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Enhancement of water self-diffusion at super-hydrophilic surface with ordered water*

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It has been well acknowledged that molecular water structures at the interface play an important role in the surface properties, such as wetting behavior or surface frictions. Using molecular dynamics simulation, we show that the water self-diffusion on the top of the first ordered water layer can be enhanced near a super-hydrophilic solid surface. This is attributed to the fewer number of hydrogen bonds between the first ordered water layer and water molecules above this layer, where the ordered water structures induce much slower relaxation behavior of water dipole and longer lifetime of hydrogen bonds formed within the first layer.

Keywords: ordered water layer, self-diffusion, dipole correlation, hydrogen bond

PACS: 01.30.–y, 05.20.–y, 05.70.Np, 05.90.+m **DOI:** 10.1088/1674-1056/27/6/060101

1. Introduction

Ordered water structures confined into two-dimensional ones have been found and extensively studied experimentally and theoretically.[1–11] It has been realized that this ordered water not only exhibits novel behavior but also affects various surface properties, such as the surface electrochemical property,[12–14] surface wetting behavior,[15–22] surface friction,[23,24] and so on. In 2009, we predicted a wetting phenomenon on a super-hydrophilic surface with a water droplet on an ordered water monolayer, termed "ordered water monolayer that does not completely wet water" at room temperature.[16,21,25–27] A similar phenomenon has been found on many real solid surfaces in several experimental[28] and computational researches,[14,20,29,30] including the metals Pt (100) and Pd (100),[17] sapphire,[28] talc,[20] Al_2O_3, SiO_2 surfaces,[30] etc. This ordered water can also induce the surface friction to decrease at a super-hydrophilic surface,[23] where the friction at this super-hydrophilic solid surface can be almost equal to that at a nonwetted surface. In the past few years, the diffusion behavior has been regarded as a key factor in the understanding of the surface lubrication,[31–35] catalysis reactions,[36] drug release rate in living organisms,[37] and recognition of biological molecules.[38] For example, faster diffusion behavior is important in the process when the drugs diffuse in blood environments and enter the tissues of the human body.[37] Usually, the diffusion of water molecules is partly determined by the interfacial interactions, which is usually the origin of the surface hydrophobicity or hydrophilicity.[39,40] Thus, it is generally accepted that there is a faster diffusion constant near the hydrophobic surfaces than near the hydrophilic surfaces.[39,41–48] Till now, considering the unexpected hydrophobicity-like behaviour of the ordered water, whether the ordered water structures can enhance the novel diffusion behavior near a super-hydrophilic surface is still unknown.

In this article, utilizing molecular dynamics (MD) simulations, we show that the water self-diffusion on the top of the first ordered water layer can be enhanced near the super-hydrophilic surface. This can be attributed to the fewer number of hydrogen bonds between the first ordered water layer and water molecules above this layer than that between the disordered water layer and the water molecules above this layer. The ordered water structures lead to a smaller water exchange rate between the first two layers, much slower relaxation behavior of water dipole and longer lifetime of hydrogen bonds formed within the first layer.

2. Simulation system and method

Using molecular dynamics simulations, we studied two types of theoretical surfaces with the planar hexagonal structure of different neighboring bond lengths (denoted as l), and the planar hexagonal structure composed of 1664 atoms. For

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these two types of surfaces, the positive and negative charges of the same quantity q ($q = 0.8e$) were assigned to the atoms that were located diagonally in neighboring hexagons (see the insert in Fig. 1(a)). Overall, the model solid surface was neutral. In this article, the type 1 surface had dimensions of 6.395 nm × 6.816 nm with a neighboring bond length l of 0.142 nm, and the type 2 surface had dimensions of 7.658 nm×8.16 nm with a bond length of 0.170 nm. These two surfaces correspond to the ordered and disordered water structures, respectively, which have been confirmed in our previous studies (see Figs. 1(c) and 1(d)).[26]

