Abstract Submitted
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Molecular Dynamics Studies of Thermal Induced Chemistry in TATB[1] JASON QUENNEVILLE, TIMOTHY GERMANN, Los Alamos National Laboratory — A reactive force field (ReaxFF[2]) is used with molecular dynamics to probe the chemistry induced by intense heating (accelerated 'cook-off') of 1,3,5-triamino-2,4,6-trinitrobenzene (TATB). Large-system simulations are desired for TATB because of the high degree of carbon clustering expected in this material. Using small, 800-atom, simulations, we will show the reaction rate as a function of temperature and density as well as the time evolution of reaction products. A larger simulation (with 14,000 atoms) will illustrate the effect of system size on both carbon clustering and reaction rate. Insight into the mechanisms of product formation will be given, as well as the chemical structure (graphitic or diamond-like) of the carbon clusters obtained. [2] A. C. T. Van Duin, et al, *J. Phys. Chem. A*, **1005**, 9396 (2001).

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