

Effect of Na⁺, Ca²⁺ on the hydration properties of quartz surface: a molecular dynamics simulation study

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Abstract: Effects of metal ions on the surface hydration of fine quartz are investigated by the theoretical methodologies. The hydration layer on the quartz surface consists of three layers of water molecules, about 8-10 Å. The interaction energy of ions changes from -1.071 eV in water to -1.821 eV (Na⁺) and -1.896 eV (Ca²⁺) when ions are present. Metal ions improve the interaction of water molecules with the quartz surface, allowing more water molecules to enter the second and third hydration layers. In the presence of Na⁺, the diffusivity of water molecules is greater than in Ca²⁺ solutions. Increased interaction between water molecules and surfaces in the order Ca²⁺ > Na⁺ is consistent with metal ions' propensity to hydrate.

Keywords: quartz, hydration layer, diffusion coefficient, interaction energy, molecular dynamics

1. Introduction

Quartz (crystalline silica mineral), is one of the most abundant minerals found on the earth. As an important industrial material, quartz has been widely used in the chemicals industry, electronic components (Zhong et al, 2021) and other industries (Lin et al., 2020). These applications are based on the purification, deep processing and modification of quartz, but the current processes of quartz purification, deep processing and surface modification are severely affected by hydration, which is also a difficult problem for the mineral processing industry to solve. When fresh hydrophilic mineral surface is exposed to aqueous solution, the neighboring water molecules have a higher viscosity and density than bulk water. Water molecules in this region are known as "structure water", which surrounds the mineral particles forming the elasticity hydration layer. The orientation and thickness of the mineral surface hydration layer plays a crucial role in many processes, such as sewage sludge treatment (Świerczek et al., 2018), sands deposition (Huang et al, 2019), petroleum (Pei et al., 2018), metallurgical (Li et al., 2020), mineral processing and wastewater treatment (Li et al., 2020; Min et al., 2015). For example, regarding slime water treatment, when particles approach a state of hydration, repulsive force prevents them from getting closer owing to the overlap of hydration layers. Combined with electrostatic and Van der Waals interactions between particles, a stable colloidal system is formed, which leads to difficulties in sedimentation and clarification of coal slurry water. For this reason, it is recognized that mineral surface hydration characteristics are the key aspect of solving the issue of difficult settlement of coal slurry.

The hydration phenomenon often involves hydration force. From the periodic hydration forces observed between mica surfaces in dilute electrolyte solutions (Pashley, 1981), it has been much studied by SFA (Schrader et al., 2015)), AFM (Butt, 1991), 3D-SFM (Miyazawa et al., 2016) and QCM-D (Chen et al., 2016) techniques. Sun studied the origin of hydration force, its date from the hydrophobic interactions and how it is shaped by the mineral surface (Sun, 2017). For the hydration model, Drost-Hansen (1977) proposed a typical three-layer structure hydration model for polar and non-polar surfaces, wherein there is a great difference in how water molecules are arranged on hydrophobic or hydrophilic surfaces. As well, the hydration layer thickness of the mineral has been researched using

experiment and simulation. Song used two methods, namely AFM and Einstein viscosity to measure the hydration layer thickness of nano silica particles immersed in aqueous solution (Song and Peng, 2005). Min et al. (2015) cited and refined the previous viscosity method to assess the thickness of the hydrated layer on the kaolinite and montmorillonite surfaces with the hydrated ions present. It is shown that the hydration layer does exist, and the hydration ability of montmorillonite is stronger than kaolinite owing to swelling. The mineral hydration layer is thicker in the Na⁺ solution than the Ca²⁺ solution. Xing et al. (2018) measured the thickness of the hydration layer on a mica surface utilizing AFM, revealing that the hydration layer on the mica surface had a thickness of 22.5 nm.

Density functional theory (DFT) is also widely used in the study of mineral surfaces and interfaces. Hydration behaviors of kaolinite (Chen et al., 2019), montmorillonite (Peng et al., 2016), hematite (Zhang et al., 2021), and cassiterite (He et al., 2021) surfaces have been intensively studied utilizing the DFT method. Liu studied water molecule adsorption on the α -quartz (001) surface and indicated that water molecule interacts with the α -quartz (001) surface by means of two hydrogen bonds between the surface active site and water molecule (Liu et al., 2019). The interaction between quartz surface and reagent adsorption is also reported, for example, various nitrogen-containing compounds on the hydroxylated α -quartz (001) and (100) surfaces are computed. Here the 2,4,6-trinitrotoluene (TNT) and 4-dinitrotoluene (DNT) are preferably adsorbed on the (001) surface of α -quartz, while 3-nitro-1,2,4-triazole-5-one (NTO) is located on both α -quartz surfaces (Tsendra et al., 2019). The DFT study revealed the depression mechanism of citric acid (CA) in sodium oleate flotation of Ca²⁺-activated quartz. Consequently, citric acid and Ca²⁺ mainly through reducing the reactive sites blocked the NaOL adsorption and in this way depressed the quartz surface (Wang et al., 2019).

