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**Simulations of water in giant planets: discovery of symmetric H-bonding in the superionic phase** NIR GOLDMAN[1], LAURENCE FRIED, Lawrence Livermore National Laboratory — We detail herein results of *ab initio* Molecular Dynamics simulations of water at conditions close to the isentropes of Neptune and Uranus (temperatures of 1000 - 2000K, and densities of 2.0.-3.0 g/cc). We have calculated the lifetimes and concentrations of molecular and non-molecular species, and ionic conductivity and vibrational spectra. Comparison is made to experiment where possible. At these conditions, we observe the onset of a "superionic phase" in which oxygen anions exhibit glassy behavior, and protons diffuse rapidly ($10^{-5}$ - $10^{-4}$ $cm^2/s$) by jumping between oxygen lattice points. We observe two distinct transitions along the superionic phase line. The first consists of a "dynamically ionized" phase, wherein $H_2O$ is the dominant species, but all species lifetimes are exceedingly short-lived such that they are better described as ensembles of transitions states, rather than molecules. At higher densities, we observe a transition to a polymeric phase, in which water has formed partially covalent, symmetric hydrogen bond networks. These results profoundly improve our knowledge of the phase diagram of water. Furthermore they have important implications for the modeling of the interiors of Neptune and Uranus and their corresponding magnetic fields.

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