Séminaire de Chimie Théorique

Salle conference ISM 3eme Est, Bat. A12
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Organic solar cells : Some Insights from Quantum Chemistry

Due to their low production costs organics-based solar cells have attracted considerable interest. Their main drawback is the low efficiency arising from the charge carrier and exciton transport properties. They strongly depend on the mutual orientation of the monomers in crystals, thin films or aggregates and the character of the electronically excited states. In the present talk these aspects are investigated for perylene based materials by means of a bottom up approach which includes appropriate quantum chemical and quantum dynamical methods. Effects arising from the environment are taken into account by appropriate hybrid approaches (QM/MM).

After discussing appropriate theoretical approaches we will focus on a new trapping mechanism for PBI aggregates as a first example. This trapping mechanism involves population transfer between neutral as well as charge-transfer states and can nicely explain the data of time-resolved experiments on a femtosecond timescale. The involved conical intersections are reached through induced stretch distortions in the monomers. In this example we will also explain why we use dimers and not monomers as the most basic unit in the description of the complex aggregates.

As a second example we will present a model which nicely explains the strong differences in the exciton diffusion lengths of □-PTCDA and DIP crystals. In the case of α-PTCDA shift motions of two neighboured molecules leads to the relaxation into an optically dark excited state through a conical intersection. This trapping mechanism can be generalized for a wide range of perylene based dyes, but our computations indicate that it cannot take place in DIP crystals due to the molecular arrangement. This may explain why DIP possesses considerably larger exciton diffusion length than □-PTCDA and also explains other experimental results. In the context we will also briefly mentioned new force fields which were necessary to describe the crystal structures of the involved molecules.

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