DFT is an accurate research method for small molecules and structures, but finds it somewhat difficult to calculate the large system. Meanwhile Molecular dynamics simulation (MD) has the advantage of describing and putting into statistics the properties of macromolecules and large systems. For this reason, MD is a good choice when studying larger-scale systems of mineral surfaces and interfaces. The dynamic statistical properties of mineral-water molecules (Li et al., 2018; Yu et al., 2021; Wang et al., 2021) and mineral-water molecules-reagents (Pei and Zhang, 2021; Yuan et al., 2021; Li et al., 2021; Chen et al., 2021) interface interactions can be simulated and analyzed. Surface wettability of montmorillonite (0 0 1) surfaces which are affected by its surface charge and exchangeable cations have been investigated through MD simulations (Yi et al., 2018). Decaethoxylated stearylamine (DEOSA) as the high-performance collector at solid-liquid interface for the selective flotation of hematite from quartz has been computed via the MD method. It emerges that quartz adsorbs much larger amounts of DEOSA than hematite owing to the electrostatic and hydrogen bonding interaction. DEOSA can significantly enhance quartz surface hydrophobics and efficiently remove quartz from hematite by selectively collecting quartz (Yang et al., 2021).

At present, the research on hydration mainly focuses on macroscopic testing and the hydration active site stage, but the cognition of the microscopic effect of actual hydration on the quartz surface and the guiding mechanism of inevitable solution metal cation is still not well understood. However, only a few studies on the MD method in the field of quartz surface hydration have been done. As mentioned above, quartz surface hydration in mine wastewater treatment and the process of deep purification is very important. In this study, MD was used to simulate the adsorption of water molecules and ions on the quartz surface. By analyzing the statistical properties of quartz-water/ion interface, such as concentration distribution, radial distribution function and diffusion coefficient, the adsorption characteristics of water/metal cations on quartz surface were analyzed. It reflects the quartz hydration properties and metal ion impact mechanisms; it would provide a theoretical basis for the control and cracking of the hydration layer on the fine mineral particles surface and the design and optimization of reagents.

2. Materials and methods

2.1. Simulation model

The simulation model is established by the Amorphous cell module in Materials Studio (MS) software. The quartz surface model is based on 7×2×1 crystal cell on α -quartz (001) surface with the volume of 34.742×34.251×17.765 Å³, and the water molecule model is SPC (Wu et al., 2006). This water molecular

model has been employed in the simulation of aqueous solution many times and exhibits good accuracy and adaptability. Furthermore, the density of water molecule clusters is controlled as 1.0 g / cm³, and the size of the box changes according to the number of water molecules. Based on the number of monolayer (ML) oxygen atoms (112) on the quartz surface, quartz-water interface structure models with water molecule coverage rates of 2 ML, 4 ML, 6 ML, 8 ML and 10 ML on the quartz surface were constructed. A vacuum layer of 80 Å should be added above the quartz-water interface model to prevent the interaction between adjacent layers from affecting the interface adsorption (as shown in Fig. 1). Based on the quartz-water interface model, a certain number of metal cations common in slurry were added to the simulation system. Furthermore, the positive charge in the corresponding anionic Cl-equilibrium system was added, so that the overall charge of the simulation system was zero. Similarly, a vacuum layer of 80 Å was added and the interface structure model of quartz/water/ion was finally constructed.

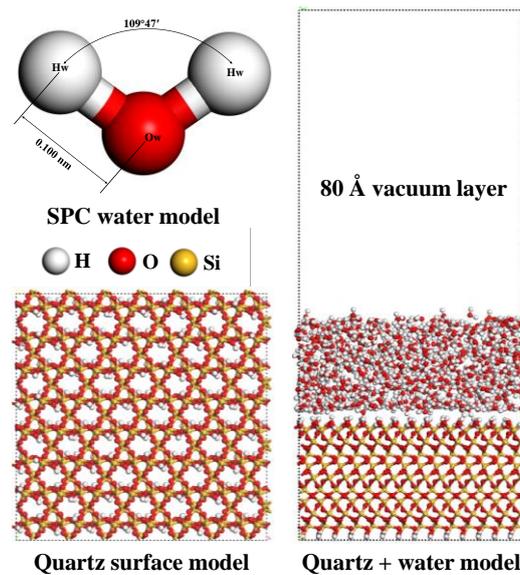


Fig. 1. Simulation model of the quartz-water interface

2.2. Simulation approach

All the dynamic simulations were done using the Forcite Plus module of Materials Studio 2017 software. We carried out molecular simulations to study structural and properties of quartz-water and quartz-water-ion interface with periodic boundary conditions. Firstly, the geometry optimization task was conducted to achieve the structural optimization and rationality of the interface models, and the conjugate gradient method served to conduct geometric optimization of the simulation system. The precision is set to fine. Convergence tolerance parameters are energy 1.0×10⁻⁴ kcal/mol, force 5.0×10⁻³ kcal/mol/Å, and displacement 5.0×10⁻⁵ Å, respectively.