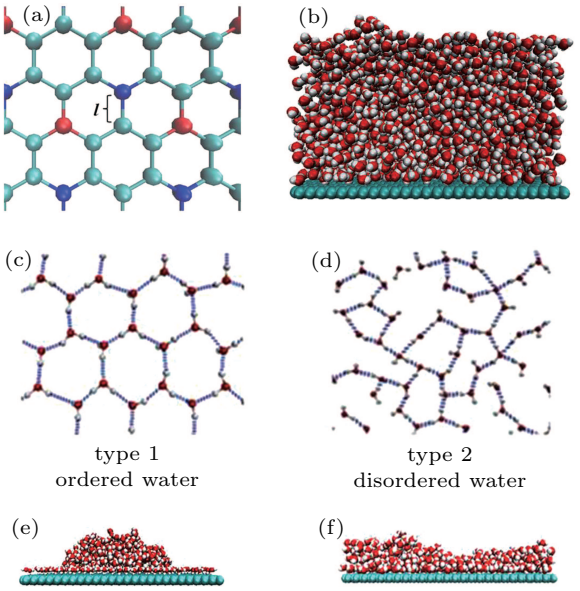


Fig. 1. (color online) (a) Geometry of solid surface model. Red and blue spheres represent solid atoms with positive and negative charges, respectively, while cyan spheres denote neutral solid atoms. (b) Side view snapshot of the first series simulation system. (c) Snapshot of ordered first water layer structure on type 1 surface ($l = 0.142$ nm), where water molecules show a regular two-dimensional ordered hexagonal structure together with H bonds (the blue lines) forming between the neighbor water molecules. (d) Snapshot of the disordered first water layer structure on type 2 surface ($l = 0.170$ nm). (e) Side-view snapshot of a water droplet on a water monolayer on type 1 surface ($l = 0.142$ nm). (f) Water film completely spreads on type 2 surface ($l = 0.170$ nm).

We simulated two series of systems. For the first series, the thickness of the water film was set to be 4.0 nm with the number of the water molecules of 5103 for the type 1 surface and 7166 for the type 2 surface, and the box sizes were set as 6.395 nm×6.816 nn×7.100 nm and 7.658 nm×8.160 nm×7.170 nm, respectively. For the second series, we added 838 water molecules on the type 1 surface and 1375 water molecules on the type 2 surface and the box sizes were 6.395 nm×6.816 nm×6.000 nm and 7.658 nm×8.160 nm ×6.000 nm, respectively. The simulation time was 5 ns, and the data in the last 1 ns were collected for analysis. All the MD simulations of our system (see Fig. 1(b)) in time steps of 1 fs were carried out with the Gromacs 4.5.4[49] in the NVT ensemble at a temperature of 300 K. The periodic boundary conditions were applied to all directions. The Lennard-Jones parameters of the solid atoms were $\varepsilon_{ss} = 0.105$ kcal/mol and $\sigma_{ss} = 3.343$ Å and we chose the rigid extended simple point charge (SPC/E) water model[50] as the explicit solvent. The particle-mesh Ewald method[52] with a real space cutoff of 10 Å was used to treat long-range electrostatic interactions, and 10-Å cutoff was applied to all van der Waals interactions. Besides, the criterion for the hydrogen bond between water molecules was that the O–O distance was less than 3.5 Å and the angle H–O···O was less than 30° simultaneously.

3. Results and discussion

For type 1 surface ($l = 0.142$ nm, $q = 0.8e$), our simulation results indicate a special wetting behavior termed "ordered water monolayer that does not wet water" at room temperature (see Fig. 1(e)), which is consistent with our previous work.[16] Although the contact angle of the water droplet on the water monolayer is 63°, characterizing the hydrophobicity of the monolayer, the solid surface is super-hydrophilic. In contrast, for type 2 surface ($l = 0.170$ nm, $q = 0.8e$), no water droplet is formed (see Fig. 1(f)). We discuss the normalized density profiles for the oxygen atoms of water molecules. As shown in Fig. 2(a), we can observe that there are two obvious peaks of oxygen atoms, which indicates that these two types of surfaces both have significant influence on the behavior of the water molecules above.

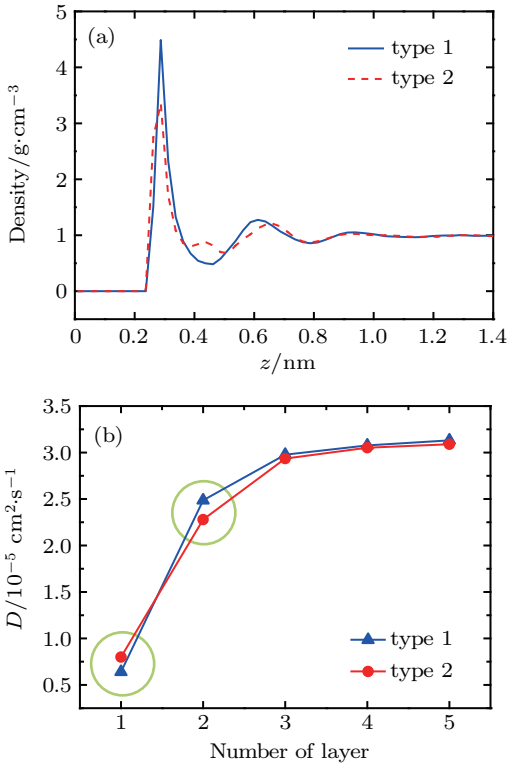


Fig. 2. (color online) (a) Normalized atom density profiles for water O atoms, $\rho(z)/\rho_0$ (ρ_0 is bulk atom density for O atoms), along z axis perpendicular to ionic surface. (b) Diffusion constant of different water layers for two types of surfaces.

