Abstract Submitted
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Signatures of Water Dissociation at Extreme Conditions in Vibrational Spectra and Ionic Conductivity from ab initio Simulations[1] VIKTOR ROZSA, University of Chicago, DING PAN, Hong Kong University of Science and Technology, GIULIA GALLI, University of Chicago; Argonne National Laboratory — Predicting the properties of water at high pressure and temperature is critical to understanding hydrogen bonding, charge transport, and phase stability of aqueous media in the Earth and outer planets. Here we employed ab initio molecular dynamics and density functional perturbation theory, as implemented in the Qbox code [1] to study ionic conductivity and infrared and Raman spectra of water at 10 and 20 GPa and 1000 K, as well as those of an amorphous solid phase at 16 GPa, and 500K. We identified specific signatures of proton hopping and molecular dissociation in the IR spectra at 20 GPa, which may be used to guide future experiments, as well as signatures of molecular diffusivity in the low frequency portion of Raman spectra, which help discern between amorphous and liquid phases at high pressure. We also computed ionic conductivities using maximally localized Wannier functions. We used our results at 20 GPa and 1000 K to address the existence of possible plastic and amorphous ice phases, recently proposed to potentially mediate the ice VII melting line.
[1] http://qboxcode.org

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