Abstract Submitted
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Photoionization of halogen atoms and singly-charged halogen anions @C_{240}[1] RUMA DE, DAKOTA SHIELDS, Northwest Missouri State University, Maryville, STEVEN T. MANSON, Georgia State University, Atlanta, HIMADRI CHAKRABORTY, Northwest Missouri State University, Maryville — The ground states of endofullerene molecules comprised of one-vacancy open-shell halogen atoms and closed-shell singly-charged halogen anions confined in the C_{240} fullerene are modeled in a spherical Kohn-Sham local density approximation (LDA). The framework is augmented by the Leeuwen and Baerends exchange-correlation functional [1]. The core of two hundred and forty 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 interaction frame. The cross sections of various levels of the molecules, in comparison with the results of free atom/anion as well as empty C_{240}, display two general spectral regions: (i) plasmon resonance enhanced low-energy domain and (ii) higher energy region of broad oscillations from the coherence of fullerene cavity and confinement effects. The results show differences in transitioning from neutral to anionic state of the central species in C_{240}. Further comparisons with corresponding calculations of C_{60} endofullerenes unravel effects of the size and electronic configuration of the fullerene cage. [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).

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Himadri Chakraborty
Northwest Missouri State University, Maryville

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