Séminaire de Chimie Théorique

Salle conférence, 3eme Est, bat. A12

Mardi 3 Mai à 11:00

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Modelling the Structural and Electronic Properties of Organic Materials in Bulk and at Interfaces in the Field of Organic Electronics

In this seminar, we will review some of our recent theoretical works addressing the structural and electronic properties of organic materials used in organic-based devices such as solar cells or transistors. We will first describe the mechanisms allowing for the modulation of the work function of electrodes in devices upon deposition of organic self-assembled monolayers and will establish useful structure-property relationships. This study will be extended to the case of dyes adsorbed on TiO_2 surfaces in dye-sensitized solar cells and to molecules sandwiched between two electrodes in the field of molecular electronics. We will show that the electronic properties of organic semiconductors can be strongly perturbed upon chemisorption on such surfaces via pinning effects, leading to a situation where the bulk electrodes dictate the alignment of the electronic levels of the molecules. In a second part, we will describe the structural properties of widely used conjugated polymer chains in the crystalline, disordered, and amorphous states by means of molecular dynamics (MD) simulations and the resulting charge transport properties at a quantum-chemical level. We will focus on four different polymers, namely the hole transporting IDTBT, PBTTT, and CDTBT and electron transporting NDITT chains. Our results highlight the unique characteristics of IDTBT associated to the fact that the torsion angles between the units along the chain are preserved when going from one phase to another; this implies that charge transport is less affected by interfaces between different regions. IDTBT also features a small and similar degree of energetic disorder in the three phases in contrast to the other polymers.

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