

Abstract Submitted
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Covalency in the superionic phase of water LAURENCE FRIED,
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National Laboratory — We detail herein results of *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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