Abstract Submitted
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High-pressure/high-temperature polymorphs of energetic materials by first-principles simulations[1] NAM LE, National Research Council Postdoctoral Fellow, U.S. Naval Research Laboratory, Washington, DC 20375, IGOR SCHWEIGERT, Code 6189, Theoretical Chemistry Section, U.S. Naval Research Laboratory, Washington, DC 20375 — Energetic molecular crystals exhibit complex phase diagrams that include solid-solid phase transitions, melting, and decomposition. Sorescu and Rice have recently demonstrated that first-principles molecular dynamics (MD) simulations based on dispersion-corrected density functional theory (DFT) can capture the α to γ phase transition in hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX) on time scales of several picoseconds [1]. Motivated by their work, we are using DFT-based MD to model the relative stability of solid phases in several molecular crystals. In this presentation, we report simulations of pentaerythritol tetranitrate (PETN) and 2,4,6-trinitrotoluene (TNT) under high pressures and temperatures and compare them with experimentally observed polymorphs [2,3]. [1] Sorescu and Rice, J. Phys. Chem. C, 120, 19547-19557 (2016) [2] Dreger and Gupta, J. Phys. Chem. A, 117, 5306-5313 (2013) [3] Dattelbaum et al., Appl. Phys. Lett., 104, 021911 (2014)

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