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Numerical Study of Water Purification Process via Improved Ni-Si Metallic Substrate with TiO_2 Nanobarriers: Molecular Dynamics Approach

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Abstract

Nanostructure refers to materials or objects with dimensions on the nanometer scale, exhibiting unique properties due to their small size, with potential applications in atomic purification procedures. In current research, we used TiO_2 nano barriers for improve water purification performance of Ni-Si metallic substrate. For this purpose, molecular dynamics (MD) approach used for 20 ns in two main phases. In first 10 ns, equilibrium phase of aqueous environment-atomic substrate detected. Next, the purification process of designed samples described with micro-canonical ensemble. MD outputs in this section predicted rectangular and cubic TiO_2 nano barriers performed appropriately. Numerically, the water purification efficiency converged to 89% and 83% by using rectangular and cubic nano barriers, respectively. Physically, this appropriate performance arises from attraction force between designed atomic substrate and H_2O molecules. Also, MD results introduced nano barriers shape as an important parameter in manipulation of water purification procedure. So, this structural parameter should be supposed in actual applications.

Keywords: Water purification; Aqueous environment; TiO_2 nano barriers; Metallic matrix; Molecular dynamics; Atomic model.

1. Introduction

Water is one of the most essential resources and is crucial for sustaining life on earth. However, the increasing population and industrialization have led to the contamination of water resources, making them unfit for consumption. Polluted water not only affects human health but also has a significant impact on the environment [1-3]. Therefore, the need for effective water purification techniques has become of utmost importance. Several water purification methods are available, such as coagulation-flocculation, sedimentation, filtration, disinfection, adsorption, ion exchange, and reverse osmosis [4-8]. Among these, adsorption is a widely used process in which contaminants are removed from the water by attaching themselves to a material surface. The effectiveness of the adsorption process depends on the adsorbent's properties and its ability to remove the targeted contaminants. Metal substrates have shown promising results for water purification, exhibiting excellent adsorption properties towards organic and inorganic pollutants, including heavy metals, dyes, pesticides, and pharmaceuticals [9-11]. This approach is particularly attractive due to metals' high surface area, chemical stability, and affinity towards several water contaminants. Moreover, metal substrates can be easily regenerated, making them a cost-effective and environmentally friendly alternative to other water treatment techniques.

In previous reports, metallic samples shows promising performance for water purification process. Lee et al. [12] introduced the design, development, and application of new metallic membranes, fabrication methods for controlling the filtration size regime, analytical tools for performance testing, and molecular modeling for transport and separation. They reported these metallic samples operate appropriately in water purification process in various initial conditions. Zhao et al. [13] focus on the describe of the multifunctional metal organic framework composite adsorbents for water purifications aims. The adsorption properties of various metal organic framework

composites are evaluated, and the interaction mechanisms between metal organic frameworks and functional components are also systematically analyzed. They reported the high stability of metal organic framework samples in aqueous environment which should be supposed in actual applications. In other work, Kavak et al. [14] introduced a water-stable ionic liquid (IL), 1-butyl-3-methylimidazolium hexafluorophosphate, [BMIM][PF_6], into a water-stable metal organic framework, MIL-53(Al), to generate the [BMIM][PF_6]/MIL-53(Al) composite. This composite was examined for water purification by studying its capacity for methylene blue (MB) and methyl orange (MO) removal from aqueous solutions having either single dye or a mixture of both. Data illustrated that the removal efficiency and the maximum adsorption capacity of MIL-53(Al) were increased several times upon [BMIM][PF_6] incorporation. Also, they reported upon [BMIM][PF_6] incorporation, the maximum MB and MO adsorption capacities of the pristine metal organic framework were increased from 84.5 to 44 mg/g to 204.9 to 60 mg/g, respectively.

More than common experimental methods, computer simulation methods can be described atomic evolution of water-based Medias in purification procedures [15-17]. Molecular dynamics (MD) method is one of the best approaches for this purpose [18-20]. So, in current computational work, we designed Ni-Si matrix (metallic sample) in presence of TiO_2 nano barriers with various shapes (cubic and rectangular arrangements). This atomic sample doesn't study in previous researches. Technically, the physical stability of modeled structures predicted by temperature and potential energy calculations. Next, the water purification performance of defined structures described by water adsorption, interaction energy, mean square displacement (MSD), root mean square displacement (RMSD), and center of mass (COM) difference calculations. We expected MD outputs for modeled Ni-Si matrixes in presence of TiO_2 nanostructures proposed appropriate atomic arrangement for water purification process in actual applications.

