

Abstract Submitted  
for the DAMOP13 Meeting of  
The American Physical Society

**Evolution of plasmonic and hybrid photoionization properties  
of alkaline earth metallofullerenes with the increasing fullerene size<sup>1</sup>**

AAKASH PATEL, HIMADRI CHAKRABORTY, Northwest Missouri State University — A theoretical study of the photoionization of endohedral fullerenes with a selection of fullerene molecules of increasing size and with confined alkaline earth atoms like Be and Mg is carried out. The fullerene ion cores, comprised of  $C^{4+}$  ions, are smudged into a continuous jellium charge distribution, while the delocalized cloud of carbon valence electrons plus the electrons of the encaged atom are treated in the Kohn-Sham local density approximation (LDA) [1]. Only the spherical geometry is considered. The photoionization spectra are calculated by the time-dependent LDA that includes essential electron correlations [1]. A systematic evolution of the mixing of valence atomic levels with states of fullerene single-electron bands is found along the sequence. This hybridization as a function of the fullerene size is seen to primarily define the properties of the subshell-differential ionization spectra both in the low energy plasmonic as well as the high energy oscillatory regions.

[1] M.E. Madjet, T. Renger, D.E. Hopper, M.A. McCune, H.S. Chakraborty, J.-M. Rost, and S.T. Manson, *Phys. Rev. A* **81**, 013202 (2010).

<sup>1</sup>Supported by NSF and DOE

Himadri Chakraborty  
Northwest Missouri State University

Date submitted: 24 Jan 2013

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