Shedding Light on Miniaturized Dialysis Using MXene 2D Materials: A Computational Chemistry Approach

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ABSTRACT: Materials science can pave the way toward developing novel devices at the service of human life. In recent years, computational materials engineering has been promising in predicting material performance prior to the experiments. Herein, this capability has been carefully employed to tackle severe problems associated with kidney diseases through proposing novel nanolayers to adsorb urea and accordingly causing the wearable artificial kidney (WAK) to be viable. The two-dimensional metal carbide and nitride (MXene) nanosheets can leverage the performance of various devices since they are highly tunable along with fascinating surface chemistry properties. In this study, molecular dynamics (MD) simulations were exploited to investigate the interactions between urea and different MXene nanosheets. To this end, detailed analyses were performed that clarify the suitability of these nanostructures in urea adsorption. The atomistic simulations were carried out on Mn$_2$C, Cd$_2$C, Cu$_2$C, Ti$_2$C, W$_2$C, Ta$_2$C, and urea to determine the most appropriate urea-removing adsorbent. It was found that Cd$_2$C was more efficient followed by Mn$_2$C, which can be effectively exploited in WAK devices at the service of human health.

INTRODUCTION

Kidney disorder is one of the fatal diseases worldwide, with 1.7 million deaths per year. Among kidney diseases, end-stage kidney disease (ESKD) is the most threatening by affecting 3 million patients annually. Although kidney transplantation is the most promising way to treat ESKD, due to the long waiting time for finding a compatible kidney and the high risk of kidney failure, researchers are about to use substitutions. Hemodialysis (HD) and peritoneal dialysis (PD) are the most common treatments for kidney patients. HD, which contains pumping the blood out of the body and pumping it back after toxin filtration with an artificial kidney, can neither remove the toxins properly from the blood nor is applicable to continuous removal of waste solute and excess water off the blood. Furthermore, the HD device’s large weight (in comparison to 175 g of the human kidney) causes difficulties in patients’ mobility and quality of social life. PD is based on sending the fluid through a catheter to the belly to remove waste solute and accumulated toxins from the body. However, the PD is an off-hospital method for kidney disease treatment. Its efficiency for blood purification is less than that of HD, and its period of treatment is limited to 30–40 min each time. Besides, PD is not a permanent treatment and is replaced gradually by HD. Another potential treatment for kidney diseases is a wearable artificial kidney (WAK). This method has been introduced in 1960s on the basis of the wearable artificial kidney that is regenerable due to the consumption of a certain amount of dialysate solution and provision of a closed loop as the human kidney does. As PD, the WAK performs dialysis outside the hospital. Despite both HD and PD, it provides an almost permanent and continuously clear bloodstream, called continuous renal replacement (CRT). An applicable WAK should be less than 2 kg to be worn in the body and also covers the requirement of a light power source with the ability to supply enough energy for an extended period without abruption as well as a sorbent system with the ability to regenerate and detoxify the bloodstream without the need for fresh dialysate to be injected in the systems. Other features such as appropriate additives, fluid removal system, and proper safety will promote the rate and efficiency of clearance of blood and consequently the quality-of-life factors, like social contribution and sleep pattern for the patients. Recently, in times of the COVID-19 pandemic, HD and PD
treatments are not that applicable due to hospitalization consideration and acute kidney injuries.10

One of the most challenging points in accordance with the dialysate is the ability to remove the waste solutes and toxic compounds. These compounds contain ions like phosphate and extra potassium, sodium, heavy metals complexes, and urea, resulting from the metabolism of proteins and other nitrogen-containing compounds. Based on the previous study, the most effective solution for ion removal from blood is activated carbon (AC) compounds that charcoal has shown to be efficient in this regard.11 Moreover, due to time extension in the CRT method, phosphate detoxification improves. In addition to structural properties like the lack of surface charge at the physiological pH of the human body, no structural reactivity, and slow hydrolysis in water compared to other compounds, the volume of urea production is approximately 240 mmol/day, making it that problematic.12 Conventional methods used two main protocols to remove urea: first, enzymatic hydrolysis, resulting in the outgassing of carbon dioxide and ammonia, and second electro-oxidation that suffers from slow kinetics and incomplete urea removal. Research shows that max phase and specific urea sorbent can play a vital role in decreasing the concentration of urea in the artificial kidney by up to 99%, which helps regeneration of the kidney.13 In this regard, the presence of a polar charged nitrogen, which intensifies the interaction of MXene and urea,14 has been found to have an eminent effect on controlling and modifying urea concentration in blood.