2. Computational Method

MD simulations are useful for a range of applications in physics, chemistry, and materials science. For instance, they can be used to study the behavior of metallic samples in aqueous environment, the wetness of materials from a liquid state, or the diffusion of atoms in a solid. The accuracy of MD simulations depends on the quality of the force field, a mathematical function that describes the interactions between the particles in the system [21]. Force fields are often derived from quantum mechanics calculations or experimental data, and they can be improved to account for specific chemical properties of the system. MD simulations can require large amounts of computational resources, especially for systems with a high number of particles or long simulation times. However, advances in computer hardware and algorithms have made MD simulations increasingly accessible to researchers in various fields. Moreover, MD simulations can provide valuable insights into the behavior of complex systems that are difficult to study experimentally.

In our MD simulations, the atomic interaction between various structures described by Lennard-Jones (LJ) potential [22],

$$U(r) = 4\varepsilon\left((\frac{\sigma}{r_{ij}})^{12} - (\frac{\sigma}{r_{ij}})^{6}\right) \qquad r \ll r_c \tag{1}$$

In which ε is the depth of the potential well and σ is the finite atomic distance at which the potential value gets to zero. Furthermore, r_{ij} is the atomic distance between simulated particles in the simulation box. These constants ratios for various atoms inside computational box listed in Table 1 [23, 24]. Furthermore, an aqueous environment in the MD simulation box is described by the TIP4P model [25]. This model has four interaction sites by adding one dummy particle near the O along the bisector of the HOH angle of the three site models. The dummy particle is massless and has a negative electric charge. This model improves the electrostatic distribution around the H_2O molecule. The bonded interaction is another type of interatomic force in the TIP4P model, which defined by harmonic oscillator equation for simple and angular bond interactions as below equations [26],

$$E_r = \frac{1}{2}k_r(r - r_0) \tag{2}$$

$$E_\theta = \frac{1}{2} k_\theta (\theta - \theta_0) \quad (3)$$

In equations (2) and (3), K_r and K_θ are the harmonic constants in harmonic oscillator equations. Furthermore, r_0/θ_0 parameter is equilibrium value of distance/angle in last equations, respectively.

Table 1. The ε and σ constants in LJ potential in current MD simulations [23, 24].

Atom type	ε (eV)	σ (Å)
Ni	0.00065	2.834
Si	0.01743	4.295
Ti	0.00007	3.175
O (TIP4P Model)	0.00672	3.154
H (TIP4P Model)	0.00000	0.000

After force-field specifies atomic structures, the computational study steps followed. For this purpose, Newton's second law's Equation is computed as the gradient of atomic force-field as below equations [27],

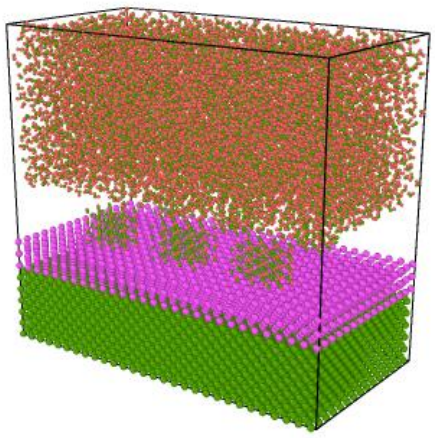
$$F_i = \sum_{i \neq j} F_{ij} = m_i \frac{d^2 r_i}{dt} \quad (4)$$

