Electronic and Vibrational Structure of Complexes Formed by C_{60} Fullerenes and Squaraine Dyes

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C_{60} fullerenes are an allotropic form of carbon known to act as efficient charge donors are acceptors, which makes them a lucrative choice in the design of organic solar power cells. A natural and straightforward way to functionalize the fullerenes would be to link them to molecular structures that convert solar radiation energy into charge in a specific region of photon energies. These conditions are satisfied by dyes, specifically squaraine dyes [1], derived from squaric acid, which form a bond with the fullerene via their central cycle.

The point of interest in this research is to study the electronic and vibrational properties of complexes formed by C_{60} fullerenes and several squaraine dyes (such as one shown on Fig. 1) in order to determine the specifics of the mechanisms, by which they interact.

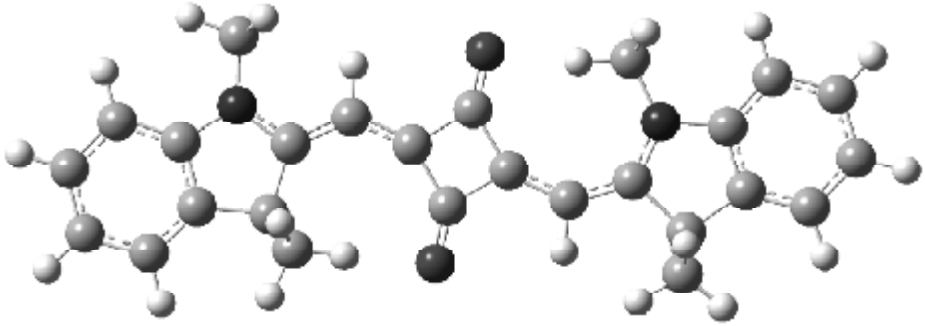

Fig. 1. A Ball and Bond Type model of a sample squaraine dye.

We use UV-VIS absorption, Raman scattering and photoluminescence measurements along with quantum-chemical calculations to explore the properties of the complexes and discuss the charge transfer, excited states, shapes of molecular orbitals and nonlinear features on experimental spectra.

Extra attention is given to the bridge that connects the squaraine dye to a fullerene, as it plays a sufficient role in the vibrational picture of the complex and the reallocation of charge.

1. G. Chen, D Yokoyama, H. Sasabe et.al., *App. Phys. Lett*, **101**, (2012), 08390.