

Congo Red
(CR)



Direct Black
(DBk)

Direct Blue
(DBu)

Figure 2. 3D Structure of Industrial Dyes

Monte Carlo adsorption locator simulations

To investigate the adsorption characteristics of the selected azo dyes on the $Ti_3C_2(OH)_2$ MXene surface, Monte Carlo-based adsorption locator simulations were employed using the Adsorption Locator module in BIOVIA Materials Studio. This module systematically searches for energetically favorable configurations by sampling various orientations and positions of dye molecules relative to the MXene surface. Each dye—Congo Red, Methylene Blue, Direct Blue 38, and Direct Black 1—was modeled in the presence of the MXene (100) crystal surface, and their interaction configurations were evaluated under periodic boundary conditions. The Universal Force Field (UFF) was applied to optimize each structure, ensuring that both the adsorbent and adsorbate reached a minimum energy configuration. Key energetic parameters were calculated, including total system energy, adsorption energy (E_{ads}), rigid adsorption energy, and deformation energy, as well as the adsorption energy per molecule (dE_{ads}/dN_i). These values provided quantitative insights into the strength and spontaneity of dye adsorption. The simulation results revealed the most stable binding configurations for each dye molecule and allowed for a comparative analysis of their affinities towards the MXene surface. This computational approach served as a critical foundation for understanding the adsorption mechanism and guiding subsequent molecular dynamics studies.

Molecular dynamics simulations

To further validate the adsorption behavior and assess the dynamic stability of dye–MXene complexes in aqueous environments, molecular dynamics (MD) simulations were performed using the Forcite module in BIOVIA Materials Studio (Version 8.0). The simulations were carried out under an NPT ensemble at 298 K and 1 atm pressure to mimic standard ambient conditions. Each system included a geometry-optimized $Ti_3C_2(OH)_2$ MXene (100) slab, a selected dye molecule (Congo Red, Methylene Blue, Direct Blue 38, or Direct Black 1), and water molecules within a periodic simulation box measuring 18.0 Å × 30.23 Å × 25.08 Å.

A time step of 1.0 femtosecond (fs) was used, and each system was simulated for 300 picoseconds (ps) to allow sufficient equilibration and conformational sampling. Berendsen thermostat and barostat were employed to regulate temperature and pressure, respectively. Long-range electrostatic interactions were computed using the Ewald summation method with an accuracy of 1×10^{-5} kcal mol^{-1}, while van der Waals interactions were treated with the same level of precision. Q_{eq} charge equilibration was utilized to compute partial atomic charges dynamically throughout the simulation [15,16]. The main objective of these MD simulations was to evaluate the adsorption energy, binding energy, and radial distribution functions (RDFs) of the dye molecules relative to the MXene surface [9]. These metrics provided quantitative and structural insights into the degree of physical versus chemical adsorption. RDF analysis, in particular, was used to estimate the most probable separation distances between dye atoms and MXene surface atoms, calculated using the following equation (1):

$$g_{xy}(r) = \frac{\rho_y(r)}{\rho_y} \quad (1)$$

Where:

- $\rho_y(r)$= local density of atoms of species Y at distance r from species X
- ρ_y = average density of species Y over the entire volume

RESULTS AND DISCUSSION

Adsorption locator studies

The adsorption behavior of the four industrial azo dyes—Methylene Blue, Congo Red, Direct Black 1, and Direct Blue 38—on the $Ti_3C_2(OH)_2$ MXene surface was investigated using the Adsorption Locator module in Materials Studio. The simulation identified the most energetically favorable dye orientations and adsorption sites on the MXene (100) surface using c vvbg a Monte Carlo algorithm. For each dye, the most stable configuration was selected and visualized (Fig. 3-6), and the corresponding adsorption energy parameters were recorded (Table 1). The total energy, adsorption energy (Eads), rigid adsorption energy, and deformation energy were calculated for each dye-MXene system, offering valuable insights into the strength and nature of interactions.

