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Ab initio molecular dynamics of hypervelocity chemistry[1] IGOR SCHWEIGERT, BRETT DUNLAP, Theoretical Chemistry Section, US Naval Research Laboratory, 4555 Overlook Ave SW, Washington, DC 20375 — Resolving chemical dynamics of decomposition of energetic molecules is crucial for understanding detonation initiation in energetic materials and predicting their sensitivity to shock and impact stimuli. We employ Born-Oppenheimer molecular dynamics driven by density-functional methods to identify possible decomposition pathways in nitric esters (including pentaerythritol tetranitrate) and to understand the effect of collision orientation and velocity. Studies of the potential energy surface in the bond-breaking region, unimolecular decomposition, and binary hypervelocity collisions of model nitric esters (methyl and ethyl nitrates) will be reported. Methodological challenges in describing extensive changes in the electronic structure that accompany decomposition will be discussed.

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