

Abstract Submitted  
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**Novel Rubidium Poly-Nitrogen Energetic Materials** ASHLEY HUFF, BRAD STEELE, IVAN OLEYNIK, University of South Florida — High-nitrogen content compounds are being actively explored with the goal of discovering new high-energy density materials with performance surpassing the conventional energetic materials such as HMX or RDX. Although pure polynitrogen compounds such as cg-N are predicted to deliver 10-fold increase in detonation pressure and detonation velocity of 30 km/s, their synthesis and recovery at ambient conditions is problematic. Doping polynitrogens with other elements is a viable route to promote metastability while reducing synthesis pressure. In this work, rubidium poly-nitrides are being investigated as candidates for high energy density materials. Using first principles evolutionary structure search methods performed at varying stoichiometries and several pressures ranging from 0 to 100 GPa, several new polynitrogen compounds have been discovered. The phase diagrams containing thermodynamically stable and lowest metastable phases are calculated and the dynamical stability of the promising materials is investigated at various pressures. Raman spectra and XRD patterns are also calculated to provide experimentally relevant information useful for identification of these compounds during their synthesis.

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