

Abstract Submitted
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New Assemblies Combining Super-halogens and Super-alkalis

SHIV KHANNA, ARTHUR REBER, Virginia Commonwealth University, A. WELFORD CASTLEMAN JR., Penn State University — An Al_{13} cluster has been shown to exhibit behaviors reminiscent of halogen atoms with an electron affinity comparable to a Cl atom while molecular units like K_3O , called superalkalis, are known to have low ionization potentials. We have carried out first principles electronic structure calculations to examine the stability and the electronic properties of compound clusters formed by combining super halogens with superalkalis. An $\text{Al}_{13}\text{K}_3\text{O}$ unit is shown to be a strongly bound ionic molecule that can be assembled into stable cluster superatom assemblies of composition $(\text{Al}_{13}\text{K}_3\text{O})_n$. It will be shown that the individual clusters maintain their identity during the growth. The nature of the super-assemblies and their electronic properties will be highlighted.

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