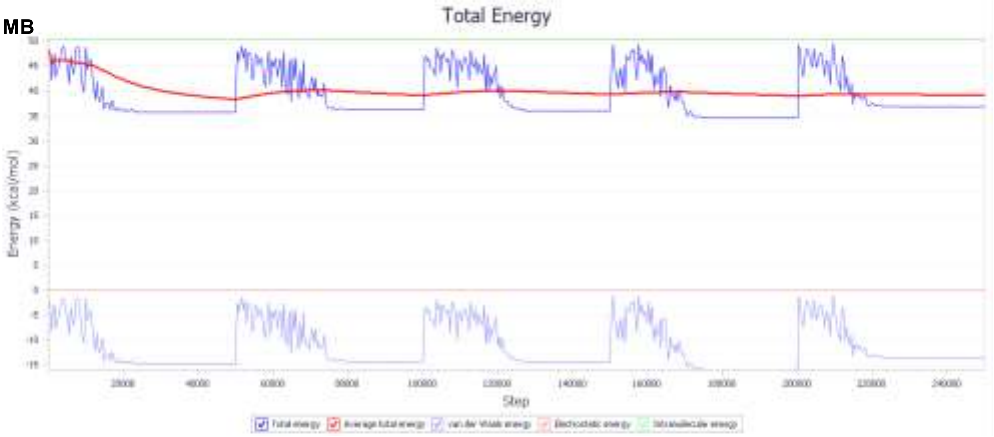


Figure 3. Total energy Monte Carlo adsorption Locator Simulations of Methylene Blue (MB)

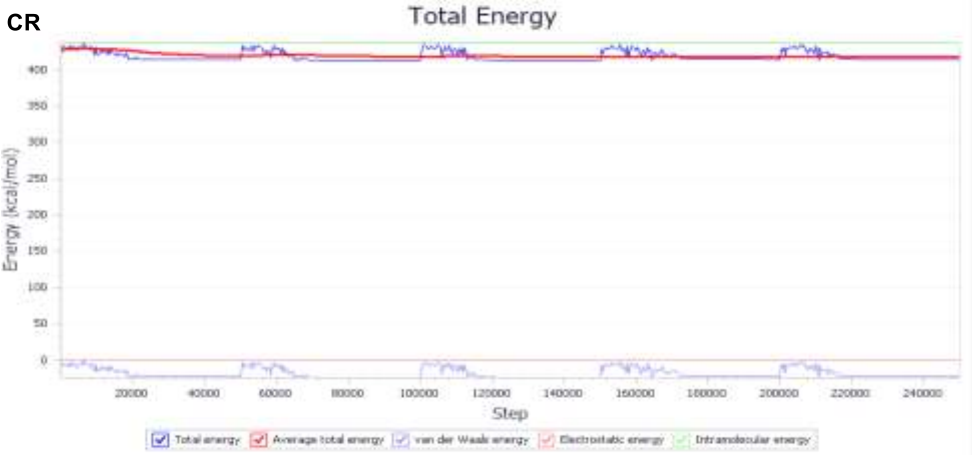


Figure 4. Total energy Monte Carlo adsorption Locator Simulations of Congo Red (CR)

