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Proton momentum distributions in water: A path integral molecular dynamics study VARADHARAJAN SRINIVASAN, JOSEPH A. MORRONE, Dept. of Chemistry, Princeton University, Washington Road, NJ 08544, DANIEL SEBASTIANI, Dept. of Spectroscopy, Max-Planck-Institut fuer Polymerforschung, ROBERTO CAR, Dept. of Chemistry/ PRISM, Princeton University — Recent neutron Compton scattering experiments have detected the proton momentum distributions of water. This density in momentum space is a quantum mechanical property of the proton, due to the confining anharmonic potential from covalent and hydrogen bonds. The theoretical calculation of this property can be carried out via "open" path integral expressions. In this work, we present an extension of the staging path integral molecular dynamics method, which is then employed to calculate the proton momentum distributions of water in the solid, liquid, and supercritical phases. We utilize the SPC/F2 empirical force field to model the system's interactions. The calculated momentum distributions depict both agreement and discrepancies with experiment. The differences may be explained by the deviation of the force field from the true interactions. These distributions provide an abundance of information about the environment and interactions surrounding the proton.

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