Oscillation phenomenon in photoionization cross section of Ar@C_{60}

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The oscillations in partial cross sections of photoionization of atomic clusters, in particular, of fullerenes C_{60}, at high photon energies was experimentally discovered more than 10 years ago [1]. These oscillations appear due to the reflection of photoelectrons at the borders of cluster potential and, as a result, the formation of spherical standing waves inside the cluster. Recently, the similar oscillation was shown to occur in the photoionization cross sections of endohedral noble gas fullerenes, in particular Ar@C_{60} [2].

The present work is devoted to the application of the consistent quantum many-body theory to the description of photoionization of endohedral noble gas fullerenes. The case study is the Ar@C_{60}. The single-electron energies and the wave functions are obtained within the jellium model with use of the self-consistent Hartree-Fock (HF) approximation. The partial and total cross sections of the photoionization are calculated within the Random Phase Approximation with Exchange (RPAE) with photon energy range up to 100 eV. The comparison between the endohedral and pristine fullerenes is performed.

Self-consistent potential of the endohedral system has a double-well profile in contrast to the single-well potential of the empty fullerene C_{60}. Due to the additional well at the centre of the system one may expect strong changes of the oscillations in the partial cross sections for endohedral fullerenes.

Preliminary analysis of the obtained results shows that the changes in the oscillatory behaviour of the partial cross sections depend on the electron density distribution between embedded atom and fullerene shell, i.e. on the hybridization of ground state orbitals.

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