

Abstract Submitted
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Toward a reaction rate model of condensed-phase RDX decomposition under high temperatures¹ IGOR SCHWEIGERT, U.S. Naval Research Laboratory — Shock ignition of energetic molecular solids is driven by microstructural heterogeneities, at which even moderate stresses can result in sufficiently high temperatures to initiate material decomposition and chemical energy release. Mesoscale modeling of these “hot spots” requires a reaction rate model that describes the energy release with a sub-microsecond resolution and under a wide range of temperatures. No such model is available even for well-studied energetic materials such as RDX. In this presentation, I will describe an ongoing effort to develop a reaction rate model of condensed-phase RDX decomposition under high temperatures using first-principles molecular dynamics, transition-state theory, and reaction network analysis.

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