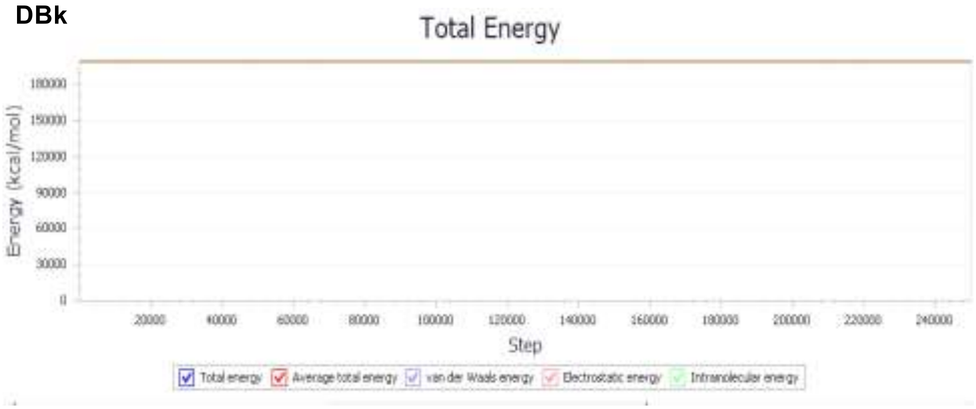


Figure 5. Total energy Monte Carlo adsorption Locator Simulations of Direct Black (DBk)

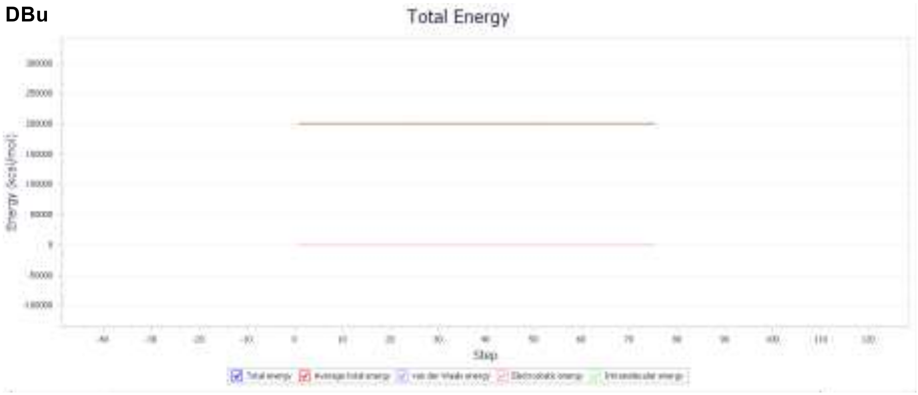


Figure 6. Total energy Monte Carlo adsorption Locator Simulations of Direct Blue (DBu)

Table 1. Adsorption Energy Parameters of Azo Dyes on $Ti_3C_2(OH)_2$ MXene Surface from Monte Carlo Adsorption Locator Simulations

Structure	**Total energy**	**Adsorption energy**	**Rigid adsorption energy**	**Deformation energy**	**dE_{ad}/dN_i**
MB	34.2	-16.35	-16.578	0.230	-16.348
CR	254.138	-22.346	-30.993	-23.353	-22.346
DBk	266.066	-23.994	-33.014	-23.993	-23.993
DBu	477.271	-46.576	-33.839	-46.578	-46.576

Methylene Blue (MB)

The adsorption of Methylene Blue (MB) on $Ti_3C_2(OH)_2$ MXene, as illustrated in Figure 3 and Table 1, revealed the weakest interaction among the four studied dyes, with an adsorption energy of –16.35 kcal/mol. MB is a relatively small, planar cationic dye containing a thiazine ring system and minimal polar functional groups. Its limited π-conjugation and lack of strongly electron-donating or withdrawing groups reduce its ability to interact strongly with the MXene surface. The deformation energy for MB is the lowest (only +0.230 kcal/mol), indicating negligible structural rearrangement upon adsorption, which is characteristic of physisorption. This weak van der Waals forces and possible limited hydrogen bonding explain its low affinity toward $Ti_3C_2(OH)_2$, confirming that MB primarily relies on surface contact rather than strong chemical interaction mechanisms.

Congo Red (CR)

Congo Red (CR) exhibited the most favorable adsorption parameters among all dyes, with a highly negative adsorption energy of –182.346 kcal/mol, as shown in Figure 4 and Table 1. CR contains two azo groups linking aromatic systems, along with two sulfonic acid groups ($–SO_3H$), which greatly enhance its hydrophilicity and ability to form hydrogen bonds. Additionally, its large, delocalized π-system promotes strong π–π stacking with the planar MXene layers. The deformation energy (–151.353 kcal/mol) is notably high, indicating significant molecular rearrangement and reorientation to optimize interaction with the surface—strong evidence of chemisorption. The combined effect of π-conjugation, polar functionalities, and structural flexibility allows CR to anchor tightly to the hydroxylated MXene, making it the most effective dye in this adsorption study.