$$F_{ij} = -\nabla V_{ij} \quad (5)$$

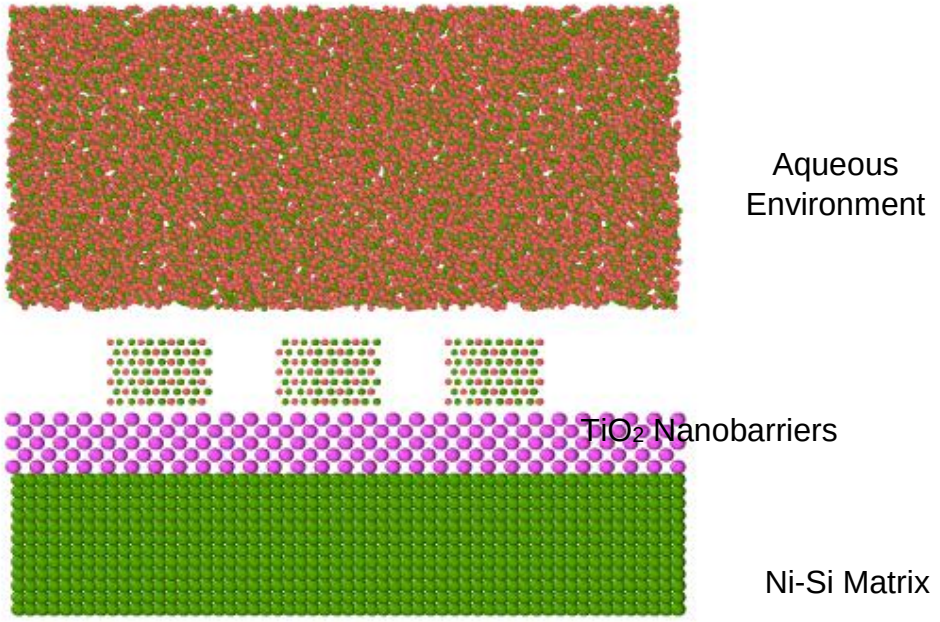
For these formalisms to be solved, the Velocity-Verlet approach implemented in the association of motion equations and physical properties of simulated nanostructures calculated in each time steps [28-30]. By using described computational details our atomic systems evolution in two main phases:

Phase A: In the first step, the equilibrium phase of modeled samples defined by using Nose-Hoover thermostat [31, 32]. The time step set to 1 fs and temperature damping ratio defined as 100value. 100000time steps defined to temperature of modeled samples which depicted in Figure 1 converged to 300 K. The box length of modeled samples set to 100×50×200 $Å^3$ and periodic boundary condition implemented in X and Y directions [33]. Also, fix boundary condition defined in Z direction.

Phase B: after equilibrium phase detection, the adsorption process of water molecules defined. In this procedure, NVE ensemble used with 0.5 fs time steps [34]. MD simulation time steps set to 10000000 until H_2O molecules in metallic matrix saturated. Also, physical stability of final sample which important for actual applications adressed in this phase. Table 2 listed our MD simulation settings in current numerical research.



(a)



(b)

Figure 1. Atomic arrangement of Ni-Si matrix in presence of a) cubic and b) rectangular TiO_2 nano barriers in aqueous environment in the first time step of MD study.

Table 2. MD simulation settings in our MD study.

MD Simulation Parameter	Parameter Setting
Computational Box Length	100×50×200 $Å^3$
Boundary Condition	Periodic and Fixed Boundary Conditions [30]
Thermostat	Nose-Hoover
Initial Temperature	300 K
Time Step	1 fs
Damping Ratio for Temperature	100
Simulation Time	11 ns

3. Results of MD simulations and Discussion

In the first step, the validation process of our used numerical method (MD simulations) for current subject introduced. For this purpose the radial distribution function (RDF) of H_2O molecules of aqueous environment calculated. RDF, denoted in equation 6 by $g(r)$, describes the probability of finding a particle at r distance from other particles. This parameter defined with below formalism [32],

$$g(r) = \frac{1}{4\pi\rho}\frac{dn_r}{dr} \quad (6)$$

where ρ is the atomic density, dn_r is a function that calculates the number of atoms within a shell of thickness dr. The RDF is strongly dependent on the type and phase of atomic structures. As show in figure 2, radial distribution function outputs in this step consistent with previous reports for aqueous environment and validated our computational approach [33].

