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Comparative study of energetic materials by classical interatomic potential ReaxFF and first-principles density functional theory IVAN OLEYNIK, University of South Florida, SERGEY ZYBIN, L. ZHANG, WILLIAM GODDARD, California Institute of Technology — Prediction of properties of energetic materials using atomic-scale simulations techniques is one of the challenging areas of energetic materials (EM) research. Molecular dynamics (MD) simulation of EM using classical reactive interatomic potentials is a powerful modeling technique that is capable of addressing sub-nanometer and sub-picosecond length and time scales of shock compression and detonation phenomena. However, the results of computer simulations can only be as reliable as the ability of the interatomic potentials to describe properly a variety of chemical effects including bond-breaking and bond-making. Recently, the reactive force field ReaxFF has been developed based on fitting of an ab-initio database of HCNO chemistry and is currently being actively used for MD simulations of EM. We performed a comparative study of static and thermodynamic properties of PETN, RDX and HMX using both density functional theory (DFT) and ReaxFF including static properties of different crystalline phases and equation of states (EOS). The transferability issues are discussed in the region of physical parameters relevant for MD simulation of initial decomposition and detonation in EM.

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