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**Atomistic and mesoscale modeling of mechanical and chemical processes in energetic materials**

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New-generation reactive interatomic potentials with molecular dynamics enable the full-physics, full-chemistry description complex thermal, mechanical, and chemical process in a wide variety of materials. I will describe the use of the first principles-based reactive force field ReaxFF to describe shock and thermal induced decomposition of various molecular energetic materials, including PETN, RDX, TATB and nitromethane. Non-equilibrium shock simulations enable the characterization of the initial chemical events under dynamical loading while equilibrium simulations at various temperatures and densities enable us to study phenomena at longer time-scales and follow the reactions to completion. These simulations provide information not only about chemical rates but also a molecular-level understanding of the complex multi-molecular chemistry involved. Furthermore, we find that decomposition time-scales of various materials have a strong correlation with their intrinsic sensitivity to ignition. While providing a very detailed description, all-atom MD simulations are computationally too intensive to simulate many important processes in molecularly complex materials such as shockwaves. Thus, we have recently developed a new mesodynamical method (where a single particle describes groups of atoms) that enables a thermodynamically accurate description of energy transfer between mesoparticles (molecules in this case) and their internal degrees of freedom. We describe the thermal role of the internal degrees of freedom of each mesoparticle using local, finite thermostats that are coupled to the local energy of the mesoparticles. The parameters entering the mesoscopic description can be obtained from all-atom simulations. We exemplify the new method via shock simulations of the crystalline polymer poly(vinylidene fluoride); the mesodynamics results are in excellent agreement with all-atom MD simulations.