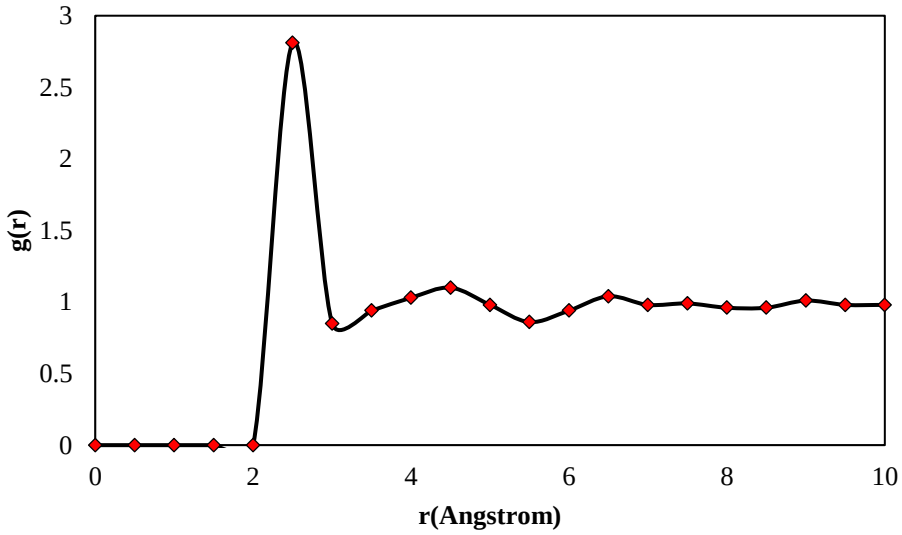
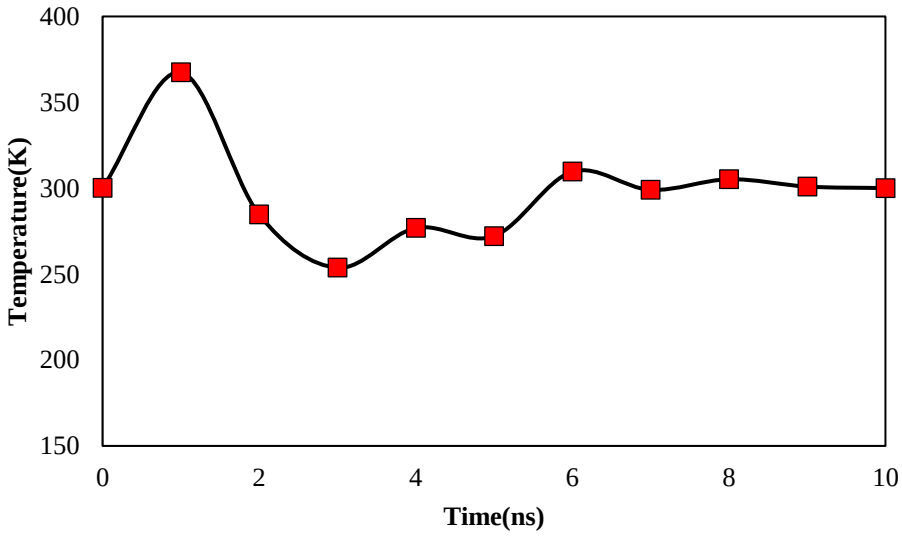
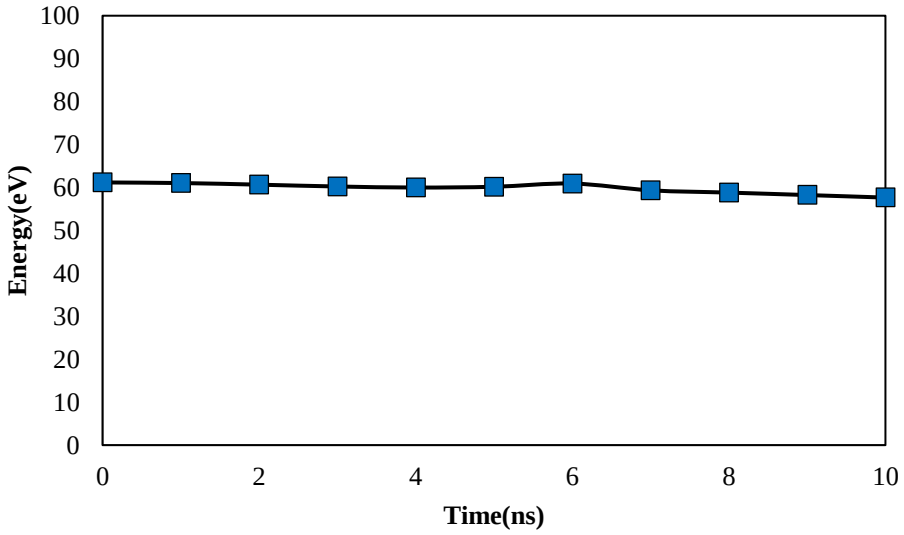


Figure 2. The RDF of oxygen-oxygen atoms in aqueous environment in the first phase of current computational research.

