Abstract Submitted
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First-Principles Constitutive Relationships in PETN and HMX under Hydrostatic and Uniaxial Compressions[1] SERGEY V. ZYBIN, California Institute of Technology, MICHAEL W. CONROY, IVAN I. OLEYNIK, University of South Florida, CARTER T. WHITE, Naval Research Laboratory — The physical mechanisms leading to shock-induced detonation at the atomic level are ultimately related to energetic materials response to uniaxial compression at the shock front. Due to the intrinsic anisotropy of the constitutive relationships, a description of the compressed state should be extended beyond hydrostatic equations of state that are frequently used for analysis of precursor states of EMs. In this presentation, we will discuss the results of first-principles density functional theory calculations of both hydrostatic and uniaxial compressions in the [100], [010], [001], [110], [101], [011], and [111] directions applied to the energetic materials PETN-I and β-HMX. A comparison will be made of available experimental data with calculated physical properties such as unit cell geometry, isothermal equations of state, and elastic constants. The presentation will focus on the anisotropic nature of the constitutive relationships in molecular crystals under uniaxial compression. The behavior of the shear stress projections on available slip systems upon uniaxial strain and their possible relationship to experimental shock-initiation sensitivity data will be discussed.

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