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Decomposition of Energetic Materials at Extreme Conditions
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— Detailed description of chemical reaction mechanisms of solid energetic materials at high-density and temperatures is essential for understanding events that occur at the reactive front of these materials, and for the subsequent development of predictive models of materials properties. In this talk, we will report the results of our ongoing ab initio based molecular dynamic simulation of the chemistry of TATB, at density of 2.9 g/cm^3 and temperature of 1500K, and at density of 2.87 g/cm^3 and temperature of 2500 K. These conditions are similar to those experienced at the CJ and von Neumann spike Following the dynamics for a time scale of up to forty picoseconds allows the construction of approximate rate laws for typical products such as H_2O, N_2, CO, and CO_2. The approximate reaction rates obtained for these products at the CJ state will be compared to those obtained recently for HMX at similar conditions. This work was performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under contract number W-7405-Eng-48.

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