From the analysis of oxygen atom density profiles, we can determine the thickness of the first water layer in contact with these two types of surfaces to be 0.40 nm. We then calculate the self-diffusion constant of water molecules near the solid surface as a function of the distance between water molecule and the plate in an equilibrium system. For simplicity, we can assume the subsequent layer thickness values of the second (0.40 nm $\leq z <$ 0.80 nm), third (0.80 nm $\leq z <$ 1.20 nm), fourth (1.20 nm $\leq z <$ 1.60 nm) and fifth layers (1.60 nm $\leq z <$ 2.00 nm) to be the same, i.e., 0.40 nm. In our study, the two-dimensional (2D) diffusion constant D in the xy plane can be obtained from the Einstein relation:

$$D = \frac{\langle |r(t) - r(0)|^2 \rangle}{4t}. \quad (1)$$

We show the self-diffusion constant D versus the different layer of water in Fig. 2(b). Due to the large partial charge quantity $q = 0.8e$, the solid surfaces are super-hydrophilic.[23] As one can observe, we find the diffusion constant corresponding to the first water layer, $D_{\text{type 1}} = 0.64 \times 10^{-5}$ cm^2/s, which is 20% smaller than $D_{\text{type 2}} = 0.80 \times 10^{-5}$ cm^2/s. These two self-diffusion values are much smaller than the bulk water self-diffusion value of 2.95×10^{-5} cm^2/s. However, to our surprise, the self-diffusion constant for layer 2 near the type 1 surface $D_{\text{type 1}} = 2.49 \times 10^{-5}$ cm^2/s, which is 9% larger than $D_{\text{type 2}} = 2.28 \times 10^{-5}$ cm^2/s. Then as z further increases, the self-diffusion constants gradually converge to 2.95×10^{-5} cm^2/s, which is close to the self-diffusion constant of the bulk water at room temperature.[40]

Why is the diffusion at the first layer (0 nm $\leq z <$ 0.40 nm) near the type 1 surface smaller than that on the type 2 surface, but the diffusion at layer 2 (0.40 nm $\leq z <$ 0.80 nm) near the type 1 surface is larger than that on the type 2 surface? We investigate the first water layer and calculate the number of hydrogen bonds, N_{HB}, formed per water molecule in the first layer with the water molecules above for type 1 and 2 surfaces (see Fig. 3). We find that $N_{\text{HB}} = 0.752$ for the type 1 surface with $l = 0.142$ nm, which is fewer than that for the type 2 surface with $l = 0.170$ nm ($N_{\text{HB}} = 0.965$). Correspondingly, the hydrogen bond number within the first layer is 2.099 for the type 1 surface, which is larger than that for type 2 surface ($N_{\text{HB}} = 2.010$). The fewer number of hydrogen bonds leads to a decrease of the attraction energy between each water molecule in the water monolayer and the water molecules above. Consequently, the fewer number of hydrogen bonds should be the physical origin of the larger diffusion constant of the second water layer contacting the water monolayer of the type 1 surface than the case of the type 2 surface.

The special arrangement of the dipoles on the solid surface has an important influence on the formation of the 2D ordered water structure as well as the number of internal hydrogen bonds. Thus, we calculate the probability distribution of water dipole orientation angle φ, which is the angle between the projection of a water molecule dipole orientation onto the xy plane and a crystallographic direction (see the insert in Fig. 4). There is a clear orientation preference of the water dipole near the type 1 surface with three peaks at 30°, 150°, and 270°, indicating a more ordered water layer for the type 1 surface. However, the peaks are much smaller for the type 2 surface with $l = 0.170$ nm, even though the charge quantity of the atoms is the same ($q = 0.8e$).

