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Thermodynamic Properties of energetic materials from density functional theory with van der Waals corrections AARON LANDERVILLE, University of South Florida, MICHAEL CONROY, Naval Research Laboratory, MIKALAI BUDZEVICH, YOU LIN, University of South Florida, CARTER WHITE, Naval Research Laboratory, IVAN OLEYNIK, University of South Florida — The calculation of thermodynamic properties for energetic materials from first-principles offers the promise to provide key parameters for mesoscopic and continuum-level simulations of explosives performance for a wide range of pressures and temperatures. While density functional theory with empirical van der Waals corrections, together with corrections for temperature and zero-point effects, can give excellent agreement between calculated and experimentally determined equations of state, quantities such as heat capacities and coefficients of thermal expansion suffer from inaccuracies in the lower frequencies of the calculated vibration spectrum. Additional approaches are discussed to account for the lowest intermolecular modes to increase the accuracy in prediction of thermal properties.

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