

Abstract Submitted  
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**Reactive Molecular Dynamics Studies of Thermal Induced Chemistry in TATB** TIMOTHY GERMANN, JASON QUENNEVILLE, Los Alamos National Laboratory — Equilibrium molecular dynamics (MD) simulation of high explosives can provide important information on their thermal decomposition by helping to characterize processes with timescales that are much longer than those attainable with non-equilibrium MD shock studies. A reactive force field is used with MD to probe the chemistry induced by intense heating ('cook-off') of 1,3,5-triamino-2,4,6-trinitrobenzene (TATB). The force field (ReaxFF) was developed by van Duin, Goddard and coworkers [1] at CalTech and has already shown promise in predicting the chemistry in small samples of RDX under either shock compression or intense heat. Large-system simulations are desired for TATB because of the high degree of carbon clustering expected in this material. We will show results of 800-particle simulations at several temperatures, and detail current capabilities for large-scale ( $10^4$  –  $10^5$  atoms) systems carried out with the massively parallel GRASP MD software developed at Sandia National Lab. Finally, we will compare the reaction timescales with those of RDX and HMX. [1] A. C. T. Van Duin, *et al*, *J. Phys. Chem. A*, **1005**, 9396 (2001).

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