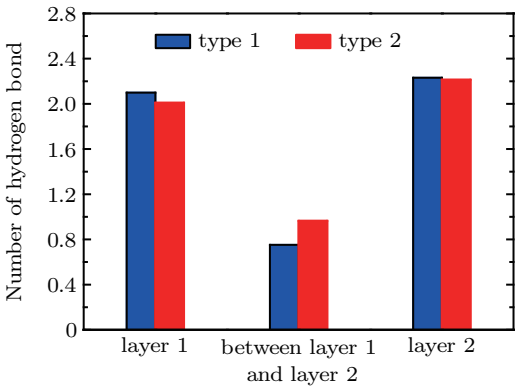


Fig. 3. (color online) Average number of hydrogen bonds formed at layer 1, layer 2, and between layer 1 and layer 2. Type 1 and type 2 are represented in blue and red respectively.

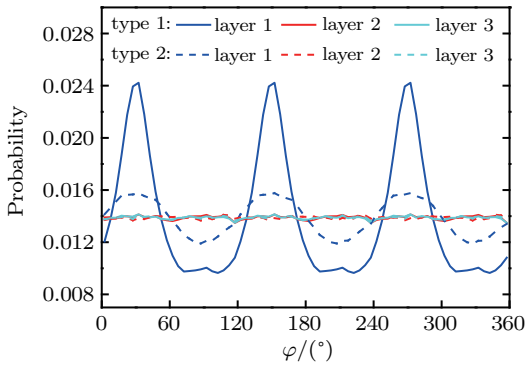


Fig. 4. (color online) Curves of angular probability distribution versus angle φ between xy plane projection of dipole orientation of each water molecule in the first water layer and axis direction for two types of surfaces.

Clearly, compared with disordered water on the type 2 surface, these ordered hexagonal configurations lead to an increase of the number of hydrogen bonds within the monolayer, and a small self-diffusion constant of water molecules near this ordered monolayer. We also calculate the exchange behavior of water molecules between layers 1 and 2 (see the inset in Fig. 5), which is characterized by the exchange number and exchange rate between the first two water layers. The exchange number is defined by the number of exchanged water from the first layer to the second layer, and the exchange rate is defined as the ratio of the number of exchanged water molecules to the number of water in the first layer. It is

obvious that both the exchange number and the exchange rate between the first layer and second layer near the type 1 surface are smaller than those of type 2, which may be due to the more ordered first water layer on the type 1 surface.

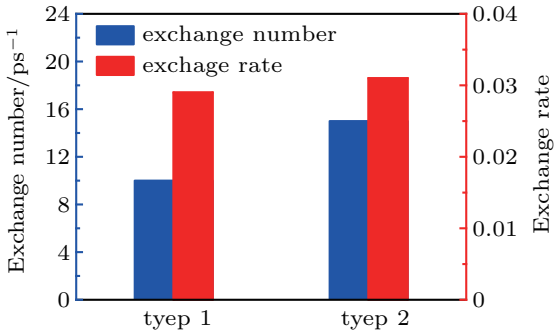


Fig. 5. (color online) Exchange behaviors of water molecules between layers 1 and 2. Blue and red columns represent the exchange number and exchange rate respectively.

In addition, we study the correlation of dipole orientation for the first layer water. And we extract the average timescale governing orientational reorganization from this dipole autocorrelation function

$$C(t) = \langle u(0) \cdot u(t) \rangle - |\langle u \rangle|^2, \tag{2}$$

where the angle brackets represent an average over all electrode-adsorbed water molecules. We note that in the bulk liquid the $\langle u \rangle$ will vanish and it does not necessarily stay at the surface. As shown in Fig. 6, water molecules on two types of surfaces yield significantly slower relaxation ($\tau_{\text{type 1}} = 35.4$ ps, $\tau_{\text{type 2}} = 30.4$ ps) than bulk water ($\tau_{\text{bulk}} = 5.1$ ps), and the relaxation of water molecules near the type 1 surface is slower than near the type 2 surface. This indicates that the relaxation dynamics of ordered water layer is slower than that of disordered water.

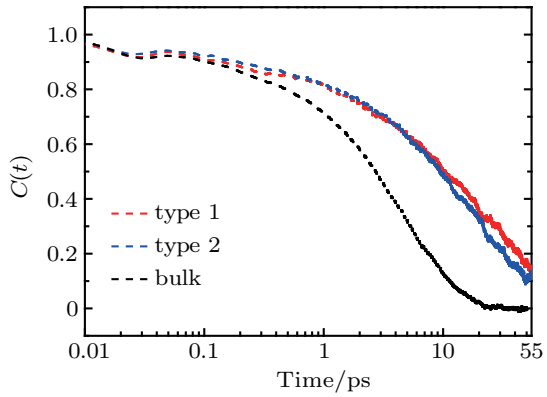


Fig. 6. (color online) Time-dependent dipole autocorrelation functions for water molecules adsorbed on the type 1 (red line) and type 2 (blue line) surface. Corresponding time-dependent function for molecules in the bulk liquid is plotted as black line.