During dynamic simulations, the pcff_interface force field is employed to depict the atomic interactions between quartz surface and the surrounding aqueous electrolyte solution. This forcefield has been successfully implemented to study the interactions and properties of inorganic-organic and inorganic-biomolecular interfaces (Heinz et al., 2013). The MD simulation is divided into two stages. The first stage aims to balance the stable molecular simulation configuration, the simulation duration is 600 ps, the ensemble is NVT, thermostat controlled by Nose algorithm, the initial velocity is random, the temperature is 298 K, step size set as 1fs. To simulate the system, energy changes and temperature changes are not measured until the system reaches a stable state. The purpose of the second phase of MD calculation is to make the properties of the simulation system stable, so as to facilitate the subsequent extraction and analysis of data.

The simulation duration was set as 300 ps, and the data was collected at intervals of 100 fs. The cut-off radius of the simulation was selected as 15.5 Å. In addition, the Ewald method calculated the electrostatic action of the system, and the Atom-based method served to calculate the Van der Waals

action. Meanwhile the structure and dispersion properties of the microcosmic interface region, such as concentration of water molecules or ions along the Z direction, radial distribution functions (RDF), mean square displacement (MSD) and self-diffusion coefficient (D) are calculated, respectively. Additionally, the interaction energy between the salt solution system and quartz surface can characterize the interaction between the two models and is calculated as follows:

$$E_{int} = E_{Q+A} - (E_Q + E_A) \quad (1)$$

where E_{int} is the interaction energy, E_{Q+A} is the total system energy, E_Q stands for the quartz surface energy, and E_A denotes energy of aqueous solution.

3. Results and discussion

3.1. Hydration properties of quartz interface

3.1.1. Concentration distribution of water molecules on quartz

The concentration distribution of water molecules in the Z direction was used to characterize the hydration structure. It is evident that the density of water molecules can be a relatively true indicator of surface hydration structure. Density distribution of water molecules in the Z direction under different water coverage models are processed based on the simulation results of the corresponding relative concentration. The distribution diagram and data of water molecules in the Z direction are obtained, as shown in Fig. 5 and Table 2, respectively.

As can be seen from Fig. 2 and Table 1, the water molecules on the quartz surface were structured and indicated hierarchical changes, and the density distribution of water molecules on the quartz surface proved the existence of the hydration layer on the quartz surface. When there are fewer water molecules on the quartz surface these molecules also form a hydration layer on the quartz surface, but only two layers formed. With the increase in the number of water molecules, three water molecule layers are formed on the quartz surface, and the structure water density increases with the rising water coverage, reaching the maximum value. When the water coverage is 6 ML, the density of interfacial water molecules realizes no significant increases with a higher water coverage such as 8 ML and 10 ML, where a slightly smaller situation is shown. It should be emphasized that the position gap between the three hydration layers is about 3 Å, which is close to the diameter of a single water molecule. Consequently, the quartz surface hydration layer consists of three layers of water molecules, the thickness being 8-10 Å. This is consistent with other studies done on the hydration layer of hydrophilic minerals.

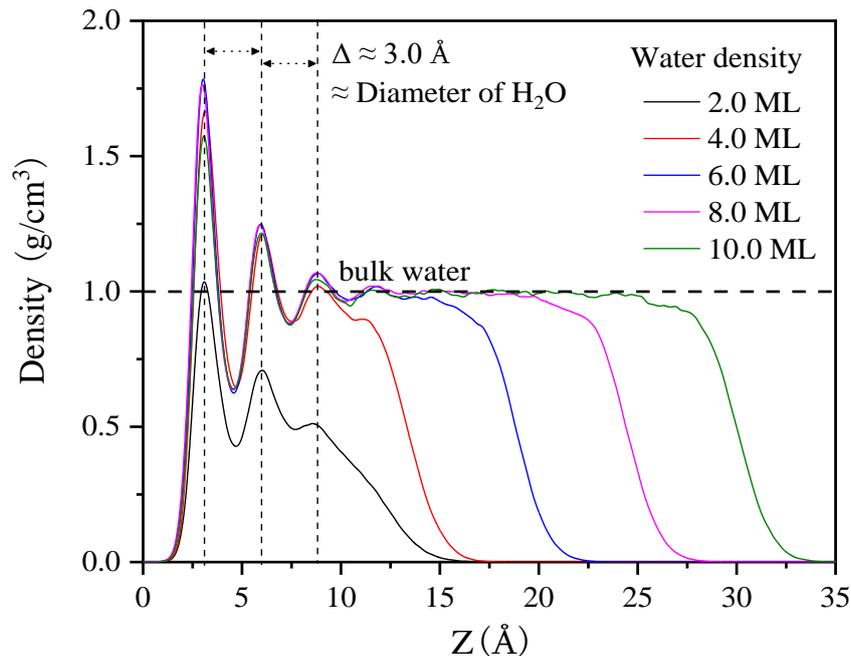


Fig. 2. Density distribution of water molecules in the Z direction under different water coverage scenarios

Table 1. Water density in hydration layer in the Z direction under different water coverage scenarios

Hydration layer	2 ML		4 ML		6 ML		8 ML		10 ML	
	Z (Å)	ρ (g/cm ³)								
1st	3.17	1.041	3.209	1.683	2.995	1.829	2.995	1.810	2.995	1.597
2nd	5.95	0.710	5.989	1.223	5.989	1.259	5.989	1.250	5.989	1.226
3rd	-	-	8.770	1.021	8.984	1.067	8.770	1.071	8.770	1.046

3.1.2 Radial distribution functions between interacting atoms

The RDF between surface atoms and water molecules can characterize the interaction between the quartz surface and water molecules to a certain extent. The peak width and peak intensity of the first peak between Os-Hw and Hs-Ow correspond to the interaction between quartz and water molecules, such as the relative distribution position and distance. Fig. 3 shows the RDFs between Os-Hw and Hs-Ow for different water coverage conditions.