Direct Black 1 (DBk)

Direct Black 1 (DBk) demonstrated intermediate adsorption strength on $Ti_3C_2(OH)_2$ MXene, with an adsorption energy of –23.994 kcal/mol, as shown in Figure 5. DBk contains azo linkages and sulfonic acid groups like CR, but with a more compact and sterically hindered molecular framework. While it does possess multiple aromatic rings, the spatial arrangement of its functional groups may restrict optimal orientation and surface contact, thus reducing overall interaction strength. The deformation energy (–23.993 kcal/mol) is relatively moderate, indicating a partial chemisorptive character, though less intense than that of CR. This suggests that DBk interacts with the MXene surface via a combination of electrostatic interactions, hydrogen bonding, and limited π–π stacking, but the overall binding is weaker due to molecular bulk and orientation constraints.

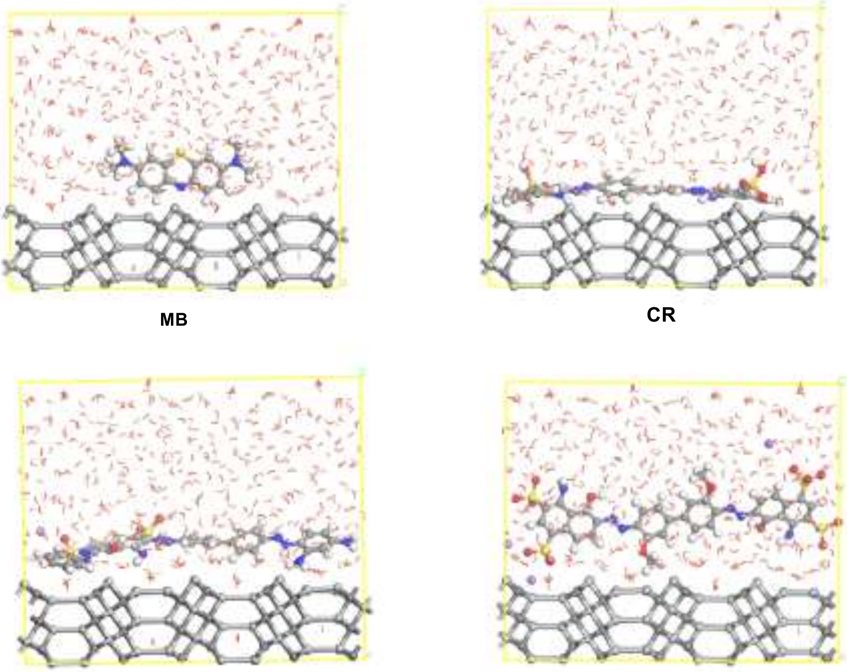
Direct Blue 38 (DBu)

Direct Blue 38 (DBu), as presented in Figure 6, displayed the second strongest interaction with the MXene surface, following CR, with an adsorption energy of –46.576 kcal/mol. DBu is a large dye molecule containing multiple aromatic rings, sulfonic acid groups, and azo linkages. These structural features enable strong π–π interactions and hydrogen bonding with the hydroxyl-terminated MXene. Interestingly, its deformation energy (–46.578 kcal/mol) is close to the adsorption energy, indicating that DBu undergoes moderate molecular adjustment to achieve a favorable adsorption geometry—evidence of a significant chemisorption component. The enhanced adsorption compared to DBk is attributed to better conjugation and more favorable spatial alignment of functional groups. Thus, DBu exhibits a stable interaction profile, supported by both molecular size and functional diversity.

