Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Pseudohalogens as Building Blocks of Hyperhalogens: A Case Study with Au(CN)$_x$ Complexes DEVLEENA SAMANTA, Virginia Commonwealth University, MIAO MIAO WU, Peking University, China, PURUSOTTAM JENA, Virginia Commonwealth University, VIRGINIA COMMONWEALTH UNIVERSITY TEAM, PEKING UNIVERSITY, CHINA COLLABORATION — Electron affinity (EA) is one of the major factors that govern reactivity. Halogen atoms possess the highest electron affinities among the elements in the periodic table since it takes only one electron to close their shell. Pseudohalogens also require one electron to close their shell and thus mimic the properties of halogens. A typical example is the CN moiety whose electron affinity (3.8 eV) is slightly larger than that of Cl. Using calculations based on density functional theory we show that when a Au atom is surrounded by CN moieties, the electron affinity of Au(CN)$_x$ complexes rise above that of CN for x$\geq$2 and reach a value as high as 8.4 eV, thus forming hyperhalogens. Electron affinities also show odd even alternation with the clusters with even x having higher EA values. Equilibrium geometries, electronic structure and spectroscopic properties of these complexes will be presented and results will be compared with available experimental data.

Devleena Samanta
Virginia Commonwealth University

Date submitted: 19 Nov 2010 Electronic form version 1.4