

Abstract Submitted
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Photoionization of open-shell Cl@C₆₀¹ 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, Atlanta, USA, HIMADRI CHAKRABORTY, Northwest Missouri State University, Maryville, USA — The ground state of the atomically open-shell Cl@C₆₀ endofullerene 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 is subsequently applied to calculate the dipole photoionization parameters of the endohedral molecule. Cross sections for the photoemission from atom-fullerene hybrid levels show the effects of both C₆₀ plasmon and atomic Coulomb dynamics, as well as the interference between them. At higher energies, the coherence of confinement and cavity oscillations dominates the structures of the spectra. Detailed comparison with the results from Ar@C₆₀, which involves the nearby close-shell atom in the periodic table, provides deeper insights into the role of a single shell-closing electron to noticeably influence the ionization dynamics. [1] R. van Leeuwen et al, Phys. Rev. A **49**, 2421 (1994); [2] M. E. Madjet et al., Phys. Rev. A **81**, 013202 (2010).

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