After validation of our used approach, we addressed about equilibrium phase of modeled samples. The temperature and potential energy convergence of these structures shows stability of these samples and proposed them to industrial applications. Figure 3a and 3b shows these parameters convergence at standard condition. As shown in Figure 3a, the temperature value converged to 300 K after 1 ns. This convergence predicted, 1 ns is a sufficient time to create equilibrium state in modeled sample. Also, temperature convergence shows amplitude of atoms inside computational box decreases by simulation time passing. So, we concluded structural divergence don't occur in atomic systems and physical stability can be expected for introduced samples in our MD simualtions. The potential every outputs shows similar performance. As shown in Figure 3b, this parameter converged to 57.64 eV in equilibrium state in presence of rectangular TiO2 nanostructures. Physically, this convergence shows attraction force between particles occur in various regions inside box.



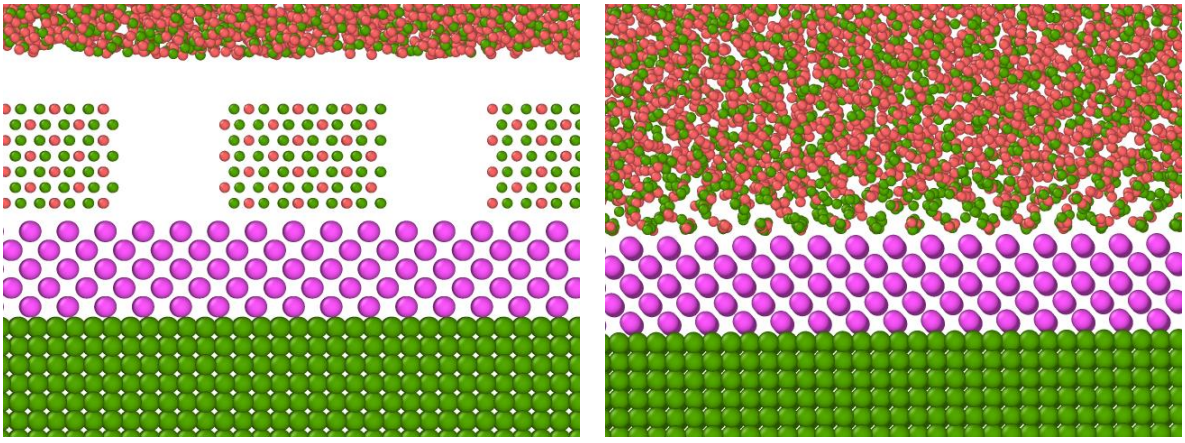
(a)



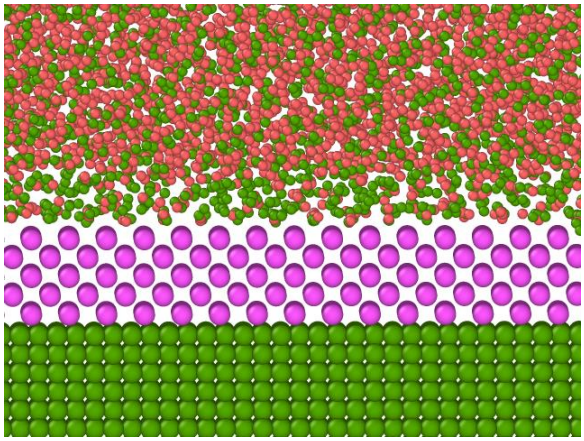
(b)

Figure 3. a) Temperature and b) potential energy changes of modeled atomic sample as a function of MD time in equilibrium phase at 300 K (as initial condition).

After equilibrium state occur inside computational box, the NVE algorithm implemented to sample. This computational changes caused aqueous environment evolution occur effectively and adsorption of H_2O molecules can be detected inside Ni-Si based matrix. This atomic evolution shows in Figure 4. Numerically, analysis of filtered sample can be reported by estimation of adsorbed atoms number with modeled matrix. MD outputs for this procedure depicted in Figure 5. These results predicted the rectangular sample shows more purification efficiency between various defined structures. Numerically, 83 % and 89% of pristine aqueous environment adsorbed with atomic matrix in presence of cubic and rectangular nanostructures, respectively. This atomic evolution arises from more attraction force creation between matrix and water molecules by defined rectangular arrisers rather to cubic one in initial condition.



