Electronic and defect structures of fullerene C_{60} molecular complex

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It is well known, that optical and electrical properties of semiconductors depend on the defective structure and the local levels in the band-gap, as a consequence. However, the information about transport properties of given fullerene based compounds is completely absent. The aim of the work was revealing and detail research of electronic and defects structures of fullerene C60 molecular complexes with copper (II) diethyldithiocarbamate $\{Cu^{II}(Etdtc)_2\}_2{\cdot}C_{60}$.

Thermostimulated currents (TSC) measurements revealed in material traps located below the LUMO level on 0.43± 0.02 eV. It allows supposing that trapping centres are caused by one type of defects. Most probably they are solution fragments donor`s molecule disordered in the hollows of the crystal lattice or defect of molecule fullerene.

To explain the peculiarities of the absorption and photoconductivity in the visible spectrum we calculated the excited electronic states of the complex $\{Cu^{II}(Etdtc)_2\}_2{\cdot}C_{60}$ in the TD-DFT/B3LYP method (*6-311G*$^{++}$ basis set). The calculation for a perfect complex allowed for a correlation of experimental optical bands (2.62, 3.09 eV according to [1]). Excited states of 2.12 eV calculation is not shown and this band in the photoconductivity spectrum of a real crystal formed by trapping centres.

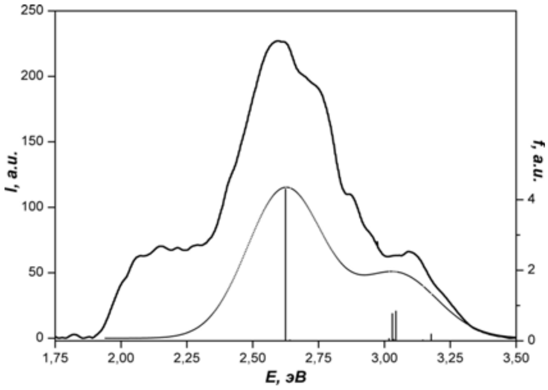

Figure. Photoconductivity spectra (solid line) and excited electronic states (dotted line) of the complex.

To test the latter hypothesis, we simulated several of the most probable types of structural defects in both the donor and fullerene molecules. It is shown that the most probable defect of real crystals is imperfect fullerene molecule.

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[1] D.V. Konarev, A.Y. Kovalevsky, S.S. Khasanov, G. Saito, D.V. Lopatin, A.V. Umrikhin, A. Otsuka, R.N. Lyubovskaya, *Eur. J. Inorg. Chem,* 1881 (2006).