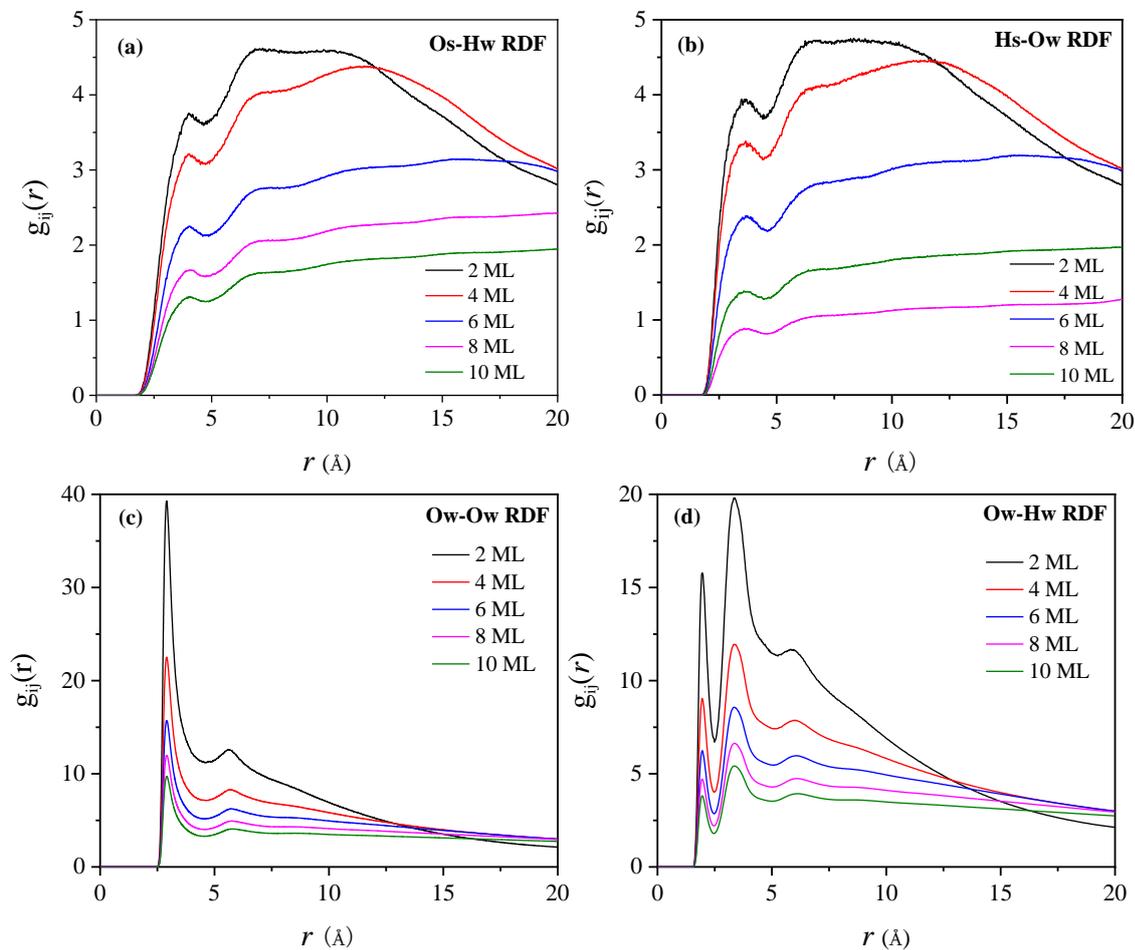


Fig. 3. Radial distribution functions between surface atoms and water molecules

As can be seen from Fig. 3 (a) and (b) the RDFs of Os-Hw and Hs-Ow both revealed a decreasing trend when the water coverage increased. Results show that when the number of water molecules increases: firstly, the interface effect between water molecules and quartz surface weakens; and secondly, the orderliness of water molecules on quartz surface diminishes.

The interaction between the interface and water molecules determines the properties of the interface water structure. The peak values of Ow-Ow and Ow-Hw RDF correspond to the distance between water

molecules and the hydrogen bond of water molecules, respectively, and also affect the order of water molecules. As can be seen from Fig. 3 (c) and (d), with the elevation in the coverage rate of water molecules, the interaction intensity between the interface and water molecules gradually weakens, and the order of water molecules also decreases.

3.1.3 Diffusion coefficient of the interface water

The mean square displacement curve of water molecules on the quartz interface is illustrated in Fig. 4.

