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The Chemistry of Shocked High-energy Materials: Connecting Atomistic Simulations to Experiments. MD MAHBUBUL ISLAM, ALEJANDRO STRACHAN, Purdue Univ — A comprehensive atomistic-level understanding of the physics and chemistry of shocked high energy (HE) materials is crucial for designing safe and efficient explosives. Advances in the ultrafast spectroscopy and laser shocks enabled the study of shock-induced chemistry at extreme conditions occurring at picosecond timescales. Despite this progress experiments are not without limitations and do not enable a direct characterization of chemical reactions. At the same time, large-scale reactive molecular dynamics (MD) simulations are capable of providing description of the shocked-induced chemistry but the uncertainties resulting from the use of approximate descriptions of atomistic interactions remain poorly quantified. We use ReaxFF MD simulations to investigate the shock and temperature induced chemical decomposition mechanisms of polyvinyl nitrate, RDX, and nitromethane. The effect of various shock pressures on reaction initiation mechanisms is investigated for all three materials. We performed spectral analysis from atomistic velocities at different shock pressures to enable direct comparison with experiments. The simulations predict volume-increasing reactions at the shock-to-detonation transitions and the shock vs. particle velocity data are in good agreement with available experimental data. The ReaxFF MD simulations validated against experiments enabled prediction of reaction kinetics of shocked materials, and interpretation of experimental spectroscopy data via assignment of the spectral peaks to dictate various reaction pathways at extreme conditions.

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