

## JAHN-TELLER SPLITTING OF MULTI-ELECTRONIC STATES IN $C_{60}$ FULLERENE ANIONS

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Fullerene  $C_{60}$  is considered as an ideal building block for novel molecular devices due to its nearly spherical symmetry and high affinity. Strong electron–lattice interaction and high icosahedral symmetry are thought to play a key role in the formation of the physical properties of alkali metal fullerenes  $A_N C_{60}$ , which range from insulating to metallic and even to superconducting [1]. In these compounds the fullerenes are in multi-charged anionic forms  $C_{60}^{-N}$  with  $N$  extra electrons, which partially fill the threefold degenerate lowest vacant molecular orbital  $t_{1u}$ . The coupling of the degenerate electronic states with certain vibrational modes of the molecule leads to a lowering of the total energy because of spontaneous molecular distortion appearing in Jahn-Teller effect [2].

We report on the results of theoretical study of static Jahn-Teller ground state splittings in icosahedral  $C_{60}^{-N}$  ( $N=1, 2, 3, 4$ ) fullerene anions with different parameterizations of electron-electron interaction [3]. Multi-electronic states of anions were determined within a quasy- $\pi$ -electron model by the symmetry adapted configuration interaction method for two active spaces of  $t_{1u}$  and  $t_{1u}+t_{1g}$  molecular orbitals [4]. Electron–lattice interaction is taken into account in a framework of Su–Schrieffer–Heeger model by linear dependence of the neighbor site resonance integrals on the corresponding length change. The calculations are performed with electron correlation potentials of two types: long-range Ohno and short-range Hubbard potentials. Contrary to the case of short-range electron repulsion the inclusion of long-range correlation can essentially change the features of the Jahn–Teller splittings. The influence of the active space expansion to  $t_{1u}+t_{1g}$  on long-range electron repulsion is shown as a change of ground state multiplicity in distorted fullerene dianion. The correlation effectively damps electron–lattice interaction favoring the electron delocalization thus destabilizing deformations. The obtained results confirm the Jahn–Teller nature of anions with charges of  $-2$  and  $-4$  providing good agreement with known theoretical [2] and experimental [5] data.

### REFERENCES

- [1] O. Gunnarsson, *Rev. Mod. Phys.* **69**, 575 (1997).
- [2] C.C. Chancey, M.C.M. O'Brien, *The Jahn-Teller effect in  $C_{60}$  and other icosahedral complexes*. New Jersey: Princeton univ. press, (1997).
- [3] O.L. Kapitanchuk, V.A. Kuprievich, *Mol. Cryst. and Liq. Cryst.* **426**, 89 (2005).
- [4] V.A. Kuprievich, O.L. Kapitanchuk, O.V. Shramko, *Mol. Cryst. and Liq. Cryst.* **427**, 23/[335] (2005).
- [5] A. Wachowiak, R. Yamachika, K.H. Khoo *et al.*, *Science* **310**, 468 (2005).