

Abstract Submitted
for the DAMOP13 Meeting of
The American Physical Society

Theoretical Study of the Photoionization of small fullerenes C_n ($n=28, 32, 40, 44, 50$) using the Time-Dependent-Local-Density Approximation (TDLDA)¹ MOHAMMAD H. JAVANI, Georgia State University, HIMADRI S. CHAKRABORTY, Northwest Missouri State University, STEVEN T. MANSON, Georgia State University — The Time-Dependent-Local-Density Approximation (TDLDA) is used to calculate total and subshell photoionization cross section of small fullerene C_n , ($n=28, 32, 40, 44, 50$). For the various C_n , which are taken to be spherical, the core of $n C^{4+}$ ions are smeared out on the sphere with known radius to form a classical jellium shell, and the resulting potential is used to treat the dynamics of the motion of the $4n$ delocalized valence electrons quantum mechanically. The theoretical methodology has been described in detail elsewhere [1]. For all cases, it is found that there are two plasmon resonances in the total cross section due to phase-coherent superposition of amplitudes that causes the enhancements in the ionization from different C_n subshells in two distinct energy regions, just as in the case of C_{60} [1]. In addition, each of the two plasmons, for each fullerene, is quite close in energy to each other and to the C_{60} case.

[1] M. E. Madjet, H. S. Chakraborty, J. M. Rost and S. T. Manson, J. Phys. B **41**, 105101 (2008).

¹This work was supported by NSF and DOE.

Steven T. Manson
Georgia State University

Date submitted: 24 Jan 2013

Electronic form version 1.4