Abstract Submitted
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Atomistic-scale simulations of energetic materials with ReaxFF reactive force fields[1] W.A. GODDARD III, S.V. ZYBIN, A.C. VAN DUIN, L. ZHANG, S. DASGUPTA, S-P. HAN, Caltech, A. STRACHAN, LANL — Understanding the response of energetic materials to thermal or shock loading at the atomistic level demands a highly accurate description of the reaction dynamics of million atom systems to capture the complex chemical and mechanical behavior involved: nonequilibrium energy/mass transfer, molecule excitation and decomposition under high strain/heat rates, formation of defects, plastic flow, and phase transitions. To enable such simulations, we developed the ReaxFF reactive force fields based on quantum mechanics (QM) calculations of reactants, products, high-energy intermediates and transition states, but using functional forms suitable for large-scale molecular dynamics simulations of chemical reactions under extreme conditions. We will present an overview of recent progress in ReaxFF developments, including the extension of ReaxFF to new nitramine- based (nitromethane, HMX, PETN, TATB) and peroxide-based (TATP) explosives. To demonstrate the versatility and transferability of ReaxFF, we will present applications to solid composite propellants such as Al/Al2O3-metal nanoparticles embedded into solid explosive matrices (RDX, PETN).

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