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Ab initio Molecular Dynamics Simulations of Water Under Shock Conditions[1] N. GOLDMAN, LLNL, C.J. MUNDY, Pacific Northwest Natl. Lab, I-F. W. KUO, E.J. REED, L.E. FRIED, LLNL, A. CURIONI, IBM Research, Zurich Research Lab — We report herein first principles simulations of water undergoing shock loading of velocities from 5 – 11 km/s. Shocked aqueous solutions are of particular interest to understanding earth and planetary sciences, and the chemical reactivity that occurs within such hot, compressed systems. The Multi-Scale Shock Method (MSSM) utilizes a Lagrangian-derived constraint dynamics to restrict a molecular dynamics simulation to the thermodynamic states found in the shock. This allows for simulations with much smaller system sizes than previously required, and for significantly longer time scales than previously achievable. Consequently, for the first time, we have been able to conduct quantum simulations of a shocked material. We show that Density Functional Theory (DFT) molecular dynamics results compare extremely well to experiments on the water shock Hugoniot. We also present results for the ionic conductivity as well as the concentrations and lifetimes of chemical species found therein. Our results represent the strongest confirmation of the accuracy of DFT at high pressure and temperature that we know of, to date.

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