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First Principles Investigation of Nitrogen-Rich Energetic Materials BRAD STEELE, IVAN OLEYNIK, University of South Florida — Energetic materials rich in nitrogen hold great promise due to their high positive heats of formation and because the products of detonation consist mostly of environmentally-friendly N_2 gas. Pure polymeric nitrogen can be synthesized at high pressures, although it has yet to be quenched to ambient conditions. By introducing a reducing agent into the crystal structure, the stability of polynitrogen compounds can be enhanced. We have investigated the stability of alkali polynitrides (R_xN_y), as well as hydro-nitrogens (H_xN_y), at high pressures and found several stable crystal structures that contain N_5 rings, N_6 rings, N_4 chains, and polymeric nitrogen chains. Using our theoretical input, cesium pentazolate salt has been synthesized for the first time by our experimental collaborators. We also consider several other ternary high-nitrogen energetic materials, containing {C, O, N}and {H, O, N}atoms. The results demonstrate the great potential for first principles structure prediction to design new energetic compounds and crystal structures, which are better, safer, and greener than traditional CHNO energetic materials.

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