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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 — Atomistic modeling of chemistry at extreme conditions remains a challenge, despite continuing advances in computing resources and simulation tools. While first principles methods provide a powerful predictive tool, 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 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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