

Abstract Submitted
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Enhancement in low energy valence photoionization of Ar confined in C_{60} HIMADRI CHAKRABORTY, Northwest Missouri State University, Maryville, MO 64468, MOHAMED MADJET, Freie Universitaet, 14195 Berlin, Germany, JAN-MICHAEL ROST, MPIPKS, 08117 Dresden, Germany, STEVE MANSOON, Georgia State University, Atlanta, GA 30303 — Encapsulation of atoms in C_{60} offers a unique possibility to examine the behavior of an atom in a nanometric confinement. We perform calculations on the photoionization of an Ar atom endohedrally confined in C_{60} . The ground state of the $Ar@C_{60}$ compound is described by the Local Density Approximation (LDA) after freezing sixty C^{2+} ions to form a classical jellium background. A time dependent LDA method is then employed to calculate the response of the compound to the dipole photon. The valence 3p ground state electron of Ar shows very little mixing with the C_{60} electrons to retain its atomic character even in the confinement. However, the low energy part of the 3p ionization cross section is found to enhance considerably, by more than an order of magnitude, when compared with its counterpart for a free atom. Further scrutiny reveals that this increase in the Ar 3p cross section is accompanied by a compensatory depletion of the surface plasmon in the ionization cross section of the confining shell, pointing to a strong dynamical coupling between the atom and the shell.

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