

Abstract Submitted
for the DAMOP20 Meeting of
The American Physical Society

Strong s,p and d level hybridization in the photoionization of noble metallofullerene molecules.¹ ESAM ALI, ANDREW DENNIS, TAYLOR O'BRIEN, Northwest Missouri State University, Maryville, Missouri, USA., STEVE MANSON, Georgia State University, Atlanta, Georgia, USA., HIMADRI CHAKRABORTY, Northwest Missouri State University, Maryville, Missouri, USA. — We calculate and study the properties of subshell photoelectron spectra of fullerene molecules endohedrally doped by noble metals. The cases of Cu@C_{60} and Ag@C_{60} have been considered. The numerical methods include the application of a gradient corrected Leeuwen-Baerends (LB) exchange-correlation functional [1] within density functional theory. The dipole coupling of the molecule with the photon is described in a linear response treatment, called the time dependent local density approximation (TDLDA) augmented by LB [2]. Metal-fullerene ground state hybridization predicted for outer electrons of s , p and d angular momentum character significantly affects the structures of photoionization cross sections of these hybrid levels. The hybridization character is not found to change appreciably for likely more stable configurations $\text{Cu}^-@\text{C}_{60}^+$ and $\text{Ag}^-@\text{C}_{60}^+$ after a fullerene electron transfers to the metal to form closed shell atomic anions. In fact, the general behavior of the hybrid cross sections also appear qualitatively similar to those of closed shell Zn@C_{60} and Cd@C_{60} in the periodic table, aside from shifts in energy. [1] R. Van Leeuwen and E. J. Baerends, *Phys. Rev. A* **49**, 2421 (1994); [2] M. E. Madjet *et al.*, *J. Phys. B* **41**, 105101 (2008).

¹Supported by the National Science Foundation grant PHY-1806206

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Date submitted: 29 Jan 2020

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