MXenes inheriting both metal and ceramic characteristics11 show elevated electrical and thermal conductivity, higher ductility, lower friction coefficient, and improved thermal stability compared to common ceramics on the one hand and higher density, rigidity, Young’ modulus, thermal resistance; outstanding strain, creep performance, and vibration; and higher thermal resistance than those of regular metals on the other hand.12,14−17 These led to their extraordinary performance in the fields of energy, electricals, optics, electronics, magnetism, molecular adsorption, catalysis, environment, sensing, as well as biomedical including drug delivery, phototherapy, diagnostic imaging, biosensing, tissue engineering, and cancer therapy.18−20 MXenes can be represented as M′X2T, MXX′T, MXX′T’, MXX′T, M′M′X′X′T, and M′M′X′T′, where T′ shows surface termination. In this regard, fluoride ions are a possible termination due to etching, in addition to −OH, −O, and other oxygen-containing groups as a result of aqueous media.22 The electrical, biological, and optical properties are highly dependent on surface functionalization.

The T’ intensifies the hydrophilic nature of MXene. Along with its high hydrophilic nature, abundant surface area makes MXene a potential option for urea adsorption. Different metal atoms in the two-dimensional (2D) MXene structure are an effective parameter in the adsorption of various compounds from aqueous media due to their capacity to bond with a certain molecule. Metal termination is necessary to reveal the supreme electronic and biological properties along with environmental applications, as electrochemical double-layer capacitors,23 water treatment agents,24 and kidney detoxifiers.13 The 2D MXenes have strong interlayer bonds and weak interlayer bonds. Due to the weak van der Waals (vdW) interlayer bonds, MXene can interact with external ions and molecules, resulting in the termination of the metal groups. For either thoroughly exfoliating the 2D MXene and making a MXene nanosheet or increasing the interlayer spacing, intercalants are necessary. Intercalation and delamination provide accessibility to the active sites due to enhancement of the pillaring effect, within which the trapping and swelling of the penetrated molecules or ions occur. Thus, through an electrochemical process, the reaction with −OH, −O, and −F groups determine them. The presence of intercalants results in increasing the interlayer spacing or, in other words, changing the c lattice parameter.24,26

In this study, an attempt has been made to thoroughly investigate the application of emerging 2D structures in urea removal. To this end, computational materials science tools have been employed to screen the novel MXene nanostructures in urea removal and blood purification. The molecular dynamics (MD) simulations were carried out on Cd-, Cu-, Mn-, Ti-, and W-based MXenes, and their viability in blood purification was accessed. In this study, we simulated different MXene structures to get a better response in this regard; as both the production and implementation of these 2D materials are expensive and sensitive, researching for different possible materials for getting a better response is necessary. However, doing laboratory research is a primary need to conduct animal study and clinical research; thus, molecular dynamics simulation can be exploited to get a deep insight into the intermolecular interactions to properly choose the most effective structures. This, in turn, prevents cumbersome and time-consuming laboratory studies. This work can enable the use of emerging nanostructures in newly developed wearable devices and accordingly improve the human’s life quality.

**RESULTS AND DISCUSSION**

**Stability.** The structures of Ti2C, Cd2C, Mn2C, Cu2C, W2C, and Ta2C had suitable minimization energies after performing the optimization process. The total energies of all MXene structures after optimizations are reported in Figure 1, indicating the stability of all considered MXene nanosheets. To clarify the viability of an emerging nanostructure in the WAK devices, it is essential to investigate the interactions between the adsorbate and urea in detail. This enables us to determine the most applicable nanostructures. In this regard, applications of the MXene nanostructures in urea removal have been studied thoroughly in terms of the adsorption energy and other factors, by which the most effective MXene type can be detected. In the following, results obtained from each analysis will be discussed.