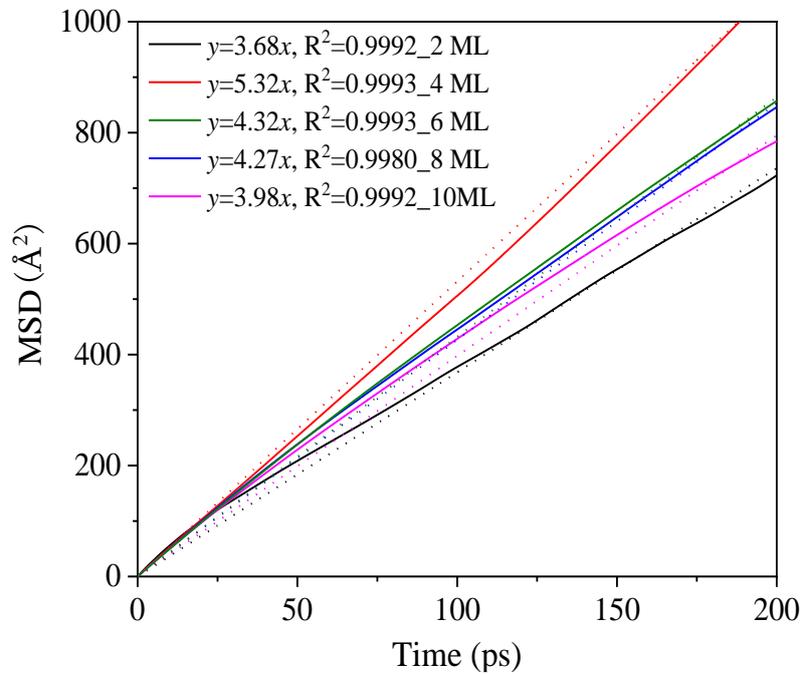


Fig. 4. MSD and linear fitting of H₂O on the quartz surface

The mean square displacement of surface water molecules varies under different water molecule coverages. It can be seen from Table 2 that the diffusion coefficient of water molecules is the largest when the water molecule coverage is 4 ML, reaching $8.87 \times 10^{-9} \text{ m}^2/\text{s}$. When the coverage of water molecules amounts to 2 ML, the diffusion coefficient of water molecules is the smallest, which is due to the slow diffusion of water molecules. This is caused by the interaction between water molecules and the surface when there are fewer water molecules. While, the surface-active sites are limited. With the increase of the number of water molecules, the surface adsorption and the cohesion between water molecules will form a coupling effect, affecting the mobility characteristics of water molecules.

Table 2. Self-diffusion coefficient (D) of H₂O on quartz (001) surface

Water coverage	2 ML	4 ML	6 ML	8 ML	10 ML
D (m ² /s)	6.13×10^{-9}	8.87×10^{-9}	7.20×10^{-9}	7.12×10^{-9}	6.63×10^{-9}

3.2. Ions' effect on interface water structure of quartz surface

3.2.1. Interfacial water and ions' distribution

The distribution of interfacial water molecules changes with the ions present, and the effect of ion type and concentration was also examined, as shown in Fig. 5. The distribution of water molecules on the quartz surface changed significantly in the presence of different metal ions. At low concentrations, the distribution of water molecules on the quartz surface is well ordered, which is due to the adsorption of metal ions on the quartz surface through electrostatic effects or in the form of hydrated cations, both of which increase the orderliness of water molecule arrangement on the quartz surface. As the

concentration increases, the active sites on the quartz surface are limited, as well as the repulsive effect between the same ions. What results is the distribution of some metal ions farther away from the quartz surface, which will attract surrounding water molecules to form hydrated cations through their own hydration ability, attracting more water molecules from the bulk phase into the second and third hydration layers. However, the greater the ion concentration, the stronger the electrostatic repulsive effect between ions, the stronger the hydration repulsive effect between hydrated cations. So, in the case of ions being highly concentrated the promotion of quartz surface hydration does not proceed smoothly. The concentration distribution curves of Na^+ and Ca^{2+} on the quartz surface show that the metal ions in the system are mainly distributed on the quartz surface (shown in Fig. 6), mainly through electrostatic adsorption, and Ca^{2+} is subject to greater electrostatic gravitational force than the monovalent ions on the quartz surface compared with Na^+ ions. So Ca^{2+} is better distributed on the surface of quartz. Ca^{2+} is still mainly distributed on the quartz surface when the concentration increases, while Na^+ gradually diffuse into the bulk water with the increase of concentration, so the relative concentration ratio of $\text{Ca}^{2+} > \text{Na}^+$ adsorbed on the quartz surface.

