Abstract Submitted
for the SHOCK11 Meeting of
The American Physical Society

Effect of pressure on nitramine dissociation: A density-functional theory study[1] IGOR SCHWEIGERT, Naval Research Laboratory — The effect of increased pressure on the initial pathways and kinetics of dimethylnitramine dissociation is studied using density-functional theory (DFT). Two competitive pathways, radical NO_2 elimination and concerted HONO elimination, are evaluated using atomic basis, hybrid DFT thermochemistry and planewave DFT molecular dynamics. The computed thermochemistry and reactive dynamics of condensed-phase dissociation are contrasted with those in the gas phase. These results are discussed in the context of developing a reduced chemical model of nitramine decomposition suitable for inclusion in mesoscale simulations.

[1]This work is supported by the Naval Research Laboratory via the Jerome and Isabella Karle Distinguished Scholar Fellowship and by the Office of Naval Research, both directly and through the Naval Research Laboratory.

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Date submitted: 16 Feb 2011 Electronic form version 1.4