Abstract Submitted
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Effects of exchange-correlation potentials in density functional descriptions of ground-state and photoionization of fullerenes[1] JINWOO CHOI, EONHO CHANG, DYLAN M. ANSTINE, HIMADRI CHAKRABORTY, Northwest Missouri State University, Maryville, USA — We study the ground state properties of C_{60} and C_{240} molecules in a spherical frame of local density approximation (LDA). Within this mean-field theory, two different approximations to the exchange-correlation (xc) functional are used: (i) The Gunnerson-Lundqvist parametrization [1] augmented by a treatment to correct for the electron self-interaction [2] and (ii) the van Leeuwen and Baerends (LB94) model potential [3] that inclusively restores electron's asymptotic properties [4]. Results show differences in the ground-state potential, level energies and electron densities between the two xc choices. We then use the ground structure to find the excited and ionized states of the systems and calculate dipole single-photoionization cross sections in a time-dependent LDA method that incorporates linear-response dynamical correlations. Comparative effects of the choices of xc on collective plasmon and single-excitation Auger resonances as well as on geometry driven cavity oscillations are found significant. [1] Gunnersen and Lundqvist, PRB **13**, 4274 (1976); [2] Madjet *et al.*, JPB **41**, 105101 (2008); [3] van Leeuwen and Baerends, PRA **49**, 2421 (1994); [4] Magrakvelidze *et al*, PRA **91**, 053407 (2015).

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