

Abstract Submitted  
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**Thermal decomposition of energetic materials by ReaxFF reactive molecular dynamics**<sup>1</sup> L. ZHANG, S.V. ZYBIN, A.C. VAN DUIN, S. DASGUPTA, W.A. GODDARD III, Caltech — Understanding the complex physico-chemical processes that govern the initiation and decomposition kinetics of energetic materials can pave the way for modifying the explosive or propellant formulation to improve their performance and reduce the sensitivity. In this work, we used molecular dynamics (MD) simulations with the reactive force field (ReaxFF) to study the thermal decomposition of pure crystals (RDX, HMX) as well as crystals bonded with polyurethane chains (Estane). The preliminary simulation results show that pure RDX and HMX crystals exhibit similar decomposition kinetics with main products (e.g., N<sub>2</sub>, H<sub>2</sub>O, CO<sub>2</sub>, and CO) and intermediates (NO<sub>2</sub>, NO, HONO, OH) in a good agreement with experiment. We also studied the effect of temperature on decomposition rate which increases at higher temperatures. With addition of polymer binders, we found that the reactivity of these energetic materials is reduced, and the polymer chains packing along different planes may also influence their thermal decomposition. In addition, we studied the thermal decomposition of TATP and hydrazine which are examples of ReaxFF development for non-nitramine based energetic materials.

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