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Equations of state for energetic materials from density functional theory with van der Waals, thermal, and zero-point energy 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 — Equations of state EOS, which establish fundamental relationships between thermodynamic variables, are important because they provide necessary input for the description of materials at the mesoscopic and continuum levels. It is shown that the introduction of zero-point energy and thermal effects to density functional theory with an empirical van der Waals correction results in a significant improvement in the prediction of equilibrium volumes and isothermal equations of state for hydrostatic compressions of energetic materials at non-zero temperatures. This method can be used to predict thermo-physical properties of these materials for a wide range of pressures and temperatures.

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