

Jahn-Teller effect in C₆₀ monoanion and monocation

ZHISHUO HUANG^{1,2}, DAN LIU^{2,3}

¹*Department of Chemistry, National University of Singapore, Block S8 Level 3, 3 Science Drive 3, Singapore 117543, Singapore.*

²*Theory of Nanomaterials Group, KU Leuven, Celestijnenlaan 200F, B-3001 Leuven, Belgium.*

³*Institute of Flexible Electronics (IFE), Northwestern Polytechnical University, 127 West Youyi Road, Xian 710072, Shaanxi, China.*

Email: zhishuohuang@gmail.com, iamdliu@nwpu.edu.cn

Fullerene ions show various types of Jahn-Teller effects. In order to quantitatively characterize the nature of the Jahn-Teller effects, we performed DFT calculations of the C₆₀ cation (C₆₀⁺) and C₆₀ monoanion (C₆₀⁻). We calculated the vibronic coupling parameters with hybrid B3LYP and CAM-B3LYP functional (including the non-local interaction correction), and based on the parameters, analyzed the static and dynamic Jahn-Teller (JT) effects. For C₆₀⁺, the global minima of adiabatic potential energy surface (APES) shows a D_{5d} Jahn-Teller deformation, with stabilization energies of 110 and 129 meV (with B3LYP and CAM-B3LYP respectively), which are two times larger than that in C₆₀⁻, implying the significance of the dynamical JT effect [1]. For C₆₀⁻, we derived the vibronic states by exactly diagonalizing dynamical JT Hamiltonian, indicating that dynamical JT effects are more significant in the first excited C₆₀⁻ than those in the ground electronic states [2]. Besides, the vibronic coupling constants calculated with CAM-B3LYP for C₆₀⁻ are closer to the coupling parameters extracted from experimental data [3] than those from B3LYP, which shows the significance of non-local interaction correction for the study of fullerene related materials.

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[3] N. Iwahara, T. Sato, K. Tanaka, L. F. Chibotaru, *Phys. Rev. B.*, 82, 245409 (2010).