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### **Atomistic Studies of Energetic Materials Under Shock Wave Loading**

THOMAS SEWELL, Theoretical Division, Los Alamos

We have recently undertaken non-equilibrium molecular dynamics studies to aid our understanding of dynamical processes in the high explosives HMX and RDX, in particular the inelastic, anisotropic response of crystals of those materials subjected to quasi-static and shock loading. The overarching goal of this work is to provide information that can serve as a foundation in basic science for the formulation of improved mesoscale constitutive models for the constituent materials in selected energetic formulations. The medium-term scientific challenge to this larger objective is to carefully identify, characterize, and quantify the dominant mechanisms of localization and dissipation in such materials, under a variety of prescribed quasi-static and dynamic loading scenarios that lead to inelastic deformation of the crystals. The focus of the present talk will be the unreactive shock response of structurally perfect, but properly thermalized, HMX and RDX crystals; and shock localization in defective RDX crystals. Effort will be made to present information of interest to the shock physics, materials science, and chemical dynamics/spectroscopy communities.