![Figure 1](https://dx.doi.org/10.1021/acsomega.0c06118)
Figure 2. continued
Energy and Gibbs Free Energy of Urea and MXene Nanosheet Reaction. The energy of intermolecular interaction can be considered to determine the adsorption energy of investigated atoms as a function of time. The more negative the energy (mmpsa), the stronger the binding of the considered MXenes and urea. Accordingly, the MXene nanosheet leading to the most negative adsorption energy value is regarded as the most effective adsorbent in the WAK devices. Furthermore, formation of strong bonds between MXene with urea helps the urea to be absorbed from the body fluid and, as a result, detoxifies the body from the wastes. As Figure 2 shows, the electrostatic interaction energies between urea and all of the investigated structures were about $-2$ mmpsa, which is negligible. Moreover, Figure 2a indicates that van der Waals (vdW) energy interaction between urea and Cd$_2$C was in the lowest level with an average of $-214.104$ mmpsa followed by that of Mn$_2$C. Based on Figure 2b–e, the energy levels were higher for Mn$_2$C, Cu$_2$C, Ti$_2$C, and W$_2$C with approximate levels of $-190.489$, $-187.9$, $-163.238$, and $-158.24$ mmpsa as a function of time. The highest vdW energy level belonged to Ta$_2$C with $-41.330$ mmpsa, as shown in Figure 2f. The observed difference can be referred to the differences between these structures’ vacant orbitals and their tendency to whether form van der Waals bonds with urea via complexing or stay in the aqueous media. The chemical complex of urea and Cd$_2$C is more potent than other structures; thus, the energy level is significantly more appropriate than other structures. Actually, energy analysis is the most appropriate index to compare the performance of various adsorbents. As discussed hitherto, the Cd$_2$C MXene is the most favorable material for urea removal in terms of the adsorption energy, which needs to be verified by other analyses.

Gibbs free energy of the reaction between urea and the above-mentioned MXenes is also (Figure 2g) an indicator of the probability of the reaction. The lower the Gibbs free energy, the more probable the reaction. As it is shown, the least Gibbs free energy belongs to the Cd$_2$C–urea reaction with a
value of $-42.32 \text{ kJ}$. Moreover, based on this diagram, the second value belongs to Mn$_2$C with a sharp increase in the Gibbs free energy value to $-25.81 \text{ kJ}$. Consequently, it can be predicted according to the energy diagrams that the highest value of Gibbs free energy belongs to Ta$_2$C with a value of $-5.02 \text{ kJ}$.

**Analysis of Radius Distribution Function (RDF) of Urea and MXene Nanosheets.** The radius distribution function (RDF) shows the density of a specific matter at a distance ($r$) around a molecule, computed through eq 1.

$$g(r) = \frac{d\rho}{4\pi r^2 \rho}$$

(1)

Here, $d\rho$ shows the number of particles in a particular shell of thickness and $\rho$ is the local density. The calculation is based on the RDF that helps us to define the coordination number and many other parameters. As the distance increases, the probability of bonding also decreases, and as a result, the coordination is less likely. Figure 3 demonstrates the RDF for the considered MXenes. As the results show, Cd$_2$C had a higher $g(r)$ peak of 10.99 at 0.474 Å, and as a result, it had a brighter coordination shell, which illustrates the higher urea intensity decreased for Mn$_2$C, Cu$_2$C, Ti$_2$C, W$_2$C, and Ta$_2$C and appeared more distant.

**Root-Mean-Square Deviation (RMSD) of Urea and MXene Nanosheets.** The root-mean-square deviation (RMSD) implies the flexibility of an atom to depart from a tagged structure or, in other words, the distance from a target that can be whether an organic molecule and protein or even a single atom. For the transformation of the hard-ball model, the RMSD can be defined as below

$$\text{RMSD}(t_1, t_2) = \frac{1}{N} \sum_{i=1}^{N} \langle ||X_i(t_2) - X_i(t_1)||^2 \rangle^{1/2}$$

(2)

In eq 2, $X_i$ is the position of atom $i$ and $X_j$ is the position of atom $j$. Although the above-mentioned equation is a function of time and in a particular $\Delta t(a)$, the RMDS may differ from this value in $\Delta t(b)$. The whole picture shows the strength and tendency of a bond to form or break. Furthermore, if $\Delta t \rightarrow 0$, then

$$\text{RMSD}(t) = \frac{a}{2}$$

(3)

where $a$ is a constant and is approximately equal to the lattice parameter of formation.

