Abstract Submitted
for the DAMOP18 Meeting of
The American Physical Society

Photoionization studies of singly-charged halogen anions @C_{60}[1]

RUMA DE, DAKOTA SHIELDS, Northwest Missouri State University, Maryville, USA, MOHAMED MADJET, QEERI, Hamad Bin Khalifa University, Doha, Qatar, STEVEN T. MANSON, Georgia State University, Atlanta, USA, HIMADRI CHAKRABORTY, Northwest Missouri State University, Maryville, USA — The ground states of endofullerene molecules comprised of atomically closed-shell singly-charged halogen anions Cl^-, Br^-, and I^- confined in C_{60} are modeled in a spherical Kohn-Sham local density approximation (LDA) by employing the Leeuwen and Baerends exchange-correlation functional [1]. The core of sixty C^{4+} ions is jelliumized [2] to ignore the carbon K-shell structures. A time-dependent LDA (TDLDA) method [3] is subsequently applied to calculate the photoionization parameters of the molecules in the dipole coupling frame. The cross sections for the bonding and antibonding hybrid levels of the molecules in comparison with the free anion valence np results display two broad energy regions: (i) plasmon-enhanced low-energy domain and (ii) higher energy region of broad oscillations from the coherence of cavity and confinement effects. However, results compared among these molecules reveal significant differences in the details. Further comparisons with the results from Ar,Kr,Xe@C_{60}, the nearby closed-shell neutrals in the periodic table, unravel effects of transitions from neutrals to anions within identical electron configurations. [1] R. van Leeuwen et al, Phys. Rev. A **49**, 2421 (1994); [2] M. E. Madjet et al., Phys. Rev. A **81**, 013202 (2010); [3] Choi et al., Phys. Rev. A **95**, 023404 (2017).

[1]The work is supported by the US National Science foundation and the US Department of Energy.

Himadri Chakraborty
Northwest Missouri State University

Date submitted: 24 Jan 2018 Electronic form version 1.4