Abstract Submitted
for the SHOCK15 Meeting of
The American Physical Society

A New Force-Matched Reactive Force Field for Bulk Water Under Extreme Thermodynamic Conditions[1] LAURENCE FRIED, LUCAS KOZIOL, Lawrence Livermore Natl Lab — A many-body classical force field is presented for water under dissociative thermodynamic conditions. The force field is optimized by force-matching to ab initio molecular dynamics (AIMD) simulations calculated with Density Functional Theory (DFT). The force field contains short-ranged central and many-body over-coordination terms, and long-range Ewald electrostatics. It is optimized and tested on water at density 1.5 g/mL and 2000 K, which is approximately 10% dissociated according to DFT. Molecular dynamics simulations closely reproduce DFT radial distribution functions, as well as the distribution of wat and dissociation products. The calculated atomic self-diffusion constants appear about 50% lower than in DFT, although precise comparison is impossible due to the short timescale accessible to AIMD (about 20 ps). The force field is also compared to ReaxFF using the CHO parameter set of Chenowith et al. ReaxFF structural and dynamical properties are in overall fair agreement with DFT, although ReaxFF water is not dissociative at these conditions.

[1]This work was 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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Date submitted: 30 Jan 2015 Electronic form version 1.4