H and D diffusion on interstellar water ices

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Studies of surface diffusion of atoms on interstellar ices are a popular topic in the field of Astrochemistry. These chemical processes occur at very low temperatures (e.g., around 10K). At low temperatures, quantum tunneling becomes a dominant factor deciding the diffusion through barriers [1]. Therefore, quantum tunneling must be taken into account in calculating rate constants. Here, I discuss the single H and D atom diffusion on crystalline (I_h) and amorphous ice surfaces (ASW). The harmonic transition state theory was used to calculate the rate constants, and the Wigner tunneling correction was employed as well as a tunneling correction based on the Eckart potential to address the tunneling effect. The adaptive kinetic Monte Carlo method was applied to analyze the random walk trajectories [2]. A range of diffusion coefficients were found at low temperatures [3].

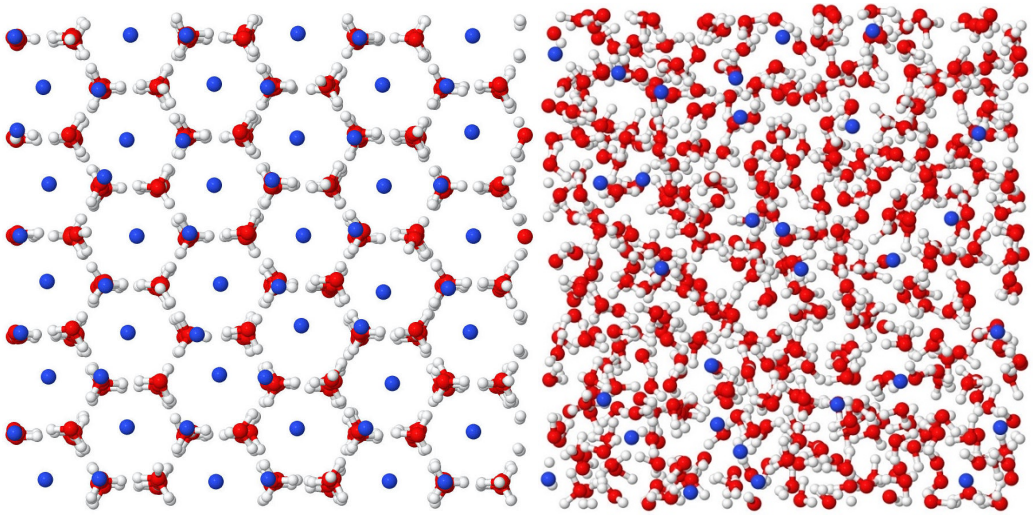

Figure 1: A map of local minima on a crystalline ice surface (left) and on an ASW surface (right). The blue dots are the local minima and the red and blue are O and H atoms of the water molecules. There are 59 local minima on the I_h surface and 30 local minima on the ASW surface.

References

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