Abstract Submitted
for the DAMOP10 Meeting of
The American Physical Society

Electron affinity of small Pt clusters[1] ZHIFAN CHEN, ALFRED Z. MSEZANE, Clark Atlanta University — The adiabatic electron affinities (AEAs) and vertical EAs (VERs) for the small (2-5 atoms) platinum clusters have been evaluated in the density functional theory. The structures of clusters for the 2, 3, 4, and 5 Pt atoms were represented, respectively by linear, equilateral triangle, tetrahedron, and trigonal bipyramid atoms. The geometric optimization was performed using the DMol package under the generalized gradients approximation (GGA) with the Perdew-Wang exchange-correlation functional (PW91). Double numerical plus polarization has been used as the atomic basis sets to describe the valence electrons. All electrons in the core were treated explicitly with some relativistic effects. The AEAs for the clusters of 2,3,4, and 5 Pt atoms are respectively, 1.89, 1.67, 2.06 and 2.39 eV. The VEAs for the above clusters are respectively, 1.87, 1.62, 2.05, and 2.37 eV. The results show better agreement with the experiment than other similar calculations do. Our calculation demonstrates the importance of the correct structure and geometry optimization involving all the electrons.

[1]Supported by DOE and AFOSR

Zhifan Chen
Clark Atlanta University

Date submitted: 14 Jan 2010 Electronic form version 1.4