Figure 4 shows the average distance between a tagged urea molecule and a part of the MXene structure. According to what has been shown, the RMSD value for Ta$_2$C fluctuated between $1.15 \times 10^{-5}$ and $7.13417 \text{ Å}$, which is a greater value compared to other structures; this illustrates the weaker bonds between urea and Ta$_2$C and more flexibility in the particle movements as a result of thermal fluctuations. On the other hand, W$_2$C fluctuates between $2.19 \times 10^{-5}$ and $7.0448 \text{ Å}$ with an increasing slope. For Cu$_2$C, Ti$_2$C, and Mn$_2$C, the RMSD values fluctuated in a more limited range with average values of $4.8559$, $4.8379$, and $4.6849 \text{ Å}$, respectively. Cd$_2$C on the other hand fluctuated in the most restricted range of $4.96 \times 10^{-5}$ to $5.53991 \text{ Å}$ with an average of $4.430084 \text{ Å}$. The finding shows that Cd$_2$C forms more resistant bonds with urea due to the limited fluctuation range, which proves that urea and Cd$_2$C bonds are the firmest and thus are more applicable in the WAKs.

**Root-Mean-Square Fluctuation (RMSF) of Urea and MXene Nanosheets.** Root-mean-square fluctuation (RMSF) is the displacement in the position of a single atom or a molecular structure of a reference atom or structure. In GROMACS, it is computed with the Poisson equation (eq 4), which goes as follows, where $M$ is the number of the frames, $t_i(t_k)$ is atom $i$ of the complex at time $k$, and $i$ is the reference atom or structure.

$$\text{RMSF} = \left[ \frac{1}{M} \sum_{k=1}^{M} (t_i(t_k) - \bar{t}_i)^2 \right]^{1/2}$$

(4)

Figure 5 shows the RMSF value for the considered MXene structures. The observation shows that the highest residue belongs to the Ta$_2$C structure with an average of 0.05689 nm. Moreover, significant fluctuations are observed for Ta$_2$C.
which, all in all, implies loose bonds such as bend, turn, and coil that introduce high flexibility, which causes the whole complex to be unstable. W₂C with 0.04856 nm is at the second position of instability and Ti₂C with a 0.01666 nm peak in the residue is the third probable unstable complex in the presence of urea. Cu₄C and Mn₄C with less fluctuation and negligible peaks are more stable than the mentioned structure. However, Cd₂C is formed with the least flexibility. This is due to the least fluctuations with an average of 0.01286 nm between the reviewed structures. In Cd₂C, π−π interactions are more durable, thus making the structure most stable.

**Number of Hydrogen Bonds between Urea and MXene Nanosheets.** Hydrogen bonds (H-bonds) are nonbinding interactions occurring through electrostatic interactions. In molecular dynamics simulations, the number of H-bonds is determined by the LINCS algorithm. Figure 6 shows the number of intermolecular hydrogen bonds for the investigated structures. Since an average of 13.27 hydrogen bonds were found for Cd₂C, it may interact with urea. Consequently, the most abundant values for hydrogen bonds of 8.18 and 2.19 belong to Cu₂C and Mn₂C. For the rest of the structures, this value is approximately zero. Since the bonding of D−H−A and their angles are of great importance in the bonding, no hydrogen bonding might be due to the lack of any bond between O and N or O/N as well as the probability of the unsuitable direction that makes urea and MXene bonding impossible. This results in weak C−H and π interactions.

Due to the high polarity of urea and its hydrophilic nature and the presence of hydrogen and oxygen atoms in the aqueous solution, aqueous media acts as a cross-linking agent for interacting MXene and urea. As the solvent-accessible surface area (SASA) of all of the studied structures is significant, the chance for cross-linking agent action is present. The formation of partially negative charges on the MXene surface due to MXene hydration may enhance the interactions. Based on the cross-linking bond capacity, the probability of bond formation varies in the studied structures.

**Density of Urea and MXene Nanosheets.** In GROMACS, the density is based on the partial density from a reference point. In other words, the determination of the reactant density from a certain point of the reference structure is calculated by three-dimensional multi-Gaussian relations of atomic density. Based on this fact, as a reaction completes or the concentration of the reactant decreases, the density function decreases as well. Figure 7 shows the density of urea around the mentioned MXenes. Figure 7a reveals that the reaction of urea and Mn₂C showed slight fluctuation, which indicates that homogeneous distribution of urea could be found around the Mn₂C structure with an average density of 18.93 kg/m³. However, Cd₂C (Figure 7b) with an average density of 18.57 kg/m³ had better urea adsorption due to the uniformity of its structure compared to Mn₂C. Based on the studied structures’ molecular dynamics simulation results, the average densities for Mn₂C, Cd₂C, Ti₂C, Ta₂C, Cu₂C, and W₂C are 18.93, 18.57, 18.47, 17.59, 16.34, and 16.34 kg/m³, respectively. Thus, urea adsorption is less likely compared to the other studied structures (Mn₂C and Cd₂C). The ups and downs in the Ta₂C, W₂C, and Cu₂C diagrams (Figure 7d–f) show a heterogeneous distribution of urea around the named structures, which is not desirable. The findings proved that Mn₂C and Cd₂C owing to the homogeneous distribution of urea around their structures and high intensity values are the most promising structures to interact with urea for effective urea removal from organs.

