SIMULATION IN ORGANIC NANOELECTRONICS: FROM SINGLE MOLECULE TO THIN FILM

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During the last decades, the organic electronic field has suffered a tremendous development due to the potential of using organic materials as active components in electronic devices that result from the possibility of tuning their electronic properties by changing the molecular structure of the organic molecules or the experimental conditions in which they are prepared. Most of the knowledge reached so far on the electronic properties of these materials occurred at the experimental level; nevertheless that research is not able to provide a deep understanding of the effect of their properties at molecular scale or the influence of the nanostructure in device performance, among other factors, separately. It is in this context that theoretical modelling reveals to be the ideal approach to understand these effects separately as well as get inside in the physics underlying the electronic processes involved. In this talk we will present some results of our work on nanoelectronic thin film and molecular devices that use small conjugated molecules and conjugated polymers. [1]

By using a quantum molecular dynamics method we study the electron transfer in a molecular device (see Fig. 1) made of a single conjugated molecule (with and without spatial symmetry) bound to two metal electrodes separated by a distance approximately 2 nm. To perform the electronic calculations we used molecular dynamics in parallel with a self-consistent quantum mechanical method since organic molecules are flexible and have strong coupling between the electronic and atomic motion. A significant difference in electron transfer through symmetric and asymmetric conjugated molecules was found to be due to molecular distortion and molecular vibrations along their axis.

To study the influence of the nanostructure, namely the molecular arrangements relative to the electrodes surface, on optoelectronic devices that uses poly(p-phenylene venylene) derivatives as the active component, we developed a nanoscale model for polymer light emitting diodes (see Fig. 2) that uses a dynamical Monte Carlo method for charge injection and transport [2,3]. Our model considers the electronic processes involved in the device functioning, namely charge injection, that depends on the barrier height at electrode/polymer interfaces, two processes for charge transport (e.g. intra-molecular charge transport along a polymer chain and inter-molecular charge transport between polymer chains), charge collection by the electrode opposite to the injection, charge trapping within the polymer layer and charge recombination. Our simulations show that by controlling the nanostructure of the polymer and the type of electrodes used it is possible to increase the performance of the device.

References:

[1] H.M.G. Correia, PhD Thesis, University of Minho, 2007.

[2] M.M.D. Ramos, H.M.G. Correia, J. Phys.: Condens. Matter, **18** (2006) S429.

[3] H.M.C. Barbosa, M.M.D. Ramos, Plasma Process. Polym., **4** (2007) S104.

Figures:

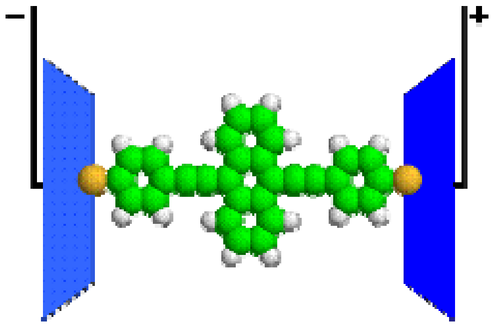

Figure 1 - Scheme of a molecular device made of a symmetric conjugated molecule bond to two gold electrodes.

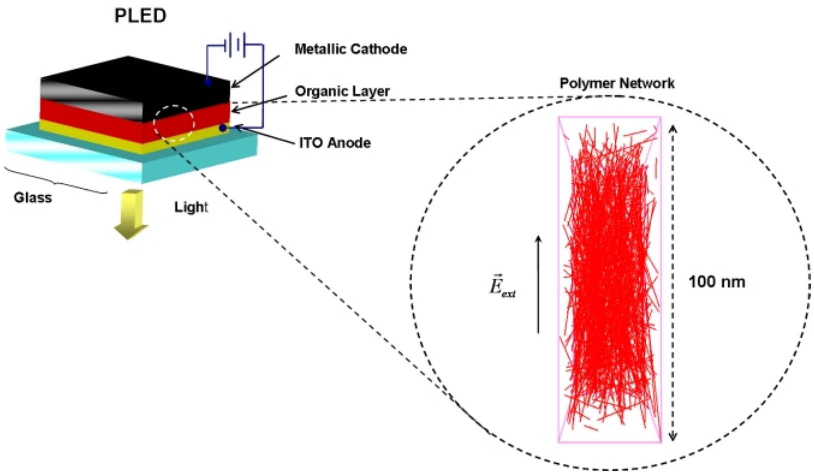

Figure 2 – Scheme of a polymer light emitting diode (PLED) where the sticks represent the different arrangements of the polymer conjugated segments relative to the electrodes surface.