

SHOCK13-2013-000802

Abstract for an Invited Paper
for the SHOCK13 Meeting of
the American Physical Society

Atomic-Scale Theoretical Studies of Fundamental Properties and Processes in CHNO Plastic-Bonded Explosive Constituent Materials under Static and Dynamic Compression¹
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The results of recent theoretical atomic-scale studies of CHNO plastic-bonded explosive constituent materials will be presented, emphasizing the effects of static and dynamic compression on structure, vibrational spectroscopy, energy redistribution, and dynamic deformation processes. Among the chemical compounds to be discussed are pentaerythritol tetranitrate (PETN), hexahydro-1,3,5-trinitro-1,3,5-s-triazine (RDX), nitromethane, and hydroxyl-terminated polybutadiene (HTPB). Specific topics to be discussed include pressure-dependent terahertz IR absorption spectra in crystalline PETN and RDX, microscopic material flow characteristics and energy localization during and after pore collapse in shocked (100)-oriented RDX, establishment of local thermodynamic temperature and the approach to thermal equilibrium in shocked (100)-oriented nitromethane, and structural changes and relaxation phenomena that occur in shocked amorphous *cis*-HTPB. In the case of shocked HTPB, comparisons will be made between results obtained using fully-atomic and coarse-grained (united atom) molecular dynamics force field models. Rather than attempting to discuss any given topic in extended detail, 3-4 vignettes will be presented that highlight outstanding scientific questions and the predictive methods and tools we are developing to answer them.

¹The U. S. Defense Threat Reduction Agency and Office of Naval Research supported this research.