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Ab initio Molecular Dynamics Simulations of Water Under Shock Compression: Chemistry Behind Shock Fronts LAURENCE FRIED, NIR GOLDMAN, Lawrence Livermore National Laboratory, ALESSANDRO CURIONI, IBM Research, Zurich Research Laboratory, CHRISTOPHER MUNDY, Pacific Northwest National Laboratory, I.-F.W. KUO, EVAN REED, Lawrence Livermore National Laboratory — We report herein first principles simulations of water under shock loading of velocities from 5 - 11 km/s. Accurate description of the plateau in the ionic conductivity at high pressures and temperatures is of particular importance to models of the planetary dynamo mechanism in Neptune and Uranus. We attribute this plateau to the exceedingly short- lived molecular and ionic states that occur in water under these extreme conditions. In particular, at the intersection of the shock hugoniot and Neptune isentrope we observe transient metallization that we attribute to the formation of short-lived negatively charged species that contribute electronic states at or around the band gap.

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