Molecular Dynamics Simulation Studies

To gain deeper insight into the adsorption mechanisms of the selected azo dyes on the $Ti_3C_2(OH)_2$ MXene surface under dynamic, aqueous conditions, molecular dynamics (MD) simulations were conducted using the Forcite module in BIOVIA Materials Studio (Version 8.0). Each simulation system consisted of a $Ti_3C_2(OH)_2$ (100) crystal slab, the dye molecule, and water molecules (solvent), all confined within a periodic simulation box measuring 18.0 Å × 30.23 Å × 25.08 Å shown in figure 7. Before the MD run, all components—including the dye molecules (Congo Red, Methylene Blue, Direct Black 1, and Direct Blue 38)—were geometry-optimized using the Universal Force Field (UFF) to ensure energy minimization and structural stability.

To complement the static adsorption analysis, molecular dynamics (MD) simulations were employed to evaluate the stability, spontaneity, and nature of dye adsorption on the $Ti_3C_2(OH)_2$ MXene surface under realistic aqueous conditions. These simulations provide dynamic insights into the interaction mechanisms by considering thermal fluctuations, solvent effects, and molecular motion over time. By analyzing adsorption and binding energies alongside radial distribution functions (RDF), this section elucidates the extent of physical versus chemical adsorption for each dye and validates the comparative adsorption trends observed in the Monte Carlo simulations.



MB CR

DBk DBu

Figure 7. Molecular dynamic simulation of Methylene Blue (MB)-MXene-water, Congo Red (CR)-MXene-water, Direct Black 1 (DBk) MXene-water, and Direct Blue 38 (DBu)-MXene-water.

Methylene Blue (MB)

The MD simulation results (Table 2 and Fig. 8) indicate that Methylene Blue (MB) shows the weakest adsorption interaction with the $Ti_3C_2(OH)_2$ MXene surface, with an adsorption energy of –895.651 kcal/mol. This relatively lower binding energy reflects a limited interaction potential, which aligns with MB’s molecular structure. MB is a planar, cationic dye containing a thiazine ring but lacks extensive π-conjugation and polar anchoring groups like sulfonates. The radial distribution function (RDF) curve in Figure 8 suggests that MB molecules maintain a slightly larger distance from the MXene surface, with less pronounced peaks, indicating weak electrostatic or van der Waals forces. The planar geometry aids in some surface contact, but the absence of strong hydrogen-bond donors/acceptors and minimal deformation upon adsorption confirms that the dye undergoes primarily physisorption. Thus, MB's interaction is governed mostly by weak non-covalent forces with limited chemisorptive character.

Table 2. Adsorption and Binding Energies of Azo Dyes on $Ti_3C_2(OH)_2$ MXene Surface from Molecular Dynamics Simulations

Obs	**E** **sol+water**	**E****dye**	**E** **total**	**E****ads**	**E****bind**
MB	-26930.875	-50.564	-27877.09	-895.651	895.651
CR	-26930.875	-283.582	-28371.625	-1157.238	1157.238
DBk	-26930.875	-297.351	-28576.79	-1348.604	1348.604
DBu	-26930.875	-500.469	-29107.669	-1676.365	1676.365

MB

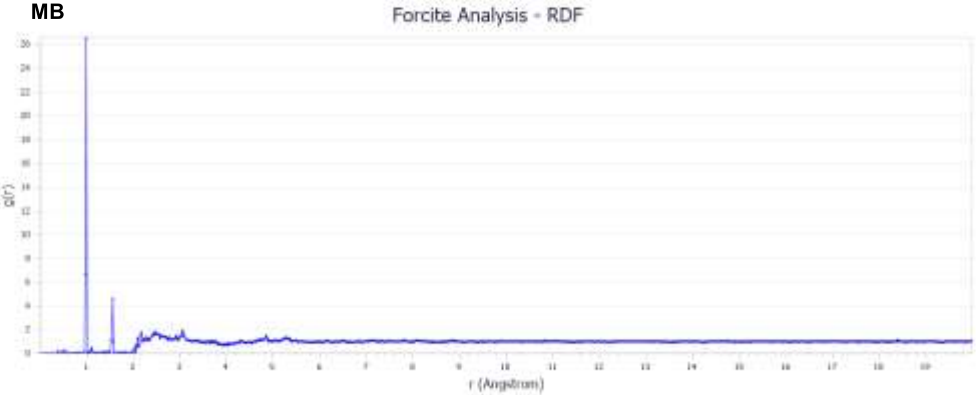


Figure 8. Radial distribution function of Methylene Blue (MB)

