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**Application of van der Waals density functional theory to study physical properties of energetic materials** MICHAEL CONROY, YOU LIN, IVAN OLEYNIK, University of South Florida, CARTER WHITE, Naval Research Laboratory — An empirical correction to account for van der Waals interactions based on the work of Neumann and Perrin [J. Phys. Chem. B **109**, 15531 (2005)] was applied to first-principles calculations of energetic molecular crystals. The calculated equilibrium unit-cell volumes of FOX-7, $\beta$-HMX, solid nitromethane, PETN-I, $\alpha$-RDX, and TATB show a significant improvement in the agreement with experimental results. Hydrostatic-compression simulations of $\beta$-HMX, PETN-I, and $\alpha$-RDX were also performed. The isothermal equations of state calculated from the results show increased agreement with experiment in the pressure intervals studied. The bulk modulus and its pressure derivative were calculated by fitting to three commonly used equations of state, and the results are within the range of reported experimental values.

Michael Conroy
University of South Florida

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