Nuclear quantum effect in the phase transition between Ice VII and ice X

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Water is one of the most abundant and essential substances on Earth, playing a critical role in the diversity of nature and natural phenomena, including the existence of life. Despite being composed of a single molecule, H_2O, ice is a complex substance with 17 different stable structures. As a result, it is an important model for studying hydrogen modeling[1]. At room temperature and pressure between 2 and 60 GPa, ice VII is a stable crystalline phase, where the oxygen atoms form a body-centered cubic structure, with the hydrogen atoms being delocalized between the two oxygen atoms (Fig. 1(a)). Infrared spectroscopy has confirmed that above 60 GPa, ice VII undergoes a phase transition to ice X, in which the hydrogen atoms lie midway between the two oxygens[2]. Although the phase transition from ice VII to ice X is a change in the symmetry of the hydrogen atom, the behavior of the hydrogen atom is still unknown due to the difficulty of conducting neutron diffraction experiments under high-pressure conditions. To address the gap, this study uses the path integral molecular dynamics method (PIMD), which can treat the nuclear quantum effect, to theoretically clarify the behavior of hydrogen atoms in the phase transition from ice VII to ice X.

We conducted three types of PIMD simulations to study the impact of the nuclear quantum effect: the simulation for hydrogen atoms (QM(H)), for deuterium atoms (QM(D)), and the classical simulation without nuclear quantum effect (CL). To analyze the phase transition, we used the difference in distance between the two oxygen atoms and the hydrogen atom (δ_{OH}) as a guide. At a lattice constant of 2.9 Å, the hydrogen atoms in the CL simulation were found to be localized on one oxygen atom, while in the QM(H) and QM(D) simulations, the hydrogen atoms were delocalized, and the distribution at $\delta_{\mathrm{OH}} = 0$ Å was increased. Across all simulations at a lattice constant of 2.9 Å, the distribution displayed two peaks, indicating the phase was ice VII. Upon reducing the lattice constant to 2.78 Å, the distribution in QM(H) displayed only one peak, suggesting that the nuclear quantum effect promotes the phase transition. Futher details will be presented in a poster.

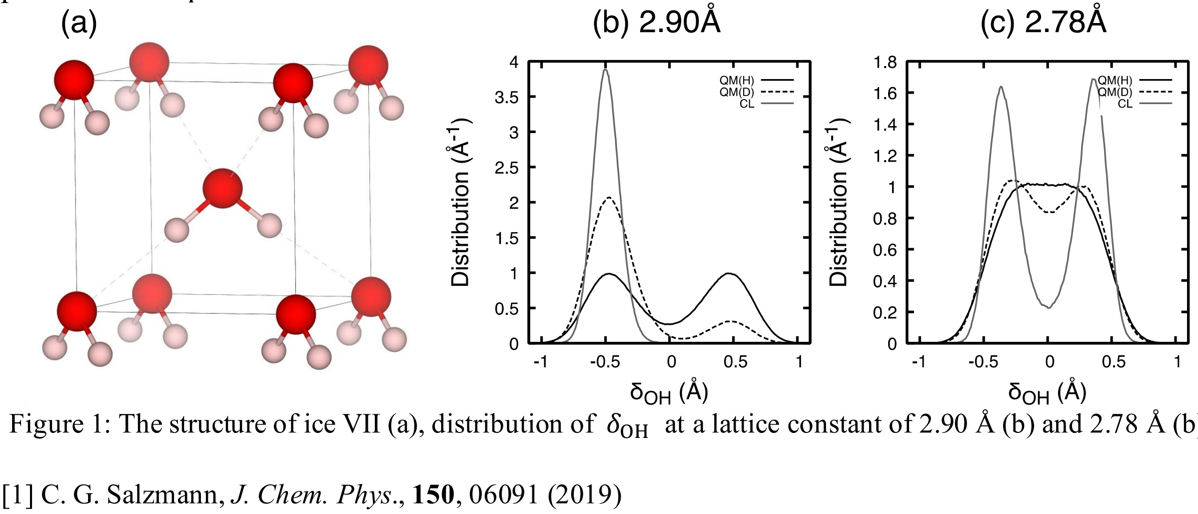

Figure 1: The structure of ice VII (a), distribution of δ_{OH} at a lattice constant of 2.90 Å (b) and 2.78 Å (b)

[1] C. G. Salzmann, *J. Chem. Phys*., **150**, 06091 (2019)
[2] K. Aoki, H. Yamawaki, M. Sakashita, and H. Fujihisa, *Phys. Rev. Let*. **76**, 5, (1996)