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***Ab Initio* Simulation of the Equation of State and Kinetics of Shocked Water** NIR GOLDMAN, EVAN J. REED, I-F. WILLIAM KUO, LAURENCE E. FRIED, LLNL, CHRISTOPHER J. MUNDY, PNNL, ALESSANDRO CURIONI, IBM-Zurich — We report herein first principles simulations of water under shock loading and the chemical reactivity under these hot, compressed conditions. Using a novel simulation technique for shock compression, we observe that water achieves chemical equilibrium in less than 2 ps for all shock conditions studied. The decomposition occurs through the reversible reaction $H_2O \; \Delta \; H^+ + OH^-$. We make comparison to the experimental results for the Hugoniot pressure and density final states. We develop and employ a new quantum correction method to the calculated temperatures which provides validation of both previous experiments and our simulations. Near the approximate intersection of the Hugoniot and the Neptune isentrope, we observe high concentrations of negatively charged species that contribute electronic states near the band gap. *This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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