Congo Red (CR)

According to the data in Table 2 and Figure 9, Congo Red (CR) demonstrates a significantly stronger interaction with the MXene surface, with an adsorption energy of –1157.238 kcal/mol. CR contains extended π-systems, azo linkages, and sulfonic acid groups (–SO_3H), which facilitate both π–π stacking and strong hydrogen bonding with the –OH-terminated MXene. The RDF profile in Fig. 9 exhibits sharp and high peaks within 2.5–3.5 Å, indicating a close and structured interaction between the dye and the surface, consistent with chemisorption. The large negative deformation energy reported in previous sections also suggests substantial molecular reorganization during binding. This indicates that CR reorients itself dynamically in solution to maximize electrostatic and hydrogen bonding interactions. Its high binding energy and favorable RDF pattern reinforce that CR exhibits strong and stable adsorption, with both structural and electronic features contributing to its robust chemisorption.

CR

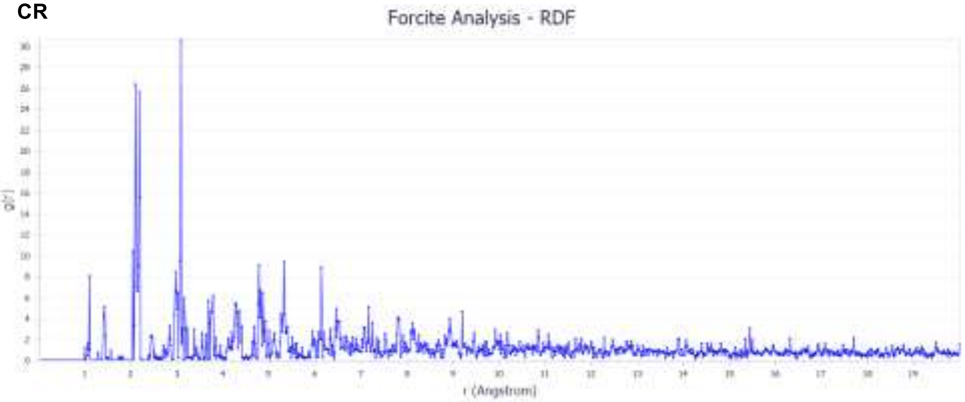


Figure 9. Radial distribution function of Congo Red (CR)

Direct Black 1 (DBk)

Direct Black 1 (DBk) exhibits an adsorption energy of –1348.604 kcal/mol (Table 2), placing it between CR and DBu in adsorption strength. From a chemical perspective, DBk features multiple aromatic rings, azo groups, and sulfonic acid functionalities, which collectively contribute to moderate-to-strong π–π and hydrogen bonding interactions with the Mxene surface. The RDF profile in Figure 10 reveals a pronounced peak around 3.0 Å, indicating that DBk maintains a fairly close and consistent orientation relative to the surface, supporting chemisorption. However, compared to CR, DBk's more sterically hindered and bulkier structure likely limits its adsorption efficiency due to less favorable spatial alignment. Nonetheless, the strong binding energy suggests that DBk still undergoes effective chemisorption, albeit with slightly lower flexibility or reorientation capability than CR.