We also calculate the hydrogen bond lifetime of the water molecules in layers 1 and 2 and between layer 1 and layer 2 for these two types of surfaces (see Fig. 7(a)). In this article, the relaxation time of hydrogen bonds is characterized by the hydrogen bond autocorrelation function

$$C(t) = \frac{\langle h(0)\, h(t) \rangle}{\langle h(0)\, h(0) \rangle}, \tag{3}$$

where $h(t) = 1$ if the tagged water pair is continuously hydrogen bonded from time 0 to time t, and $h(t) = 0$ otherwise. $C(t)$ describes the probability with which a pair of water molecules becomes hydrogen bonded at time $t = 0$ and continuously hydrogen bonded at time t. As shown in Fig. 7(b), we show that for water molecules at layer 1, their hydrogen bond lifetime of the type 1 surface is 24.43 ps,which is larger than that 16.32 ps of the type 2 surface, but for water molecules between layer 1 and layer 2, their hydrogen bond lifetime of the type 1 surface is 6.69 ps smaller than that of the type 2 surface (8.85 ps). This is mainly attributed to the fact that the water molecules in the first layer of the type 1 surface prefer to form hydrogen bonds with the water molecules in the first layer, rather than between the monolayer and the water molecules above. This is quite consistent with the slower relaxation behavior of the ordered water and the larger number of hydrogen bonds formed within the monolayer than the number of hydrogen bonds formed between the ordered water monolayer and the water molecules above.

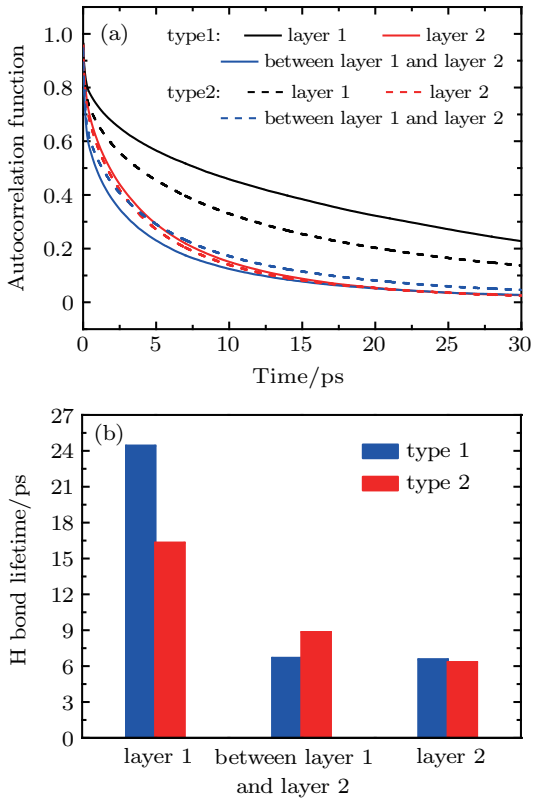


Fig. 7. (color online) (a) Plots of time-dependent hydrogen bond autocorrelation function $C(t)$ for type 1 (solid lines), type 2 (dashed lines) of layer 1 (black lines), layer 2 (red lines), and between layer 1 and layer 2 (blue lines). (b) Average relaxation times of water molecules at layer 1, layer 2, and between layer 1 and layer 2 for these types of surfaces.

4. Conclusions

In this work, we have studied the diffusion behaviors, the dynamics of hydrogen bonds, and the structures of water molecules on different types of surfaces via molecular dynamic simulations. We find that the water molecules diffuse faster on the top of the ordered water molecules near the surface, which is due to the reduction of hydrogen bonds between the water molecules in the ordered water layer and the water molecules above this layer. These water molecules with the ordered water structures also characterize the much slower relaxation time of water dipole and the longer lifetime of hydrogen bonds in the first layer. Our view in the present work is different from the conventional view of slower self-diffusion near the hydrophilic solid surface and provides a new way to enhance the water self-diffusion near the hydrophilic surfaces. Considering that the room temperature ordered water has been found to extensively exist on a variety of material surfaces,[14,16,19,20,26,28,29,52] we believe that this work will soon evoke more extensive experiments.

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