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First-Principles Studies of Anisotropic Constitutive Relationships in Nitromethane and RDX MICHAEL CONROY, IVAN OLEYNIK, University of South Florida, SERGEY ZYBIN, California Institute of Technology, CARTER WHITE, Naval Research Laboratory — One of the goals of energetic materials (EMs) research is to obtain accurate equations of state (EOS). These EOS establish fundamental relationships between thermodynamic variables and provide necessary input for the description of materials at the mesoscopic and continuum levels. Ultimately, these EOS are governed by interactions at the atomic scale, and the investigation of these relationships provides an opportunity to connect the shock sensitivity of EMs with underlying atomic-scale structure. In order to investigate this fundamental structure-property relationship, we performed first-principles density functional theory studies of hydrostatic and uniaxial compressions in several crystallographic directions of nitromethane and RDX. Equilibrium properties, including lattice parameters and elastic constants, as well as the hydrostatic equation of state obtained from our calculations are compared with experiment. The shear stresses upon uniaxial compression will be examined, and the possibility of a correlation of their behavior with shock sensitivity will be discussed.

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