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Self-consistent Tight-binding Molecular Dynamics Simulations of Shock-induced Reactions in Hydrocarbons MARC CAWKWELL, EDWARD SANVILLE, ANDERS NIKLASSON, STEPHEN SHEFFIELD, DANA DATTELBAUM, Los Alamos National Laboratory — Shock-induced reactions in liquid hydrocarbons have been studied using quantum-based, self-consistent tight-binding (SC-TB) molecular dynamics simulations with an accurate and transferable model for interatomic bonding. Our SC-TB code LATTE enables explicit simulations of shock compression using the universal liquid Hugoniot. Furthermore, the effects of adiabatic shock heating are captured precisely using Niklasson's energy conserving extended Lagrangian Born-Oppenheimer Molecular Dynamics formalism. We have been able to perform relatively large-scale SC-TB simulations by either taking advantage of the sparsity of the density matrix to achieve $O(N)$ performance or by using graphical processing units to accelerate $O(N^3)$ algorithms. Simulations of liquid methane, benzene, and tert-butylacetylene are used to illustrate these capabilities. In particular, in accord with recent experiments we show that tert-butylacetylene undergoes radical chain polymerization reactions under shock compression.

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