Abstract Submitted for the SHOCK11 Meeting of The American Physical Society

Equation of State and Kinetics of Shock Compressed Water,  $\alpha$ -Quartz and Diamond from Density Functional Tight Binding Simulations NIR GOLDMAN, LARRY FRIED, Lawrence Livermore National Laboratory — We present equation of state and chemical kinetics data from density functional tight binding (DFTB) molecular dynamics simulations of covalently bonded materials shock compressed to high pressure and temperatures. DFTB holds promise as an alternative to standard quantum simulations due to its increase in computational efficiency which allows for simulations of up to  $\sim 1$  ns while retaining the accuracy of quantum codes. However, its accuracy at extreme conditions remains largely unknown. Using a new extension to the Multi-Scale Shock Technique, we have simulated shock compression in water,  $\alpha$ -quartz and diamond up to high densities where these materials experience significant thermal electronic excitations and quartz and diamond are in a dense fluid state. Our simulations show good agreement with experimentally measured Hugoniot pressures, densities, and temperatures (where available) for all materials. In addition, our simulations of water yield accurate dissociation kinetics over a wide range of pressures. DFTB simulations have the potential to answer open experimental questions for a variety of materials, including the anomalous heat capacities measured in shock compressed  $\alpha$ -quartz and the transition to a high pressure BC8 phase in diamond.

> Nir Goldman Lawrence Livermore National Laboratory

Date submitted: 17 Feb 2011

Electronic form version 1.4