(a) (b)



(c)

Figure 4. The atomic evolution of water purification process in presence of TiO_2 nano barriers.

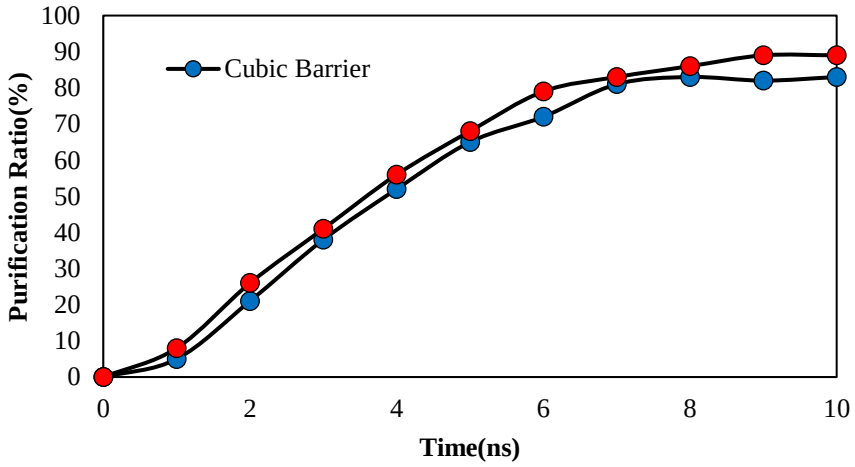


Figure 5. The water atoms adsorption ratio in Ni-Si metallic substrate with cubic and rectangular TiO_2 nanobarriers.

The COM outputs is another which can be described water purification process in current research. The COM parameter is the point within a system or object where the mass is evenly distributed in all directions. It is the average position of all the individual parts of the system or object, taking into account their masses and positions. Physically, the COM can be used to analyze the motion and stability of the system or object. In this step distance between aqueous environment and atomic substrate COMs reported as a function of simulation time. As shown in Figure 6 by MD time passing, the COM distance decreases. This procedure estimated water molecules diffused inside atomic substrate. Numerically, COM distance converged to 26.05 Å and 23.06 Å in presence of cubic and rectangular nano barriers respectively. So, we concluded atomic diffusion maximized by rectangular nano barriers defining. Figure 7 depicted atomic position in H_2O molecules after purification process done. From these figures the physical stability of water molecules after purification process can be detected.

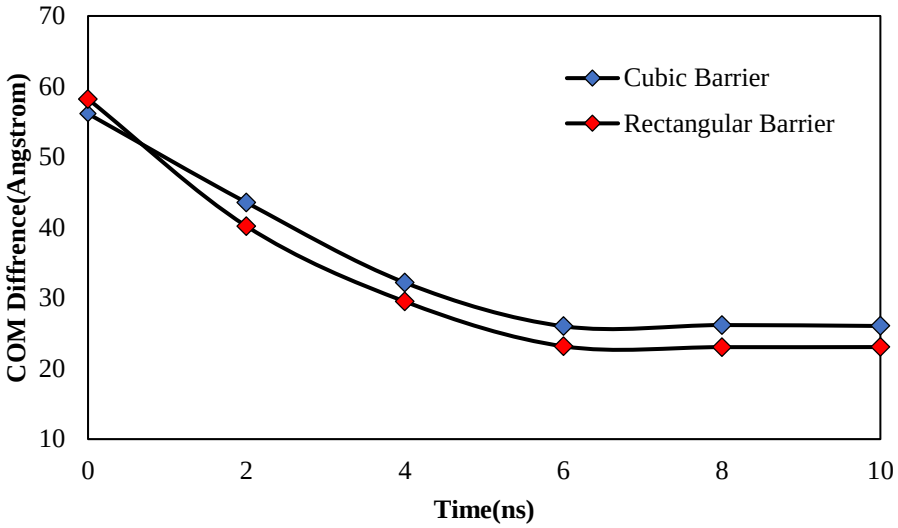
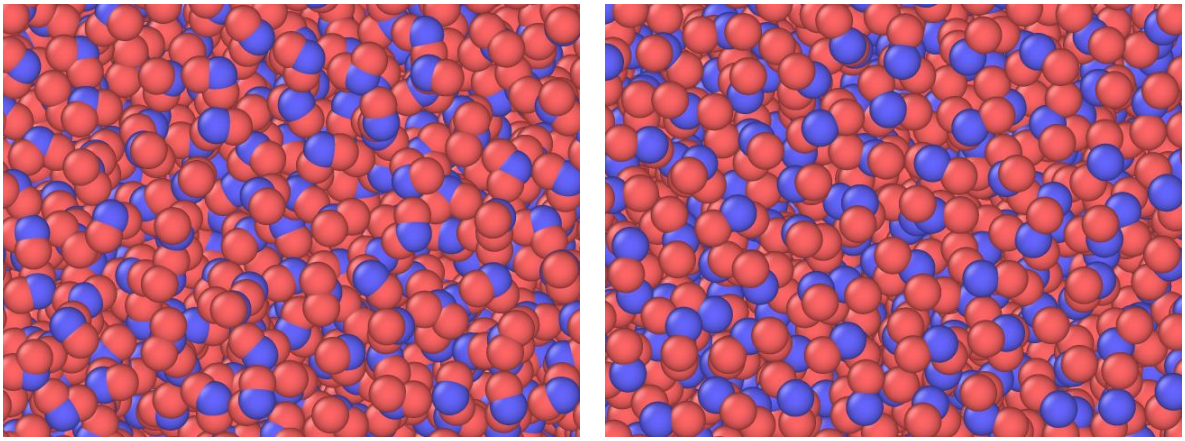


