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Metalloid Clusters as Novel Energetic Materials: Progress and Challenges. SUFIAN ALNEMRAT, JOSEPH HOOPER, Naval Postgraduate School — Integration of combustible metals is a standard route for increasing the energy density of explosive and propellant formulations. Bulk metals, however, have well-known limitations. As a rather different route, we have been studying molecular scale metalloid clusters that contain a core of low-valence metal surrounded by a layer of organic ligands. These materials may retain the high energy density of bulk metals but offer substantially faster reaction kinetics. In this talk we present recent computational results on the stability and decomposition of these clusters. We compare molecular dynamics simulations of the oxidation of a prototype aluminum metalloid cluster to recent experimental thermally programmed reaction data; both show that oxygen reacts with the metal core and not the ligands. As a route to larger-scale fabrication of these clusters, we present simulations of the nucleation and growth of small metalloid systems on functionalized graphene layers. The simulations demonstrate that spontaneous cluster nucleation and growth is favorable on many graphene defects, suggesting a means of templated growth of clusters and nanoparticles.

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