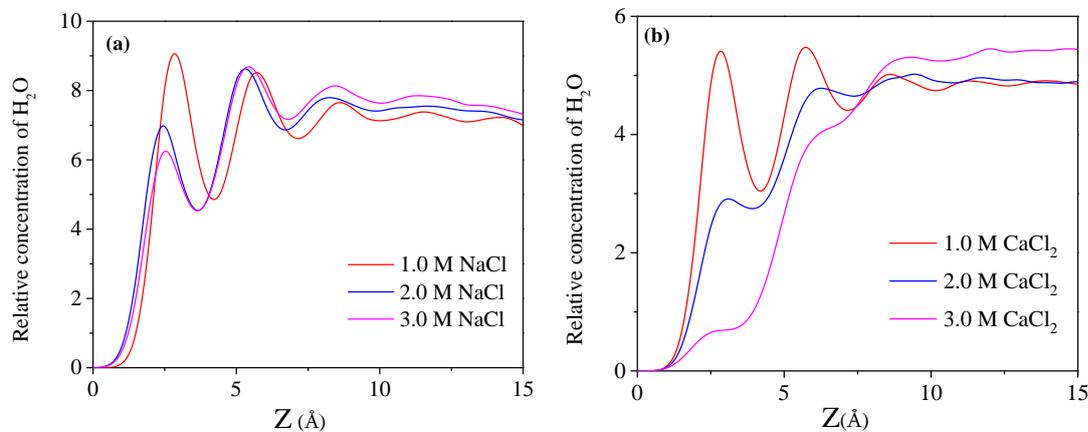


Fig. 5. Effect of metal ions on the interface water molecule distribution (a) NaCl, (b) CaCl_2

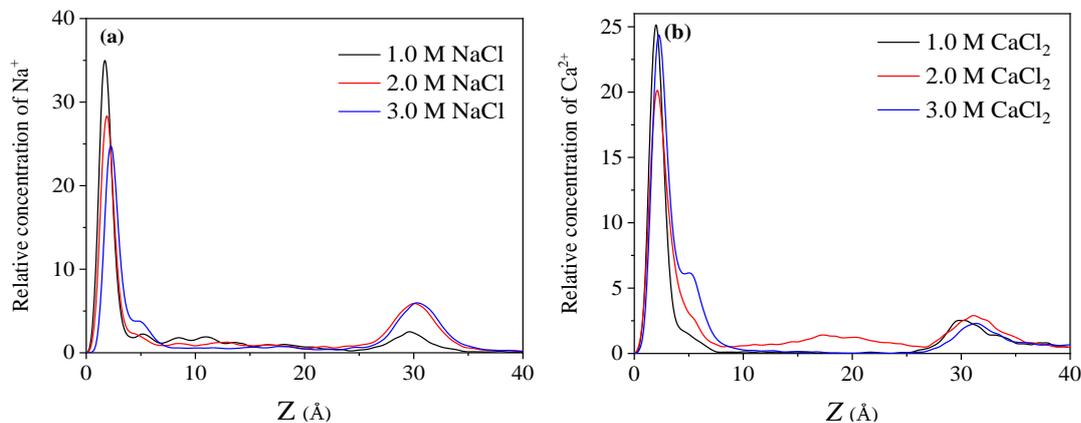


Fig. 6. Concentration profile of metal ions near the quartz surface (a) NaCl, (b) CaCl_2

3.2.2. Ions's effect on the interaction between surface and water molecules

In aqueous solution, ions can easily interact with water molecules owing to their surface charge, which affects the interaction between water molecules and the surface. Take Na^+ as an example to illustrate the effect of ion concentration on the interaction between water molecules and quartz surface (see Fig. 7). The analysis strongly suggests that in the presence of Na^+ , the distribution of water molecules around the surface changes. From the RDF, the concentration of Na^+ enables water molecules to be more distributed in the second and third hydration layers of the hydration layer on the quartz surface. This is consistent with the law of the concentration distribution curve of water molecules on the quartz

surface in the presence of ions. However, the higher the concentration, the stronger the mutual repulsion between ions, resulting in a decline in the ability of high concentration ions to promote interaction between water molecules and the quartz surface.

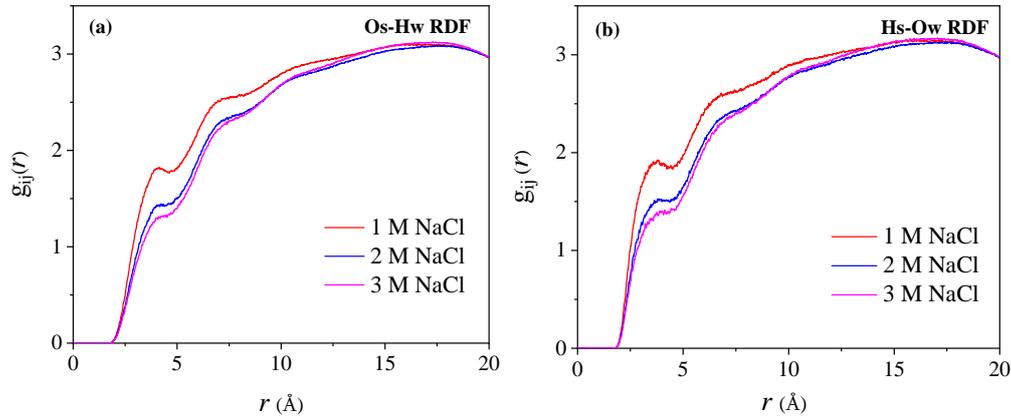


Fig. 7. Effect of ion concentration on the RDFs of Os-Hw (a) and Hs-Ow (b)

