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Nuclear momentum distribution and potential energy surface in hexagonal ice¹ LIN LIN, Princeton University, JOSEPH MORRONE, Columbia University, ROBERTO CAR, Princeton University, MICHELE PARRINELLO, ETH Zurich — The proton momentum distribution in ice Ih has been recently measured by deep inelastic neutron scattering and calculated from open path integral Car-Parrinello simulation. Here we report a detailed investigation of the relation between momentum distribution and potential energy surface based on both experiment and simulation results. The potential experienced by the proton is largely harmonic and characterized by 3 principal frequencies, which can be associated to weighted averages of phonon frequencies via lattice dynamics calculations. This approach also allows us to examine the importance of quantum effects on the dynamics of the oxygen nuclei close to the melting temperature. Finally we quantify the anharmonicity that is present in the potential acting on the protons.

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