Figure 6. The water and atomic substrate COMs distance as a function of simulation time in presence of cubic and rectangular TiO_2 nano barriers.



(a) (b)

Figure 7. The atomic arrangement of water molecules in presence of a) cubic and b) rectangular TiO_2 nano barriers.

In the final step of current research, the interaction energy and MSD of samples calculated. These parameters can be more introduced the atomic performance of modeled structures. Interaction energy predicted the interatomic force which implemented to water molecules from substrate. Simulations shows this parameter increased to -28.61 eV by change nano barriers to rectangular shape (see Figure 8). So, this interatomic parameter directly shows appropriate performance of designed samples. Furthermore, MSD is a measure of the average distance that a particle or molecule travels from its initial position over a given period of time. It is defined as the average of the squared displacements of the particle from its initial position. MSD is commonly used in the study of diffusion and other types of random motion, and can provide insight into the underlying physical processes. It is calculated by taking the average of the squared distances between the initial position and subsequent positions of the particle over a given time interval. As shown in Figure 9 and Table 3, this parameter for H_2O molecules converged to 2.24 $Å^2$ and 2.63 $Å^2$ by using TiO_2 nano barriers with cubic and rectangular shapes, respectively. Also, RMSD parameter converged to 1.50 Å and 1.62 Å values in presence of cubic and rectangular nano barriers, respectively.

Finally, from Table 3 results, we concluded by nano barriers shape change the water purification efficiency can be manipulated for actual applications.

