

Abstract Submitted
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First-principles molecular reactive dynamics of energetic materials AARON LANDERVILLE, IVAN OLEYNIK, University of South Florida, CARTER WHITE, Naval Research Laboratory — The understanding of initiation chemistry of shock-compressed energetic materials on the atomic scale is of fundamental importance for developing a predictive theory of initiation of detonation. We have performed first-principles density-functional modeling of reactive molecular collisions of PETN and RDX molecules aimed at elucidating the first chemical events that trigger the chemistry behind the shock wave front. We will discuss fundamental mechanisms responsible for the transformation of mechanical energy from the shock wave into molecular degrees of freedom that result in excitation of a reaction mode and eventual bond breaking. We will also discuss the stereochemistry of initial reaction events, unimolecular, bi-molecular or multi-molecular nature of initial reactive events and the relationship of the simulated reactive collisions with a non-equilibrium shock wave environment.

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