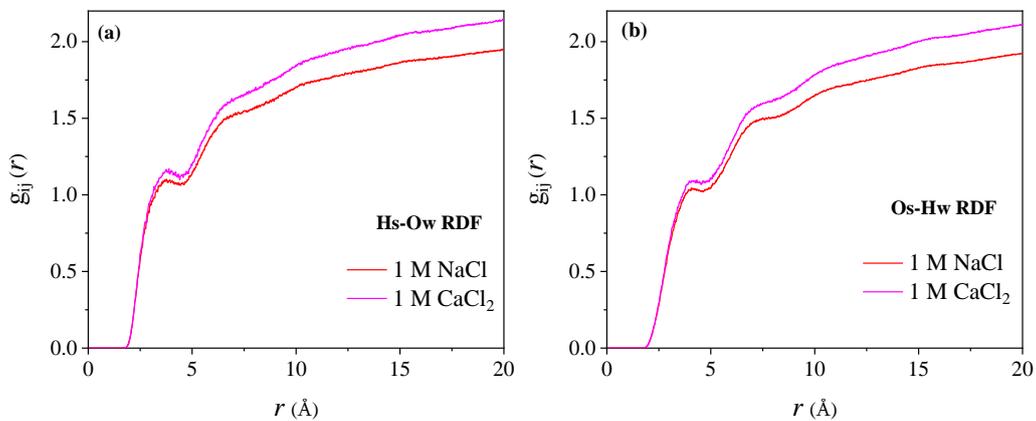


Fig. 8. Effect of ion types on the RDFs of Hs-Ow (a) and Os-Hw (b)

The ion types are also simulated and analyzed with the results depicted in Fig. 8. The hydration ability of different metal ions varies and their capacity to bind water molecules in aqueous solution is different, and so will be their influence on the interaction between quartz surface and water molecules. As shown in Fig. 8, under the action of Na⁺ and Ca²⁺, the interaction between water molecules and the surface has also altered. It is obvious that under the action of Ca²⁺, the arrangement order of water molecules on the surface of quartz is higher than that with Na⁺ present. Therefore, the order of promoting the hydration degree of quartz surface is Ca²⁺ > Na⁺. The influence of ion species on the interaction energy of the system is calculated and shown in Table 3.

It can be seen from Table 3 that the interaction energy of water molecular clusters on the quartz surface is -1.071 eV. When Na⁺ exists, the interaction energy of the system becomes -1.821 eV. In the presence of Ca²⁺ the interaction energy of the system is the largest, which is -1.896 eV. The interaction energy is relatively close to that in the presence of Na⁺, but slightly stronger. Results show that in the presence of metal ions, the interaction between quartz surface and water molecules is stronger, and ions hydration promotes the water molecules and quartz surface combining. The degree of strengthening the interaction between water molecules and quartz surface in the order of Ca²⁺ > Na⁺, is consistent with the order of hydration ability of metal ions as Ca²⁺ > Na⁺.

Table 3. Effect of ions on the interaction energy

Adsorption system	quartz/H ₂ O	quartz/H ₂ O/Na ⁺	quartz/H ₂ O/Ca ²⁺
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E_{int} (eV)	-1.071	-1.821	-1.896
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3.2.3. Effect of $\text{Na}^+/\text{Ca}^{2+}$ on on interfacial water structure

The RDF of the interaction between water molecules in the presence of metal ions was described in detail in Fig. 9, because the RDF related to how Hw removes the influence of the atoms on water molecules. Here, the RDF is the atoms in one water molecule relative to those in other water molecules. The presence of ions obviously enhances the interaction between water molecules. The existence of metal ions encourages molecules to gather more closely and become more orderly. This can be seen from the RDF curves of Ow-Ow and Ow-Hw. Under the action of metal ions, the probability of other water molecules around water molecules is significantly higher than that in bulk water. Because of its strong hydration ability, Ca^{2+} can significantly enhance the interaction and order of water molecules while forming hydrate cation. The existence of Na^+ enhances the interaction between water molecules, however, the effect is not as good as Ca^{2+} , which is determined by its hydration ability.

After studying the influence of ions on the hydrogen bond of their water structure in aqueous solution, some scholars put forward the concept of structure manufacturing and structure destruction ions, which initially refers to the increase or decrease of viscosity near ions. It is defined that ions with high charge density (high ion charge and small in size) are structure makers, while large ions with low charge density are structure destroyers (Marcus, 2009). However, Soper and Weckström (2006) pointed out that this definition is not accurate when looking at the research, because it was found that some large ions with low charge density destroyed the hydrogen bond in the water structure. Nonetheless, they formed a stronger interaction near the ions than the hydrogen bond. In this paper, Ca^{2+} obviously belongs to structural manufacturing ions, but according to the definition, alkali metal ions such as Na^+ belong to spheres with low charge density and mainly form electrostatic interaction in the solution. Some authors have documented that Na^+ is a weak structural manufacturing ion (Marcus, 2009), which is consistent with the view of this paper.

