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First-principles reactive molecular dynamics of initiation chemistry in energetic materials AARON LANDERVILLE, IVAN OLEYNIK, University of South Florida, MORTKO KOZHUSHNER, Institute of Chemical Physics, Russian Academy of Sciences, CARTER WHITE, Naval Research Laboratory —
Understanding of initiation chemistry of shock-compressed energetic materials on the atomic scale is one of the outstanding problems for shock wave and energetic materials community. Using first-principles density functional theory, we have performed molecular dynamics simulations of the reactive molecular collisions of several energetic molecules such as PETN and RDX aimed at elucidating the first chemical events that trigger the chemistry behind the shock wave front. These results provide an insight into 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, bond breaking and subsequent events taking place under non-equilibrium conditions of the shock wave environment.

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