Abstract Submitted
for the DAMOP13 Meeting of
The American Physical Society

**Photoabsorption spectrum of the Ce@$C_{82}$ endohedral fullerene**[1]
ZHIFAN CHEN, ALFRED Z. MSEZANE, Clark Atlanta University — The absolute differential oscillator strengths (DOS's) for the photoabsorption of the Ce atom encapsulated in the $C_{82}$ have been evaluated using the time-dependent-density-functional-theory (TDDFT). The geometry optimization was performed for the $C_{82}$ and Ce@$C_{82}$. The atomic coordinates were obtained by minimizing the total energy until the change in energy was less than $5x10^{-4}$ eV. The final position of the Ce atom was found at 1.85 Å off the center along the $C_2$ axis. A supercell of 23.8 Å was constructed. The Kohn-Sham equation was solved to yield the eigenvalues and eigenvectors for the ground state. The dynamical polarizability of the ground state due to the external electric field perturbation was evaluated using TDDFT. The results demonstrate that the peak of the free Ce 4d giant resonance was reduced and shifted to the lower energy side. Comparison with the experimental data [1] shows great suppression of the 4f decay process for the encaged Ce atom. This calcultion confirms the experimental result which observed no confinement resonance in the Ce@$C_{82}$ endohedral fullerene photoionization.

[1] A Müller et al, Phys. Rev. Lett. **101,** 133001 (2008)

[1]Supported by DOE, AFOSR and Army Research.

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Date submitted: 23 Jan 2013 Electronic form version 1.4