Abstract Submitted
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Molecular dissociation under extreme conditions[1] IGOR SCHWEIGERT, US Naval Research Laboratory — Molecular dissociation under extreme temperatures and pressures is the first step towards thermal or shock initiated decomposition of energetic materials. Fast dissociation rates are challenging to measure, but amenable to first principles calculations. We combine transition-state theory with molecular dynamics simulations based on density-functional theory to predict the temperature-dependent dissociation rates in the gas and the condensed phase. Current applications focus on gas-, solution-, and liquid-phase thermal dissociation of nitramines. These studies will be discussed in the context of developing mesoscale models of initiation of energetic materials.

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