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Fast Quantum Molecular Dynamics Simulations of Simple Organic Liquids under Shock Compression MARC CAWKWELL, ANDERS NIKLASSON, VIRGINIA MANNER, SHAWN MCGRANE, DANA DATTELBAUM, Los Alamos National Laboratory — The responses of liquid formic acid, acrylonitrile, and nitromethane to shock compression have been studied using quantum-based molecular dynamics simulations with the self-consistent tight-binding code LATTE. Microcanonical Born-Oppenheimer trajectories with precise energy conservation were computed without relying on an iterative self-consistent field optimization of the electronic degrees of freedom at each time step via the Fast Quantum Mechanical Molecular Dynamics formalism [A. M. N. Niklasson and M. J. Cawkwell, Phys. Rev. B, **86**, 174308 (2012)]. The input shock pressures required to initiate chemistry in our simulations agree very well with recent laser- and flyer-plate-driven shock compression experiments. On-the-fly analysis of the electronic structure of the liquids over hundreds of picoseconds after dynamic compression revealed that their reactivity is strongly correlated with the temperature and pressure dependence of their HOMO-LUMO gap.

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