**Radius of Gyration of Urea and MXene Nanosheets.** The radius of gyration is an indicator of the compactness of a structure and its change as a function of time. In Figure 8, the radius of gyration is shown for different modeled MXene
structures. Since the radius of gyration for Cu$_2$C was 2.84861 Å, it can be stated that Cu$_2$C was less compact in comparison to Cd$_2$C, Mn$_2$C, Ta$_2$C, W$_2$C, and Ti$_2$C with \( R_g \) values of 2.64254, 2.38891, 2.24154, 2.11727, and 1.94982 Å, respectively. So, the adsorption of urea by Ti$_2$C may be the strongest due to the tight bonds, while the weakest adsorption was achieved for Cu$_2$C for which loose bonds are anticipated. Moreover, a slight decrease in the bond distance in Cd$_2$C from

Figure 6. Number of hydrogen bonds between urea and (a) Cd$_2$C, (b) Cu$_2$C, (c) Mn$_2$C, (d) Ti$_2$C, and (e) W$_2$C, and (f) Ta$_2$C.
Figure 7. continued
2.939321 to 2.3972 Å demonstrates that the adsorption of urea and Cd2C increased with time, while other structures were stable since their radii of gyration were not fluctuating with time sharply.

**Adsorption Capacity. Solvent-Accessible Surface Area (SASA) of Urea and MXene Nanosheets.** The term solvent-accessible surface area (SASA) refers to the capacity of a material in an aqueous media to be surrounded by water molecules. The SASA is calculated through eq 5

\[ \Delta G = \sum \Delta \sigma_i A_i \]  

where \( i \) is a specific atom indiector and \( \Delta \sigma_i \) is its atomic solvation parameter and \( A_i \) shows its SASA. As the SASA increases, the active sites of the adsorbate increase as a function of higher capacity; moreover, the free energy transfer increases and adsorption of nonpolar molecules is enhanced, and this means that the detoxification of the body fluid will be affected as well. Figure 9 demonstrates that the SASA value for Cd2C was about 97.7964 nm² with an adsorption percentage of 60%. An improvement was observed in the SASA for other structures, especially for Ta2C, which reached 111.5022 nm², while its adsorption percentage falls to 6.25%. The SASA values for W2C, Ti2C, Cu2C, and Mn2C were 109.0914, 108.7972, 103.6181, and 101.2825 nm², respectively. The observed differences are due to the size of the molecules. As smaller molecules provide a higher surface area, the SASA is the highest for Ta2C with the Ta ion radius of 31 pm and the lowest for Mn2C with 97 pm radius. Although the SASA value reveals the ability of an adsorbent to be accessible to the adsorbate molecules, it is not an absolute index to compare the MXenes and it just verified the acceptable performance of all MXenes in providing enough accessible area to remove urea and detoxify the blood. However, comparing the adsorption percentage in Figure 9c, it is found that Cd2C shows the best performance.

**Evaluation of Urea Adsorption Rate.** In this section, the urea adsorption rate by MXenes was investigated. To do this, the amount of urea adsorbed by MXenes during the simulation is shown in Figure 10. The intensity of urea adsorption versus time is shown in Figure 10, so the rate of urea adsorption can be compared by investigating the slope of these graphs. According to the obtained results, Cd2C and Mn2C diagrams had the highest slope. This indicates a higher urea adsorption rate by these two structures. On the other hand, since the slope of the graphs decreased with time, it is inferred that the intensity of urea adsorption by MXenes decreased with time. The decrease in the urea adsorption rate may be due to decreasing urea concentration in solution with time as well as limited MXenes’ surface (Table 1).

