Covalency in the superionic phase of water LAURENCE FRIED, Lawrence Livermore National Laboratory, NIR GOLDMAN, Lawrence Livermore National Laboratory — We detail herein results of \textit{ab initio} Molecular Dynamics simulations of water at temperatures of 1000 – 2000K, and densities of 1.8 – 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. We observe the onset of a superionic phase at much lower temperature and pressure than previously calculated. Results indicate that at these conditions, water undergoes several transformations in which at higher densities, the oxygen atoms form a glassy state, and the hydrogens diffuse extremely rapidly by jumping between oxygen “lattice” points. We also find that at the superionic phase transition, molecular species are too short lived to be described as molecules or ionic conductors, and are better described as ensembles of transitions states. We argue that water in the so-called superionic phase is best described as consisting of extensive transient networks of O—H bonds, which are predominantly covalent.

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