

<< **ELECTRON CORRELATION EFFECTS IN MULTICHARGED IONS OF
ICOSAHEDRAL C₆₀ FULLERENE** >>

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Fullerene C₆₀ is considered to be promising active material for various electronic devices. Its unique physical properties are determined in the first place by the size and icosahedral symmetry causing the high degeneracy of levels. One of the questions, important for understanding of fullerene electronic properties but still discussed concerns the role of correlation effects in the C₆₀ molecule and its ions. In this report the results of the symmetry-adapted SCF-CI calculations for C₆₀ ions with charges -4 to +3 are reported. Two different CI active spaces built on h_u HOMO and $t_{1u}+t_{1g}$ LUMOs are considered for the cases of fullerene cations and anions, respectively. The many-electron states of C₆₀ ions are calculated within the spatial π -electron model with three different parametrizations for electron-electron (e - e) potentials known in literature, some of them are proposed to account for the polarization of carbon atoms in C₆₀. The manifestation of electron correlation in ion excitation spectra and correlation functions are discussed in the relation to e - e potential shape. As it is shown, all the e - e potentials predict alike energy-charge dependencies of parabolic form, however, only long range potential caused strong electric correlation leads to right quantitative predictions the energies of C^{-N}₆₀ anions.

The results show, particularly, the essential role of long-range interactions and electron correlations for predicting the observed order of ground-state energies of the multicharged anions thus suggesting the restricted applicability of Hubbard model and one-electron approaches for the calculations of many-electron states of fullerene and fullerenes.



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