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First-Principles Reactive Molecular Dynamics of Chemistry in Detonating Energetic Materials AARON LANDERVILLE, IVAN I. OLEYNIK, University of South Florida, MORTKO A. KOZHUSHNER, Russian Academy of Sciences, CARTER T. WHITE, Naval Research Laboratory — We investigated the initial chemistry of shock compressed energetic materials that results from intermolecular collisions behind the shock wave front by performing first-principles MD simulations of bimolecular collisions for PETN and RDX with different crystallographic orientations and velocities. For each orientation, we determined the threshold collision velocity for reaction, the reaction timescales, and the products of decomposition. We find that the calculated threshold velocities lie within the range of typical particle flow velocities in detonating materials. Owing to the extremely short reaction timescales ($\sim 10^{-13}$s), these initial chemical events are largely driven by the direct collision dynamics, instead of temperature.

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