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Vibrational Energy Relaxation in Common High Energy Density Materials Through Reactive Molecular Dynamics Simulations MITCHELL WOOD, ALEJANDRO STRACHAN, Purdue University — We use molecular dynamics with the reactive force field ReaxFF to study the decomposition and subsequent reactions of the nitramine HMX under induced by electric fields and temperature. We find that electric fields of appropriately chosen frequencies can trigger chemical decomposition for total energy input significantly smaller than thermally excited systems. In addition, the energy barriers associated with exothermic chemical reactions are also dependent on the character of the excitation for electric field driven samples. We are able to characterize the frequency-dependent energy input and subsequent equilibration using the power spectra of atomic velocities and we find that the non-equilibrium nature of the energy distribution obtained via electric field excitations is responsible for the dependence of energy threshold for decomposition on type of perturbation. Timescales and decay pathways for vibron energy are discussed for HMX and other energetic materials.

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