

Abstract Submitted
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Atomistic-scale simulations of the initial chemical events in triacetoneperoxide (TATP) detonation ADRI VAN DUIN, California Institute of Technology, YEHUDA ZEIRI, Hebrew University, WILLIAM GODDARD, California Institute of Technology — To study the initial chemical events related to the detonation of triacetoneperoxide (TATP) we have performed a series of molecular dynamics (MD) simulations using the ReaxFF reactive force field [1,2], extended to reproduce the quantumchemical (QM)-derived relative energies of the reactants, products, intermediates and transition states related to the TATP unimolecular decomposition. We find excellent agreement between the reaction products predicted from QM and those observed from ReaxFF unimolecular cookoff simulations. Furthermore, the primary reaction products observed in the unimolecular cookoff simulations match closely with those observed from a TATP-condensed phase cookoff simulation, indicating that unimolecular decomposition dominates TATP-condensed phase initiation. [1] A.C.T. van Duin, S. Dasgupta, F. Lorant and W.A. Goddard (2001), *J. Phys. Chem. A* **105**, 9396-9409. [2] A. Strachan, A.C.T. van Duin, D. Chakraborty, S. Dasgupta and W.A. Goddard III (2003) *Phys. Rev. Letters* **91**, 09301.

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