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Ion diffusion on amorphous ice surface

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In interstellar molecular clouds, various molecules (for instance, H2O, NH3, CO, CO2, and so on) are formed from elements such as H, C, O, and N [1]. Most of H2O exists as a thin shell of amorphous ice around dust grain. The molecules undergo chemical evolutions to organic molecules through various processes on the surface of amorphous ice [2]. Thus, the surface structure of amorphous ice is an important factor to understand the molecular evolution of organic molecules in molecular clouds [3]. To investigate the effects of adsorption of ion on the surface structure of amorphous ice, the molecular dynamics (MD) calculations of amorphous ice with ions (H+, NH4+, and NO3−) were performed.

The MD calculations were performed using an atom-atom potential model, KAWAMURA potential model [4]. The amorphous ice was prepared by quenching of a liquid phase consisting of 2760 water molecules from 280 to 235 K with 2.5 K/fs in cooling rate. After annealing at 235 K, the system was cooled to 10 K with 2.5 K/fs. To equilibrate the fundamental cell, the MD code was run for 40 ps at 10 K. Then, an ion (H+, NH4+, or NO3−) was put in a position, such the center of ion was at a distance of 0.5 nm from the outermost hydrogen atom in surface. Then, the temperature was changed to a temperature in the range of 15–130 K to analyze the ion diffusion. An infinite surface was simulated by replicating the cell in the directions parallel to the surface using periodic boundary conditions. The pressure was kept at 0.1 MPa. The layer with 0.5 nm in thickness from the outmost atom was analyzed as the surface layer.

From an observation of the trajectory of ion on the surface, the diffusion mechanism was analyzed. The result shows that the adsorbed H+ diffuses on the surface with formation and dissociation of H3O+. Using the frequencies of the formation and dissociation of H3O+, the activation energy of diffusion of H+ was estimated. On the other hand, no diffusion hop was observed for NH4+ and NO3− in the simulation period of 80 ps. The adsorbed NH4+ (or NO3-) forms four (or three) hydrogen bonds with water of the surface layer. Therefore, the activation energies for the ions are extremely higher than that for H+. The atomic displacement parameters (ADP) of oxygen and hydrogen of water molecules in surface layer increase during the adsorption of NH4+ and NO3−. This suggests that, the rotational motion of water is one of the driving forces of hops for NH4+ and NO3−. The effects of ion adsorption might have important implications for surface reaction in interstellar molecular clouds.

References

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Significance statement

To investigate the effects of ion adsorption on surface structure of amorphous ice, the molecular dynamics calculations of amorphous ice with ions (H+, NH4+, and NO3-) were performed. From the results, the processes and mechanisms of adsorption and diffusion are discussed.

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