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Molecular Dynamics Simulation of Amorphous Ice on Interstellar Dust

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Interstellar dust has a silicate core and a mantle of amorphous ice. It is supposed that organic molecules are synthesized on the amorphous ice. In order to investigate the details of the synthesizing process, the structure of the amorphous ice at the atomic scale should be known. However, it is still unclear. Some laboratory experiments were carried out to create a simulated amorphous ice by vapor-depositing onto the surface of a base material. Recently, atomic force microscopy observed the detailed structure of the simulated amorphous ice [1]. A theoretical study using Monte Carlo simulations has created an amorphous ice model with a spherical model of water molecules, ignoring the explicit shape of the water molecule [2]. Therefore, the detailed atomic-scale structure remains unknown. In this study, we conducted a molecular dynamics simulation that explicitly treats water molecules to simulate the formation process of simulated interstellar dust surface amorphous ice. We obtained results consistent with the previous Monte Carlo simulation [1] and the observations [2].

References

[1] T. Tomaru et al. (2024), *Phys. Chem. Chem. Phys.* 26, 15232–15239.

[2] A.R. Clements et al. (2018), *Phys. Chem. Chem. Phys.* 20, 5553–5568.