THEORETICAL STUDY OF ELECTRONIC PROPERTIES IN ORGANIC PHOTOVOLTAIC MATERIALS

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Abstract

It has been proved that fullerene derivatives, in which an oligophenylenevinylene (OPV) group is attached to C₆₀, present an interesting photophysical phenomenon and can be incorporated into photovoltaic cells. In these systems, the OPV acts as electron donor upon excitation, and then fullerene absorbs photoexcited electrons. This new organic semiconductor materials offer the prospect of lower manufacturing costs and they present several advantages: easy fabrication, large area, flexible and light weight devices when compared to the inorganic counter parts.

In the present theoretical study, oligomeric chains of p-phenylenevinylene (n-PPV, n = 3 - 8 units) and C₆₀-OPV hybrids, have been studied by Density Functional Theory (DFT) and Time Dependent – Density Functional Theory (TD-DFT). The electronic properties such as: Electronic absorption and emission spectrum of these systems were calculated in order to determinate as the increasing of spectroscopic units affects their electronic behavior. All the theoretical calculations of the structural properties of n-PPV and hybrids of OPV were obtained using PBE1PBE/6-31G and ONIOM2 method, a two-layered version, respectively. Absorption and emission spectra were obtained by TD-DFT in Gaussian 03W.

Keywords: DFT, Time Dependent-DFT, electronic transference, donor-acceptor system, electronic spectrum.