**Refurnishing the Surface of MXene after Urea Adsorption.** To verify the application of MXenes in urea removal and blood purification, the reusability of the MXene adsorbents must be studied. In the literature, some methods have been investigated to regenerate the MXenes used in the removal of various contaminants. Mechanochemical (MC) etching on Ti3C2Tx for methylene blue removal from water proved to be useful, which could be regenerated using Al powder as a regeneration agent. Another research showed that MXene has a great absorption-desorption capacity while using 0.1 M NaOH as an effective regeneration agent. Moreover, the absorption capacity of MXene was more than 80% after six cycles. Another method to refurnish the spent MXene surface is the thermal desorption method. In this regard, the active surface sites will be regenerated as the temperature increases. To investigate the effect of thermal desorption, a simulation has been conducted at 150 °C for occupied Cd2C to clarify the rate of urea desorption (Figure 11). Moreover, the energy value, RDF, RMSD, RMSF, area, number of hydrogen bonds, and the radius of gyration (Table 2) have been calculated to

Figure 7. Density fluctuations of urea around (a) Mn2C, (c) Cd2C, (f) Ti2C, (g) Ta2C, (h) W2C, and (i) Cu2C and fluctuation of urea in (b) Mn2C and (d, e) Cd2C.

Figure 8. Radii of gyration for Mn2C, Cu2C, Cd2C, Ti2C, Ta2C, and W2C.
support the given information in Figure 11. As can be detected, the urea desorption cycle can be completed in 30 ns.

The average energy value for urea desorption shows that the reaction (urea release) is thermodynamically desirable (due to the negative value for urea desorption). Moreover, decreasing the number of particles around a tagged particle (RDF), the number of hydrogen bonds, and the compactness of the structure (radius of gyration) and increasing the flexibility of a structure (RMSD), the instability of the residue (RMSF), and solvent-accessible surface area (SASA) are all indicators of thermal desorption of urea from the Cd_{2}C surface.

Validation. A comparison between experimental (reported in the literature) and simulated urea adsorption is shown in Figure 12a. The results are in accordance with the experimental reference data. In the report by Meng et al.\textsuperscript{13} urea adsorption on Ti_{3}C_{2}T_{x} was investigated. The volume of urea solution used in the experiment was equal to 6 mL, along with 0.155 g of MXene. The urea concentration in the simulation was determined according to the laboratory conditions and was in proportion to the volume of the simulation boxes (which is equal to 1000 nm\textsuperscript{3}). Moreover, simulations have been performed according to the experimental conditions (37 °C and different laboratory concentrations). Validation of diagrams in Figure 2e from the experimental work is reported in Figure 12b and validation of diagrams in Figure 3 from the experimental work is reported in Table 1. A good agreement of the experimental data with the data obtained from the simulation is shown in Figure 12b and Table 1. The amount of urea adsorbed by Ti_{3}C_{2}T_{x} in the simulation was lower than the experimental adsorption. This is due to the limited simulation time. On the other hand, urea adsorption by Cd_{2}C has been investigated using molecular
dynamics simulations. Figure 12b shows the concentration of urea in solution at the beginning of the simulation and after adsorption by Cd₂C. The results show high urea adsorption by Cd₂C and the effectiveness of this structure in eliminating urea.

CONCLUSIONS

In this study, through performing MD simulations on a set of emerging 2D nanostructures, the viability of employing MXenes in purifying the blood from urea was assessed. To this end, different MXene types including Mn₂C, Cu₂C, Cd₂C, Ti₃C₂Tₓ, Ta₂C, and W₂C were considered for the urea removal process. Applicability of nanosheets in detoxifying the blood through removing urea was investigated from stability and adsorption capacity perspectives, which include different parameters like adsorption energy, solvent-accessible surface area, RDF, RMSD, RMSF, and radius of gyration. The finding attested to the fact that all considered MXenes have acceptable performance in urea removal and being exploited in the WAK devices. In this regard, Cd₂C possessed the best performance with respect to adsorption and stability followed by Mn₂C. It was clarified that Cd₂C is a suitable option due to the lowest energy level of −214.04 mJ/mol compared to other systems. Moreover, the least flexibility as well as homogeneous distribution of urea around the system, high probability of bonds formation, and reasonable compactness, which have been driven from RMSD, RMSF, number of H-bonds, density, gyration, and SASA of 0.86871 Å, 0.01286 nm, 13.27, 18.57 kg/m³, 2.64 Å, and 97.7964 nm², respectively, proves that using Cd₂C will benefit us from different aspects. This work concentrates that MD simulations can be effectively utilized to develop nanomaterials with direct applications in enhancing the human’s quality of life.

