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Photoionization of the Zn@C_{60} endofullerene: Atom-fullerene ground-state orbital hybridization of d-d character[1] JAYKOB MASER, Northwest Missouri State University, MOHAMMAD JAVANI, Georgia State University, RUMA DE, Northwest Missouri State University, MOHAMED MADJET, CFEL/DESY, Hamburg, Germany, HIMADRI CHAKRABORTY, Northwest Missouri State University, STEVE MANSON, Georgia State University — A detailed theoretical study of the subshell photoionization of Zn endohedrally confined in C_{60} has been performed. The fullerene molecular core of sixty C^{4+} ions is modeled by a classical jellium smearing, while the delocalized cloud of 240 carbon valence electrons, *plus* the encaged Zn atom placed at the center of the cage, are treated in the time-dependent local density approximation (TDLDA) [1]. A powerful hybridization of the Zn 3d state with the 2d orbital near the low end of C_{60} electronic band are unraveled. Cross sections for these hybrid states at both low photon energies, overwhelmed by electronic collective motions, and high energies of dominant single-electron behavior are presented. The results exhibit rich structures and are radically different from the cross sections of free atomic or free fullerene states participating in the hybridization process.

[1] M.E. Madjet et al., *Phys. Rev.* A **81**, 013202 (2010).

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