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**Chemistry away from local equilibrium: shocking high-energy and energy absorbing materials**

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In this presentation I will describe reactive molecular dynamics and coarse grain simulations of shock induced chemistry. MD simulations of the chemical reactions following the shock-induced collapse of cylindrical pores in the high-energy density material RDX provide the first atomistic picture of the shock to deflagration transition in nanoscale hotspots. We find that energy localization during pore collapse leads to ultra-fast, multi-step chemical reactions that occur under non-equilibrium conditions. The formation of exothermic products during the first few picoseconds of the process prevents the hotspot from quenching, and within 30 ps a deflagration wave develops. Quite surprisingly, an artificial hot-spot matching the shock-induced one in size and thermodynamic conditions quenches; providing strong evidence that the dynamic nature of the loading plays a role in determining the criticality of the hotspot. To achieve time and lengths beyond what is possible in MD we developed a mesoscale model that incorporates chemical reactions at a coarse-grained level. We used this model to explore shock propagation on materials that can undergo volume-reducing, endothermic chemical reactions. The simulations show that such chemical reactions can attenuate the shockwave and characterize how the characteristics of the chemistry affect this behavior. We find that the amount of volume collapse and the activation energy are critical to weaken the shock, whereas the endothermicity of the reactions plays only a minor role. As in the reactive MD simulations, we find that the non-equilibrium state following the shock affects the nucleation of chemistry and, thus, the timescales for equilibration between various degrees of freedom affect the response of the material.