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Non-equilibrium Reaction Kinetics in Molecular Solids MITCHELL WOOD, ALEJANDRO STRACHAN, Materials Engineering, Purdue University — We explore the possibility of non-statistical chemical reactions in condense-phase energetic materials via reactive molecular dynamics (MD) simulations. We characterize the response of three unique high energy density molecular crystals to different types of insults: electric fields of various frequencies (100-4000cm^{-1}) and strengths and direct heating at various rates. We find that non-equilibrium states can be created for short timescales when energy input targets specific vibrations through the electric fields, and that equilibration eventually occurs even while the insults remain present. Interestingly, for strong fields these relaxation timescales are comparable to those of the initial chemical decomposition of the molecules. Details of how this vibrational energy localization affects the preferred uni- or multi-molecular reactions are discussed. These results provide insight into non-equilibrium or coherent initiation of chemistry in the condensed phase that would of interest in fields ranging from catalysis to explosives.

Mitchell Wood
Materials Engineering, Purdue University

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