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Towards validated chemistry at extreme conditions: reactive MD simulations of shocked Polyvinyl Nitrate and Nitromethane[1] MD MAHBUBUL ISLAM, ALEJANDRO STRACHAN, Purdue University — A detailed atomistic-level understanding of the ultrafast chemistry of detonation processes of high energy materials is crucial to understand their performance and safety. Recent advances in laser shocks and ultra-fast spectroscopy is yielding the first direct experimental evidence of chemistry at extreme conditions. At the same time, reactive molecular dynamics (MD) in current high-performance computing platforms enable an atomic description of shock-induced chemistry with length and timescales approaching those of experiments. We use MD simulations with the reactive force field ReaxFF to investigate the shock-induced chemical decomposition mechanisms of polyvinyl nitrate (PVN) and nitromethane (NM). The effect of shock pressure on chemical reaction mechanisms and kinetics of both the materials are investigated. For direct comparison of our simulation results with experimentally derived IR absorption data, we performed spectral analysis using atomistic velocity at various shock conditions. The combination of reactive MD simulations and ultrafast spectroscopy enables both the validation of ReaxFF at extreme conditions and contributes to the interpretation of the experimental data relating changes in spectral features to atomic processes.

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