COMPUTATIONAL METHODS

Theory. Molecular dynamics simulation is a computational method to direct laboratory studies at a microscopic scale based on general physics rules and is widely used in different fields of science, from biology to materials science. Two families of simulations are accessible in this regard, molecular dynamics (MD) simulation and Monte Carlo (MC). MD is more favorable due to the time dependency which gives results on rheological properties, diffusion of particles, turbulence, transport coefficient, etc. To determine the positions of atoms, it considers individual particle motion and interatomic interactions on a scale of time. This results in an investigation of the numerous possible conditions of atoms binding, folding, and conformational changes.

Classic MD simulation has been constructed based on the idea of no bond formation or breaking, where Newton’s equation of motion based on the interaction potential for the periodic behavior of a one-dimensional inharmonic chain (Fermi–Pasta–Ulam) and three-dimensional hard-sphere model (Alder–Wainwright) (eq 6) is applied. Ab initio molecular dynamics (AIMD), density functional molecular dynamics (DFMD), and such simulations have been developed since that classic MD does not consider the complex chemical formation as a matter of time; besides, it also ignores the effect of geometrical importance on developing different structure models. Quantum mechanics/molecular mechanics (QM/MM) simulations, which are constructed on...
the computation of the wave equation of Schrödinger, contain local density approximation (LDA) of the Hartree–Fock and Kohn–Sham LDA theory\(^\text{39}\) (eq 7). This theory involves numerous numerical stability checks in each step on a scale as short as a few femtoseconds\(^\text{38}\) using the perturbation theory.\(^\text{36}\) Rules of motion are applied to define each atom’s position as a function of time in each step. Consequently, they are updated repeatedly based on the computation of interaction between phonons\(^\text{38}\) for a long range of structures (eq 8).\(^\text{40}\)

\[
\text{MR} = -\nabla E^{\text{eff}} \quad (6)
\]

where \(M\) is the atomic mass, \(R\) is the degree of freedom, and \(E\) is the Ehrenfest potential.

\[
H\varphi = E\varphi \quad (7)
\]

where \(H\) is the Hamiltonian operator of the system and the initial state of \(\varphi\).\(^\text{49}\)

\[
Q(t) = Q e^{-\left(\omega + \Delta - \nu\right)t} \quad (8)
\]

where \(\omega\) is an indicator of the unperturbed harmonic frequency, \(\Delta\) is the frequency shift, and \(r\) is the frequency linewidth.

\[
r = \frac{\int_0^\infty \langle \delta n(t) \delta n(0) \rangle \, dt}{\langle (\delta n)^2 \rangle} \quad (9)
\]

where \(n\) is the phonon occupation number and \(\delta n\) is the fluctuation of \(n\).

\[
r = (2\pi)^{-1} \quad \text{Eq. 10}
\]

However, the whole story is based on the approximation of motions and actions on an atomic scale. It is a powerful method due to position calculation as a function of time and careful control of atoms’ possible conditions based on the structural equilibrium and fluctuations.\(^\text{41}\)

Simulation Details. In this study, GROMACS software was used for molecular dynamics simulations and data analyses.\(^\text{36,42}\) To this end, a 32-core X5670 CPU and a 1080 Ti graphics card with a Ubuntu 18.04.1 operating system were used\(^\text{43}\) and all of the molecular structures were modeled by Avogadro software. MXene adsorbent structures were designed via Avogadro software and the most stable state was reached using Gaussian software. The structure of the Ti\(_2\)C nanosheet was downloaded from the Materials Project website with ID mp-10721, for which the energy stability of the Ti\(_2\)C structure has been reported.

Validation. In this study, we validated our simulation results by comparing them with an experimental study by Meng et al.\(^\text{13}\) For this purpose, three simulations for three MXene molecules (Ti\(_3\)C\(_2\)T\(_x\), Mo\(_2\)TiC\(_2\)T\(_x\), and Ti\(_2\)CT\(_x\)) have been performed in a 10 \times 10 \times 10 nanocube for 300 ns with GROMACS 2020.1 in the all-atom optimized potential for liquid simulations (OPLS-AA) force field. MXene structures were downloaded from the Materials Project website and changed based on the reference. The changes in the structures were applied using Avogadro software. Gaussian software has been used for atomic charge calculation based on the electrostatic potential (ESP). For each MD simulation, a certain MXene nanosheet and ten urea molecules were simulated, and the mass ratio of the absorbed urea per studied MXene has been calculated.

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