Abstract Submitted
for the SHOCK13 Meeting of
The American Physical Society

Quantum mechanical simulations of condensed-phase decomposition dynamics in molten RDX[1] IGOR SCHWEIGERT, Naval Research Laboratory — A reaction model for condensed-phase decomposition of RDX under pressures up to several GPa is needed to support mesoscale simulations of the energetic material's sensitivity to thermal and shock loading. A prerequisite to developing such a model is the identification of the chemical pathways that control the rate of the initial dissociation and the subsequent decomposition of molecular fragments. We use quantum mechanics based molecular dynamics simulations to follow the decomposition dynamics under high-pressure conditions and to identify the reaction mechanisms. This presentation will describe current applications to the liquid-phase decomposition of molten RDX.

[1]This work was supported by the Naval Research Laboratory, by the Office of Naval Research, and by the DOD High Performance Computing Modernization Program Software Application Institute for Multiscale Reactive Modeling of Insensitive Munitions

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Date submitted: 04 Mar 2013 Electronic form version 1.4