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Vibrational and Thermophysical Properties of PETN from First Principles JOSEPH GONZALEZ, AARON LANDERVILLE, IVAN OLEYNIK, University of South Florida, Tampa, FL, 33620 — Thermophysical properties are urgently sought as input for meso- and continuum-scale modeling of energetic materials (EMs). However, empirical data in this regard are often limited to specific pressures and temperatures. Such modeling of EMs can be greatly improved by inclusion of thermophysical properties over a wide range of pressures and temperatures, provided such data could be reliably obtained from theory. We demonstrate such a capability by calculating the equation of state, heat capacities, coefficients of thermal expansion, and Gruneissen parameters for pentaerythritol tetranitrate (PETN) using first-principles density functional theory, which includes proper description of van der Waals interactions and zero-point and thermal free energy contributions to pressure, the latter being calculated using the quasi-harmonic approximation. Further, we investigate the evolution of the vibration spectrum of PETN as a function of pressure.

Ivan Oleynik
University of South Florida, Tampa, FL, 33620

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