Abstract Submitted
for the SHOCK15 Meeting of
The American Physical Society

Modeling the stability and growth of metalloid clusters for energetic materials JOE HOOPER, SUFIAN ALNEMRAT, Naval Postgraduate School — Metal and metalloid clusters are currently under study as energetic materials that may retain the high energy density of bulk metals but offer substantially faster reaction kinetics. Ligand-stabilized aluminum clusters have received particular attention in this regard, but experimental synthesis of these clusters with tailored ligands or new structures has proven extremely challenging. Here we present density functional theory and quantum molecular dynamics simulations to examine the stability and cluster-forming behavior of metalloid Al and related systems. A proposed magic-number shell closure model is examined to determine the importance of electronic structure stability versus other effects during synthesis. Metadynamics simulations are used to study the initial stages of cluster oxidation in a computationally efficient fashion, and are shown to be in good agreement with recent experimental gas phase oxidation studies. We discuss prospects and initial simulations for constrained cluster growth on nanoporous frameworks or templated surfaces.

Joseph Hooper
Naval Postgraduate School

Date submitted: 30 Jan 2015 Electronic form version 1.4