Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Anion Photoelectron Spectroscopy and First-Principles Study of PbxIny Clusters[1] S. VINCENT ONG, Virginia Commonwealth University, JOSHUA MELKO, UJJWAL GUPTA, The Pennsylvania State University, J. ULISES REVELES, Virginia Commonwealth University, JONATHAN D'EMIDIO, The Pennsylvania State University, SHIV KHANNA, Virginia Commonwealth University, A.W. CASTLEMAN, The Pennsylvania State University, DEPARTMENT OF PHYSICS, VIRGINIA COMMONWEALTH UNIVERSITY COLLABORATION, DEPARTMENTS OF CHEMISTRY AND PHYSICS, THE PENNSYLVANIA STATE UNIVERSITY COLLABORATION — Anionic and neutral Pb_xIn_y clusters containing up to 5 Pb and up to 7 In atoms have been investigated using negative ion photodetachment spectroscopy along with first-principles electronic structure studies within a gradient corrected density functional approach. The stability and electronic properties of these clusters have been characterized through studies of the detachment energies, gaps in the electronic spectrum, variations in binding energy, and nature of the electronic states. Particularly stable clusters have been grouped into two families of stable species. $PbIn_3^-$, Pb_2In_2, and Pb_3In_2 exhibit enhanced stability compared to their neighbors and the stability is linked to the aromatic character identified in their molecular orbitals. On the other hand, $PbIn_5^-$ and Pb_2In_4 exhibit enhanced stability associated with filled electronic shells within a confined nearly free electron gas.

[1]We acknowledge support from the U.S. Department of the Army through a MURI Grant W911NF-06-1-0280.

Shiv Khanna
Virginia Commonwealth University

Date submitted: 30 Nov 2010 Electronic form version 1.4