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Force Field Accelerated Density Functional Theory Molecular Dynamics for Simulation of Reactive Systems at Extreme Conditions REBECCA LINDSEY, NIR GOLDMAN, LAURENCE FRIED, Lawrence Livermore Natl Lab — Understanding chemistry at extreme conditions is crucial in fields including geochemistry, astrobiology, and alternative energy. First principles methods can provide valuable microscopic insights into such systems while circumventing the risks of physical experiments, however the time and length scales associated with chemistry at extreme conditions (ns and μm, respectively) largely preclude extension of such models to molecular dynamics. In this work, we develop a simulation approach that retains the accuracy of density functional theory (DFT) while decreasing computational effort by several orders of magnitude. We generate n-body descriptions for atomic interactions by mapping forces arising from short density functional theory (DFT) trajectories on to simple Chebyshev polynomial series. We examine the importance of including greater than 2-body interactions, model transferability to different state points, and discuss approaches to ensure smooth and reasonable model shape outside of the distance domain sampled by the DFT training set. 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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