DBk

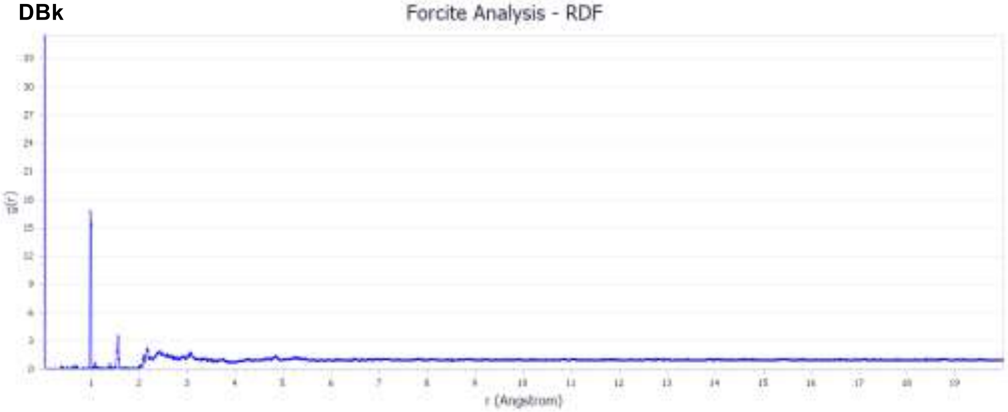


Figure 10. Radial distribution function of Direct Black 1 (DBk)

Direct Blue 38 (DBu)

Among all studied dyes, Direct Blue 38 (DBu) demonstrates the highest adsorption energy of –1676.365 kcal/mol (Table 2), clearly indicating the most favorable interaction with the $Ti_3C_2(OH)_2$ surface. Chemically, DBu possesses multiple conjugated aromatic systems, sulfonic acid groups, and azo linkages, providing abundant sites for π–π stacking, hydrogen bonding, and electrostatic interactions. Figure 11 shows an RDF curve with highly pronounced peaks in the 2.5–3.5 Å region, confirming very strong and close-range interactions—hallmarks of dominant chemisorption. The dye's planar segments likely align well with the MXene layers, maximizing surface contact and interaction energy. Moreover, the large negative deformation energy observed earlier reinforces that DBu undergoes significant reconfiguration to adopt a stable adsorbed state. Overall, DBu exhibits the most thermodynamically favorable and chemically intensive interaction, making it the best-performing dye in terms of spontaneous, stable adsorption on the MXene surface.

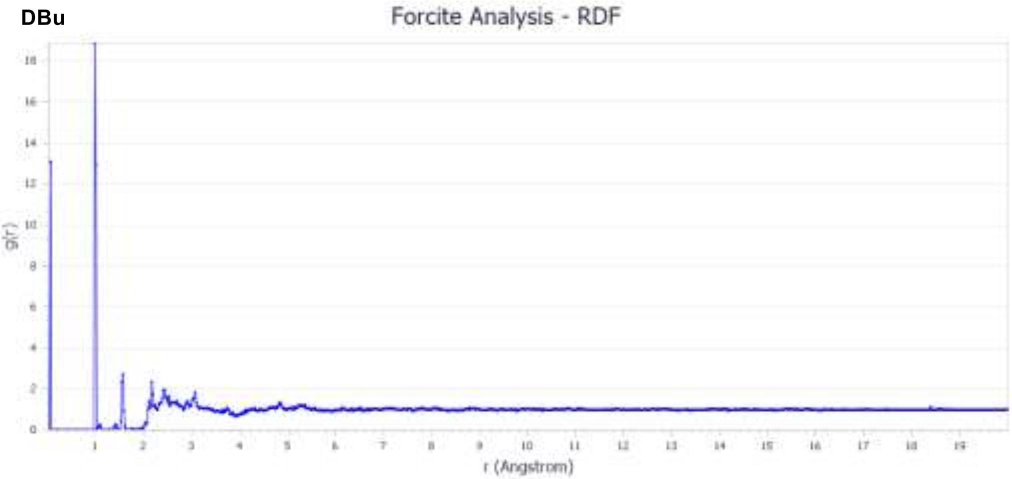


Figure 11. Radial distribution function of Direct Blue 38 (DBu)

