TITLE: Superionic water at planet interior conditions—an ab initio molecular dynamics study

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ABSTRACT:

The phases and equation of states of water have been of interest in physics and planetary science. Over the past few years, there has been numbers of work on this subject using density functional theory which significantly improve our knowledge in these aspects. This includes new ground-state structures[1], formation of hydrogen-rich non-stoicheometric H-O compounds at 13 Mbar[2], and decomposition into H_2O_2 and a hydrogen-rich phase at 50 Mbar[3], etc. At megabar pressures, with increasing temperature, solid ice transforms into a superionic phase before fully melting. In this superionic phase, the oxygen lattice has been assumed to have bulk-centered cubic symmetry until recently, when a face-centered cubic phase was reported[4]. In this work, we perform molecular dynamics simulations on several different superionic structures and calculate their Gibbs free energy using the thermodynamic integration method. Our result show more possible superionic phases at higher pressures. We also calculated the equation of states for these water phases, which are of importance for modeling the interiors of giant planets such as Uranus and Neptune[5].

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