

Abstract Submitted
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Photoionization of atom-fullerene hybrid levels in $F@C_{60}$ versus $F^-@C_{60}^+$.¹ TAYLOR OBRIEN, ANDREW DENNIS, ESAM ALI, Northwest Missouri State University, Maryville, Missouri, USA., STEVE MANSON, Georgia State University, Atlanta, Georgia, USA., HIMADRI CHAKRABORTY, Northwest Missouri State University, Maryville, Missouri, USA. — A density functional study to model the ground state structure and to calculate the photoionization properties of the $F@C_{60}$ endohedral molecule is performed. The method goes beyond the local density approximation by employing the Leeuwen-Baerends (LB) exchange-correlation functional [1] and the interaction of the molecule with the radiation field is described in a linear response framework [2]. The study primarily focusses on the photodynamics of atom-fullerene hybrid levels of *p* angular momentum character. It is found that this hybridization is weak for $F@C_{60}$ as well as for $F^-@C_{60}^+$ formed after an electron transfers to F from most any of the C_{60} levels. However, when this electron originates from the C_{60} hybridizing level itself, the hybridization is strengthened dramatically. This contradicted the hole-level universality found for $Cl^-@C_{60}^+$ earlier [3]. Consequently, significant variations in photoionization cross sections at the plasmonic energies of the spectrum and beyond emerge. Detailed results will be presented in the conference. [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); [3] D. Shields, R. De, M. E. Madjet, S. T. Manson, and H. S. Chakraborty (submitted) [arXiv:1907.04881](https://arxiv.org/abs/1907.04881) [physics.atm-clus].

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