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First-principles density-functional theory investigation of FOX-7

BRIAN VOHASKA, MICHAEL CONROY, IVAN OLEYNIK, University of South Florida, CARTER WHITE, Naval Research Laboratory — Due to the expense and difficulty of experimental investigation of the chemical and physical properties of energetic materials (EMs), computational methods provide a unique opportunity for accurate determination of the chemical and physical properties of EM molecular crystals based on underlying atomic structure. In this presentation, we discuss the results of first-principles density functional theory (DFT) calculations of hydrostatic and uniaxial compression of the important energetic material, FOX-7. The calculated equilibrium properties, such as lattice parameters, elastic constants, and the bulk modulus will be reported and compared with experiment, as well as the isothermal equation of state. Due to the anisotropic nature of energetic molecular crystals, physical properties such as cohesive energy, band gap, and stress-strain relationships are reported as functions of each uniaxial compression studied. In addition, the shear stress behavior upon uniaxial compression will be discussed, as well as its possible relation to anisotropic shock-sensitivity in FOX-7.

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