Abstract Submitted
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From Designer Clusters to Synthetic Crystalline Nano-Assemblies[1] MEICHUN QIAN, S. KHANNA, A. REBER, Dept. of Physics, Virginia Common. Univ., A. CASTLEMAN, A. SEN, A. UGRINOV, K. DAVIS, S. PEPPERNICK, M. MERRITT, Dept. of Chemistry and Physics, Penn. State Univ. — Clusters have the potential to serve as building blocks of materials, enabling the tailoring of materials with novel properties. We have recently proposed a new protocol that combines gas phase investigations to examine feasible units, theoretical investigations of energy landscapes to identify potential motifs, and synthetic chemical approaches to synthesize cluster assemblies. We had earlier applied the protocol to As_7^{3-} based cluster assemblies. In this work, we extend our investigations to cluster assembled materials based on As_{11}^{3-} units as building blocks. By varying the alkali cation and introducing crypts, it is possible to form materials with arsenic clusters arranged to form one dimensional chain, two dimensional layers or three dimensional lattices and X-ray studies provide information on bond lengths etc. Theoretical studies have been carried out to examine their microscopic structure and electronic properties. It will be shown that these new compounds have the tunable electronic and optical properties. The theoretical predictions on the As_{11}^{3-}Crypt(K)$_3$ and $[As_{11}Cs_2]^{1-}$Crypt(K) are in good agreement with the experimental observations.

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Meichun Qian
Dept. of Physics, Virginia Common. Univ.

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