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Hypervelocity reactive dynamics in detonating PETN, RDX, and HMX energetic materials AARON LANDERVILLE, IVAN OLEYNIK, University of South Florida, CARTER WHITE, Navel Research Laboratory — Despite intensive experimental and theoretical efforts, the first chemical events that trigger the chemistry behind the shock wave front in detonating materials are still largely unknown. We investigate the chemical initiation of detonation in shock compressed PETN, RDX, and HMX which results from intermolecular collisions behind the shock wave using first-principles reactive molecular dynamics. The reaction dynamics of bimolecular collisions were studied as a function of collision velocities and crystallographic orientations. For each orientation, threshold collision velocities of reaction, and products of decomposition were determined. The timescale of reaction was determined and used to understand whether these initial chemical events are largely driven by reaction dynamics, or temperature. Bond dissociation energies were calculated for each molecule and used to rationalize the outcome of the chemical events in the course of the reaction dynamics. A correlation between the order in which products are formed and the relative strengths of the bonds within the bimolecular complexes was investigated. Finally, the relationship between orientation dependent sensitivities and steric factors is discussed.

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