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Nonlinear THz signatures of energetic molecular crystals DAVID MOORE, Los Alamos National Laboratory, MITCHELL WOOD, Purdue University, DIEGO DALVIT, Los Alamos National Laboratory — Several methods exist for detecting energetic materials, yet no method is available to surmount the simultaneous challenges of rapid screening, areal coverage, sensitivity and selectivity. Nonlinear coupling of penetrating THz radiation to explosives is a promising new tool for stand-off detection. Here, we report on reactive molecular dynamics simulations of the emission spectra of energetic molecular crystals under electromagnetic insults. The THz emission spectrum, calculated from the time dependent dipole accelerations, is altered due to anharmonic coupling between modes in the material, providing a unique fingerprint for each material. The efficiency of the nonlinear frequency conversion mechanism is studied as a function of various parameters of an incoming electromagnetic pulse, including its carrier frequency, polarization, peak power, and duration. Two common energetic materials, PETN and RDX, were studied wherein we have found unique emission peaks in the frequency range of 0-10THz that arise from select carrier frequencies.

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