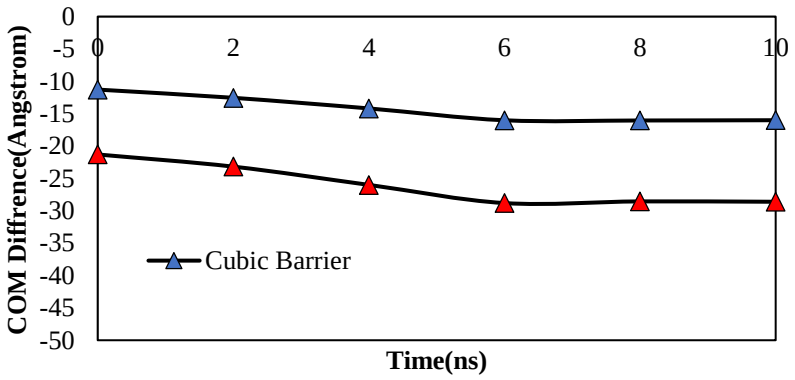
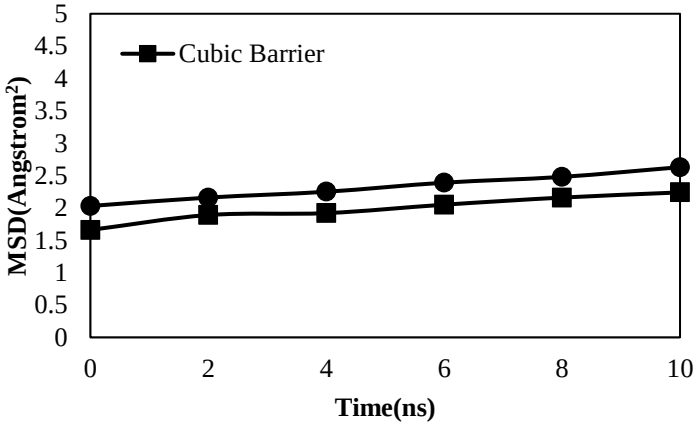
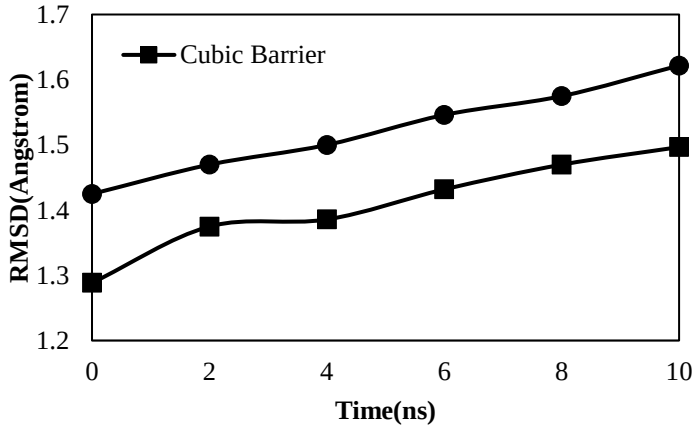


Figure 8. The water and atomic substrate interaction energy changes in presence of TiO_2 nano barriers with cubic and rectangular shapes.



(a)



(b)

Figure 9. a) MSD and b) RMSD parameters of H_2O molecules as a function of nano barriers shape and MD time.

Table 3. MD outputs for water purification ratio, COMs difference, interaction energy, and MSD/RMSD changes as a function of modeled TiO_2 nano barriers in the final time step of current research.

Physical Parameter Type	Cubic Nano barriers	Rectangular Nano barriers
Water Purification Ratio (%)	83	89
COMs Difference (Å)	26.05	23.06
Interaction Energy (eV)	-16.01	-28.61
MSD ($Å^2$)	2.24	2.63
RMSD (Å)	1.50	1.62

Conclusion

Water purification is the process of removing contaminants and impurities from water to make it safe for consumption or other uses. The process involves various physical, chemical, and biological methods, such as sedimentation, filtration, disinfection, and reverse osmosis. The goal of water purification is to remove harmful substances, including bacteria, viruses, chemicals, and pollutants, while retaining essential minerals and nutrients. Today, this process has importance in various scales. Nanotechnology is an effective way to done this process in various conditions. In current computational study, we used molecular dynamics method to describe the TiO_2 nano barriers effect in water purification process by using Ni-Si metallic substrate. Technically, MD simulations done in two main phases. Firstly, the equilibrium phase of pristine sample reported by temperature and potential energy calculations. MD outputs shows these parameters convergence to 300 K and 57.64 eV, respectively. Next, purification process in equilibrated structure reported by adsorption ratio and center of mass (COM) difference changes in side computational box. Simulation results predicted TiO_2 nano barriers with rectangular shape has more efficiency in water purification process. Numerically, purification ratio converged to 83% and 89% by using cubic and rectangular nano barriers, respectively. Also, COM of optimized system decreases to 23.06 Å. This atomic performance arises from attraction force between H_2O molecules and atomic matrix changes in defined conditions. The maximum ratio of interaction energy inside computational box reached to -28.61 eV. Finally, we concluded the water purification efficiency with Ni-Si metallic substrate can be manipulated with TiO_2 nano barriers shape changes. This evolution should be supposed in actual applications.

Declarations

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Conflicts of interest/Competing interests: The authors declare that they have no conflicts of interest.

Ethics approval: N/A

Consent to participate: N/A

Consent for publication: N/A

Availability of data and material: Data available on request from the authors.

Code availability: LAMMPS main inputs available on request from the authors.

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