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Ab initio Raman spectroscopy of water under extreme conditions

VIKTOR ROZSA, DING PAN, QUAN WAN, GIULIA GALLI, Institute for Molecular Engineering, University of Chicago — Water exhibits one of the most complex phase diagrams of any binary compound. Despite extensive studies, the melting lines of high-pressure ice phases remain very controversial, with reports differing by hundreds of Kelvin. The boundary between ice VII and liquid phase is particularly disputed, with recent work exploring plasticity and amorphization mediating the transition. Raman measurements are often used to fingerprint melting, yet their interpretation is difficult without atomistic modeling. Here, we report a study of high P/T water where we computed Raman spectra using a method [1] combining ab initio molecular dynamics and density functional perturbation theory, as implemented in the Qbox code [2]. Spectra were computed for the liquid at 10 and 20 GPa, both at 1000 K, and for solid ice VII (20 GPa, 500 K). Decomposing the spectra into inter and intra molecular contributions provided insight into the dynamics of the hydrogen-bonded network at extreme conditions. The relevance of our simulation results for models of water in Earth, Uranus, and Neptune will be discussed, and an interpretation of existing experiments at high pressure will be presented. [1] Wan, Q., Spanu, L., Galli, G., Gygi, F., J. Chem. Theory Comput. 9, 4124. (2013) [2] http://qboxcode.org

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