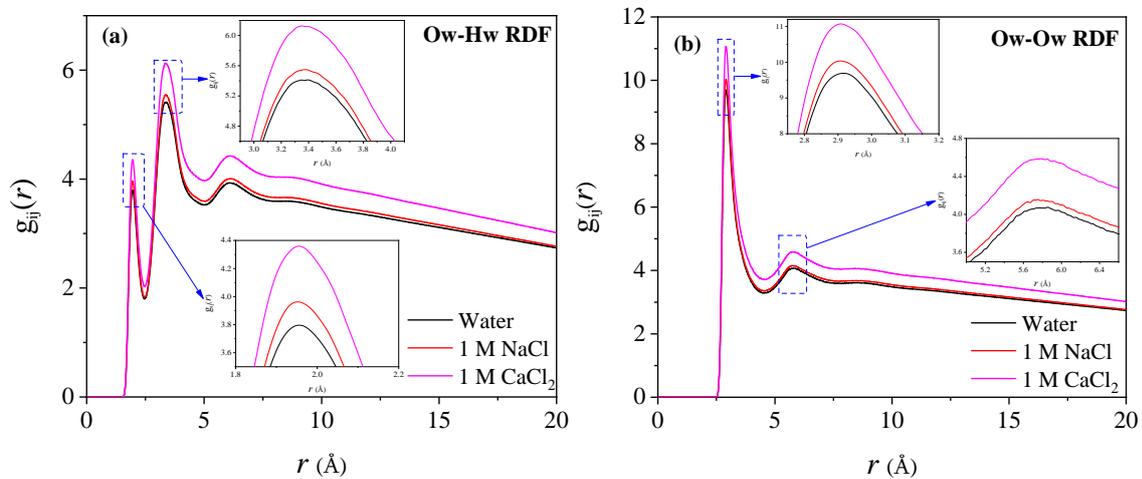


Fig. 9 Effect of ions species on the RDFs of Ow-Hw (a) and Ow-Ow (b)

3.2.4. Ions's effect on diffusion characteristics of water molecules

The mean square displacement curve of water molecules in the presence of different ions is calculated and shown in Fig. 10.

The self-diffusion coefficient of water molecules is 7.64×10^{-9} m²/s in water, and with the introduction of ions, the interaction between water molecules and quartz surface is enhanced. The interaction between water molecules is also improved, resulting in the enhancement of the order of water molecules, so that the movement of these molecules is bound to a certain extent, and the level of enhancement of Na^+ and Ca^{2+} on the interaction between water molecules and quartz surface is $\text{Ca}^{2+} > \text{Na}^+$. Therefore, in the presence of Na^+ and Ca^{2+} , the corresponding self-diffusion coefficients of water

molecules are $7.51 \times 10^{-9} \text{ m}^2/\text{s}$, and $7.11 \times 10^{-9} \text{ m}^2/\text{s}$, respectively. This is consistent with the conclusion that ions enhance the interaction between water molecules and quartz surface, and the effect on the order of water molecules

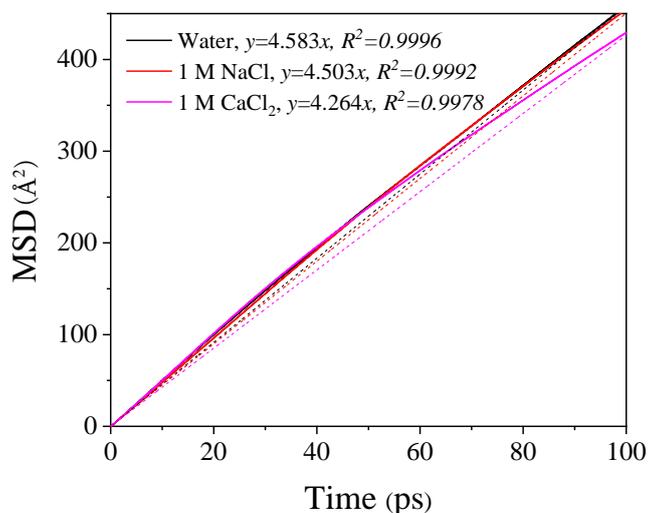


Fig. 10. Diffusion characteristics of H₂O with different ions present

4. Conclusions

Molecular dynamics simulation results show that the hydration layer on the surface of quartz is composed of three layers of water molecules, and the thickness of the hydration layer is 8-10 Å. Due to the quartz surface active sites and interface effect, the hydration layer on the quartz surface does not increase when the number of water molecules on the quartz surface rises. When the water molecule coverage is 6 ML, the interfacial water molecule density reaches its maximum. The interfacial water molecule density does not increase with bigger water coverage, but in fact falls slightly. The strength of the hydration layer follows the same rule.

In the presence of ions, the interaction energy changes from -1.071 eV in pure water to -1.821 eV (Na⁺) and -1.896 eV (Ca²⁺), respectively. The comparative analysis shows that the order of the enhanced interaction between water molecules and surfaces is Ca²⁺ > Na⁺, which is consistent with the hydration ability of metal ions. At low ion concentration, metal ions enhance the interaction between water molecules and the surface, and promote more water molecules to enter the second and third hydration layers on the quartz surface. With the increase of metal ion concentration, due to the combination of electrostatic action and ion hydration layer, more ions diffuse into bulk water, weakening ions' promotion of hydration. With the introduction of ions, the interaction between water molecules and the quartz surface is enhanced, as is the order between water molecules, resulting in a certain binding effect on the movement of water molecules. The degree of enhanced interaction between water molecules and quartz surface follows the order of Ca²⁺ > Na⁺. Therefore, in the presence of Na⁺, the diffusivity of water molecules is greater than that of water molecules in Ca²⁺ solutions.

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