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Quantum-based Molecular Dynamics Simulations of Shock-induced Reactions with Time-resolved Raman Spectra MARC CAWKWELL, EDWARD SANVILLE, JOSHUA COE, ANDERS NIKLASSON, 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 graphics processing units to accelerate $O(N^3)$ algorithms. We have developed the capability for the on-the-fly computation of Raman spectra from the Fourier transform of the polarizability autocorrelation function via the density matrix perturbation theory of Niklasson and Challacombe. These time-resolved Raman spectra enable us compare the results of our simulations with identical diagnostics collected experimentally. We will illustrate these capabilities with a series of simulations of shock-induced reaction paths in a number of simple molecules.

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