First-principles studies of hydrostatic and uniaxial compression of a new energetic material – an energetic nitrate ester

MICHAEL CONROY, AARON LANDERVILLE, IVAN OLEYNIK, University of South Florida, CARTER WHITE, Naval Research Laboratory — Density functional theory calculations with an empirical vdW correction were performed on a new energetic material (EM), a nitrate ester, that was recently synthesized by Chavez et al. [Angew. Chem. Int. Ed. 47, 8307 (2008)]. This EM was shown to have physical properties superior to another nitrate ester, PETN. The equilibrium structure was calculated by vdW-DFT in excellent agreement with experiment (to within about 0.1% of the equilibrium volume of the unit cell). From the hydrostatic-compression simulation, the isothermal EOS and bulk modulus were predicted prior to any known experimental results. In addition, uniaxial compressions were simulated in the $<100>$, $<010>$, $<001>$, $<110>$, $<101>$, $<011>$, and $<111>$ directions to examine the anisotropic quality of the constitutive relationships. The calculated physical properties of the nitrate ester at extreme conditions are compared with other important energetic materials.

Michael Conroy
University of South Florida

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