

Abstract Submitted
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A simple model to describe C_{60} photoemission measurements by the inclusion of atomic carbon emissions.¹ MAIA MAGRAKVELIDZE, University of Mary Washington, HIMADRI CHAKRABORTY, Northwest Missouri State University — We previously used Kohn-Sham time-dependent local density approximation (TDLDA) [1] with Leeuwen and Baerends exchange-correlation functional [2] to calculate the total photoionization cross section of C_{60} where the core of sixty C^{4+} ions is smeared in a spherical jellium shell. This implied 240 valence electrons to be entirely delocalized by being oblivious to Coulomb potentials of C atoms. While the result qualitatively showed two plasmon resonances, as observed in experiments [3,4], the absolute value of the cross sections veered far from the measurements. This must be due to the effect of emissions from sixty C centers omitted in the jellium theory. To test, we calculate the photo cross section of a C atom in TDLDA and admix this result, times sixty, with the C_{60} jellium result by ensuring that the total oscillator strength stays conserved in order to retain participations of the same 240 electrons. Even though the scheme misses the interference between C_{60} and C emissions, the fit has produced a far improved quantitative agreement with experiments above 15 eV photon energy. [1] Choi et al, PRA 95, 023404 (2017) [2] van Leeuwen et al, PRA 49, 2421 (1994) [3] Hertel et al, PRL 68 784 (1992) [4] Reinkoster et al, JPB 37 2135 (2004)

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