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Accelerated electronic structure-based molecular dynamics simulations of shock-induced chemistry

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The initiation and progression of shock-induced chemistry in organic materials at moderate temperatures and pressures are slow on the time scales available to regular molecular dynamics simulations. Accessing the requisite time scales is particularly challenging if the interatomic bonding is modeled using accurate yet expensive methods based explicitly on electronic structure. We have combined fast, energy conserving extended Lagrangian Born-Oppenheimer molecular dynamics with the parallel replica accelerated molecular dynamics formalism to study the relatively sluggish shock-induced chemistry of benzene around 13-20 GPa. We model interatomic bonding in hydrocarbons using self-consistent tight binding theory with an accurate and transferable parameterization. Shock compression and its associated transient, non-equilibrium effects are captured explicitly by combining the universal liquid Hugoniot with a simple shrinking-cell boundary condition. A number of novel methods for improving the performance of reactive electronic structure-based molecular dynamics by adapting the self-consistent field procedure on-the-fly will also be discussed. The use of accelerated molecular dynamics has enabled us to follow the initial stages of the nucleation and growth of carbon clusters in benzene under thermodynamic conditions pertinent to experiments.