Hexagonal ice density dependence on inter atomic distance changes due to nuclear quantum effects

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Hexagonal ice is the most common form of ice as it is that appears at standard structure, impacting fields like atmospheric chemistry, cryobiology, and materials science.[1] Despite its simple chemical structure, their density displays anomalous behavior, and the nature of its hydrogen bonds remains not fully understood.[2] While classical models have been useful in studying ice phases, their accuracy is often limited. Advances in *ab initio* molecular dynamics (AIMD) offer more precise simulations, though they are constrained by system size and computational demands. In this way, machine learning potentials offer an efficient way to represent the potential energy surface, and thus are appealing for performing molecular dynamics (MD) by integrating the accuracy of *ab initio* calculations with computational efficiency comparable to classical MD.[3] Nuclear quantum effects (NQEs), particularly significant for light atoms like hydrogen, can alter the properties of water and ice. Recent studies have shown that including NQEs enhances the structural properties of ice.[4] This work aims to explore the impact of NQEs on structural properties of {\iceIH} through Deep Potential Molecular Dynamics (DP-MD) and Deep Potential Path Integral Molecular Dynamics (DP-PIMD), revealing that NQEs influence bond lengths and intermolecular distances, ultimately increasing equilibrium density across various exchange-correlation functionals.

References

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Figures

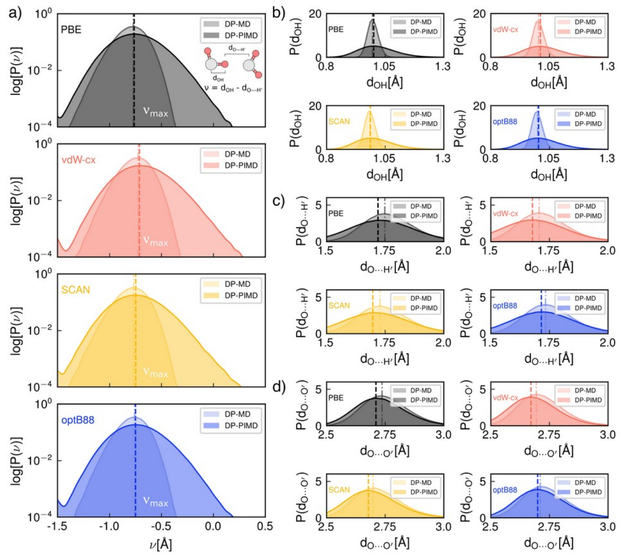

Figure 1. Distributions of a) proton transfer coordinate $\ nu$ and bond distances of b) intramolecular oxygen-hydrogen (\$\rm{d_{OH}}\$), c) intermolecular oxygen-hydrogen (\$\rm{d_{O\cdots H}}\$) and d) oxygen-oxygen (\$\rm{d_{O\cdots O}}\$) obtained via DP-MD and DP-PIMD simulations for different XC functionals. For all distributions, the dashed (dash-doted) line represents the most probable value for the bond length of DP-PIMD (DP-MD) simulations.