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COMPUTATIONAL MODELING OF MATERIALS AND PROCESSES IN HYBRID/ORGANIC PHOTOVOLTAICS

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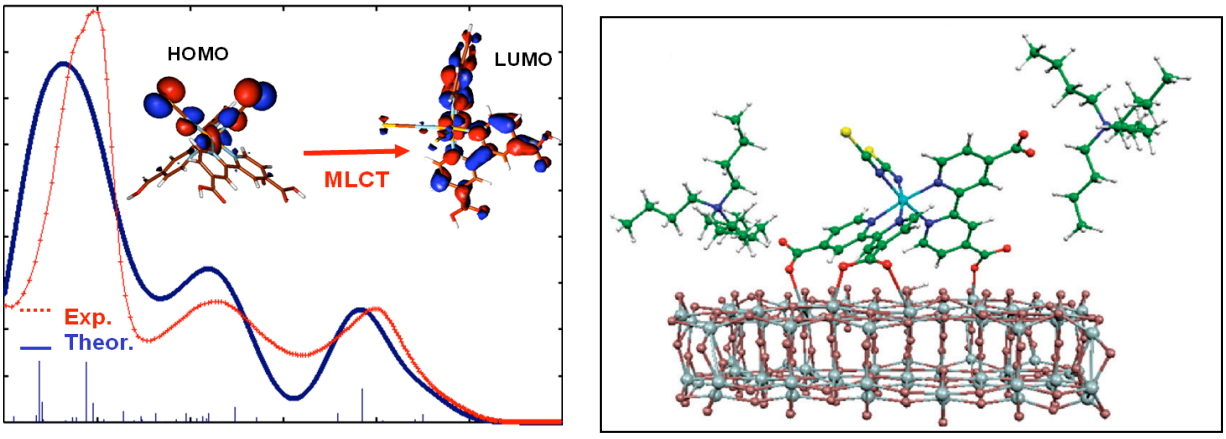
ABSTRACT I:

We present the potential of computer simulations based on ab initio methods applied to the investigation of the structural, electronic and spectroscopic properties of materials of interest in the field of hybrid/organic photovoltaics (HOPV). In the specific field of dye-sensitized solar cells one needs to accurately simulate hybrid/organic interfaces involving a dye-sensitized semiconductor and a liquid environment containing the electrolyte. In addition to ground state properties, excited states of the combined system need to accounted for, thus calling for an appropriate methodology set-up along with a proper modeling strategy. We devised over time a computational strategy based on DFT, DFT-based molecular dynamics and Time Dependent DFT which allows the accurate calculation of ground and excited state properties of large systems in condensed phase. The ingredients of our computational strategy are presented and the potential of computer simulations are discussed in direct connection to available experimental data. Due to the implemented methodological advances, theory is today a predictive tool, allowing us to scrutinize and screen the properties of organic and inorganic materials even before their synthesis, simulating, at the same time, the fundamental processes of light-harvesting and charge injection central to HOPV technology.

Figure 1. Comparison between the calculated and experimental absorption spectra and orbital contributions for the N3 Ru-dye in solution (left) and its adsorption on TiO_2 (right).



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