CONCLUSION

This study offers a molecular-level perspective on the chemisorption behavior of four widely used industrial azo dyes—Congo Red, Methylene Blue, Direct Black 1, and Direct Blue 38—on hydroxyl-functionalized Ti_3C_2 MXene surfaces. By employing a dual computational strategy of Monte Carlo adsorption locator simulations and molecular dynamics under aqueous conditions, we unveil that dye–MXene interactions are governed by a synergy of π–π stacking, hydrogen bonding, and surface-induced molecular reorganization. Among the dyes, Congo Red and Direct Blue 38 consistently demonstrated the most favorable energetics, not only in static conditions but also under dynamic environments, suggesting their adsorption is both spontaneous and structurally adaptive—a hallmark of strong chemisorption. Notably, the deformation energy analyses provided insight into the extent of structural adjustments dyes undergo, revealing the importance of molecular flexibility and functional group orientation in determining adsorption strength.

These findings extend beyond comparative adsorption metrics, offering mechanistic insights that highlight the role of dye architecture—such as planarity, electron-donating groups, and steric hindrance—in influencing dye–MXene affinity. The significant binding energy profiles suggest that $Ti_3C_2(OH)_2$ MXene is not merely a passive adsorbent but an active participant in the dye capture process. Future directions should aim at correlating these theoretical predictions with experimental adsorption isotherms and kinetics, as well as exploring surface functionalization strategies to further tune selectivity and efficiency. This work thus establishes a foundational framework for the rational design of MXene-based adsorbents in advanced wastewater treatment technologies.

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Izvod

MEHANIZMI HEMISORPCIJE INDUSTRIJSKIH BOJA NA POVRŠINI TI$_3$C$_2$ MXENE ZA PRIMENU U PREČIŠĆAVANJU OTPADNIH VODA: TEORIJSKI PRISTUP

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Ispuštanje azo boja iz industrijskih otpadnih voda predstavlja ozbiljan ekološki i zdravstveni rizik zbog njihove postojanosti i otpornosti na biorazgradnju. MXeni funkcionalizovani hidroksilnim grupama $Ti_3C_2(OH)_2$ pojavili su se kao obećavajući adsorbensi zahvaljujući velikoj specifičnoj površini, hidrofilnosti i raznovrsnoj površinskoj hemiji. U ovoj studiji primenjene su Monte Karlo i simulacije molekulske dinamike za ispitivanje adsorpcionog ponašanja četiri industrijske boje — Kongo crvena (CR), Metilen plava (MB), Direktna crna 1 (DBk) i Direktna plava 38 (DBu) — na površinama MXena $Ti_3C_2(OH)_2$.

Rezultati Monte Karlo lociranja adsorpcije pokazali su da CR ima najpovoljniju statičku energiju adsorpcije (–182,346 kcal/mol), zatim slede DBu (–46,576 kcal/mol), DBk (–23,994 kcal/mol) i MB (–16,35 kcal/mol). Posebno je značajno da je energija deformacije CR iznosila –151,353 kcal/mol, što ukazuje na jaku hemisorpciju usled značajne molekulske reorganizacije. Simulacije molekulske dinamike u vodenom medijumu dodatno su potvrdile ove trendove, pri čemu je DBu pokazala najveću dinamičku energiju adsorpcije (–1676,365 kcal/mol), zatim DBk (–1348,604 kcal/mol), CR (–1157,238 kcal/mol) i MB (–895,651 kcal/mol). Energije vezivanja pratile su sličan redosled, potvrđujući da su π–π interakcije, vodonične veze i površinski indukovana reorijentacija dominantni mehanizmi interakcije.

Ova saznanja pružaju uvid na molekulskom nivou u odnos između strukture i funkcije koji upravlja adsorpcijom boja na MXenima i ističu $Ti_3C_2(OH)_2$ MXen kao efikasan materijal za selektivno i održivo uklanjanje boja iz otpadnih voda.

Ključne reči: Azo boje, Ti_3C_2 MXen, Energija adsorpcije, Hemisorpcija, Molekulska dinamika, Prečišćavanje otpadnih voda.