

Abstract Submitted
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Effects of inter-fullerene π -band mixings in the photoexcitation of hybrid plasmons in the $C_{60}@C_{240}$ molecule¹ RUME DE, Northwest Missouri State University, MOHAMED MADJET, CFELS, DESY, Germany, HIMADRI CHAKRABORTY, Northwest Missouri State University — We perform a detailed study of the ground state electronic structure of a two-layer fullerene onion molecule $C_{60}@C_{240}$. Calculations are carried out in a quantum mechanical framework of local density approximation (LDA) where the onion's ion-core of sixty C^{4+} ions from C_{60} and two hundred and forty of those from C_{240} is smeared into a classical jellium distribution [1]. Significant inter-fullerene mixing between the bands of single-node radial symmetry, the π -bands, is found. We then compute the photoionization from all the levels of the system using a time-dependent version of LDA at photon energies where the ionization is dominated by the inter-layer hybridization of collective plasmon resonances [2]. It is determined, by comparing the isolated fullerene cross sections with the cross section of the onion system for both π and σ (having nodeless radial waves) symmetry, that the π -band mixing is predominantly responsible for the production of plasmon hybrids.

[1] M.E. Madjet, H.S. Chakraborty, J.-M. Rost, and S.T. Manson, *J. Phys. B* **41**, 105101 (2008);

[2] M.A. McCune, R. De, M.E. Madjet, H.S. Chakraborty, and S.T. Manson, *J. Phys. B* Fast Track Comm. **44**, 241002 (2011).

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