

Abstract Submitted
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Photoemissions from hybrid states in metastable halogen-endofullerene molecules¹ DAKOTA SHIELDS, RUMA DE, 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 — For the Cl@C₆₀ endofullerene we consider the transfer of a C₆₀ π electron of p angular character to the outer $3p$ shell of confined Cl forming a metastable molecule Cl⁻@C₆₀⁺. The ground state of this molecule is modeled in a spherical local density approximation (LDA) augmented by the Leeuwen and Baerends exchange-correlation functional [1] where the core of sixty C⁴⁺ ions is jelliumized [2]. A time-dependent LDA (TDLDA) method [3] is subsequently applied to calculate the dipole photoionization parameters of the molecule. Cross sections for the photoemission from levels hybridized between the C₆₀ level containing the p hole and the Cl⁻ $3p$ level show the coherence between C₆₀ plasmonic and atomic Coulomb dynamics. At higher energies, the mixing of confinement and cavity oscillations [4] determines the structures in the spectra. Calculations are also extended to similar hybrid levels of metastable Br⁻@C₆₀⁺ and I⁻@C₆₀⁺. Detailed comparison among the results provides deeper insights into the role of evolving halogen structures to influence the molecular photoionization. [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); [4] Potter et al., Phys. Rev. A **82**, 033201 (2010).

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