Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Computational Investigations of a Possible New Class of Materials: A Superatom Ionic Solid KARL SOHLBERG, VIOLETA NASTO, Drexel University — A "superatom" is a cluster of atoms that shows high stability. High stability can arise from the geometric arrangement of the atoms in the cluster. For example, when atoms are close packed, clusters containing an integer number of closed shells of atoms, (i.e. 13, 55, 137... atoms) exhibit enhanced stability and are termed "magic clusters." High stability can also arise from the electronic structure. High symmetry metal clusters that have exactly 8, 20, 40..., valence electrons show enhanced stability. Superatoms can act chemically like a single atom of a different element. We have used electronic structure calculations to test the idea that a new class of materials may be formed based on the periodic arrangement of superatom ions, instead of the typical atomic or polyatomic ions of a conventional ionic solid. A solid is formed based on crystalline packing of anionic ($Al@Cu_{54}^{-}$) and cationic ($Ce@C_{60}^{+}$), nearly spherical superatom species that show exceptional stability. According to radius-ratio rules, these ions will favor a CsCl crystal structure with a body-centered (bcc) type of unit cell. Calculations on this material suggest that it is stable, semiconducting and less dense than common metal oxides, but that the metal anion clusters deform within the material.

Karl Sohlberg
Drexel University

Date submitted: 04 Dec 2012 Electronic form version 1.4