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Anisotropic constitutive relationships in energetic materials: nitromethane, RDX, and TATB IVAN OLEYNIK, MICHAEL CONROY, University of South Florida, CARTER WHITE, Naval Research Laboratory — We extend our first-principles studies of isotropic equation of states (EOS) of energetic materials to include stress-dependent relationships that describe the anisotropic materials response upon dynamic loading. We will discuss the results of first-principles density functional theory calculations of the energetic materials nitromethane, RDX, and TATB. The behavior of the materials is investigated upon both hydrostatic and uniaxial compressions along different crystallographic directions and compressions resulting in pressures up to 50 GPa. We will examine the equations of state for each material, its structural and electronic properties as a function of compression ratio, and compare with available experimental results. The behavior of shear stresses upon uniaxial compression will be discussed in relationship with the sensitivity properties of these materials.

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