MO 27: Poster: Theory: Quantum Chemistry

Time: Thursday 16:00–18:00 Location: P1

MO 27.1 Thu 16:00 P1

Ab initio study on limitations of excitation energy transport in pi-stacked organic dyes — •Volker Settels, Reinhold F. Fink, and Bernd Engels — Institut für Physikalische und Theoretische Chemie, Am Hubland, D-97074 Würzburg

The energy conversion efficiency of organic bilayer solar cells depends crucially on the excitation energy transfer (EET) in the employed dyes. For certain perylene-tetracarboxylic-bisimde (PBI) aggregates the authors provided evidence that the EET is quenched by relaxations of excited aggregate structures [1]. In the quenching process the excitation in the optically bright state reaches a dark state via an intermolecular relaxation path. In this dark state the exciton is trapped due to the loss of energy and the strongly reduced oscillator strength. In this poster the EET quenching mechanism is generalized for a wider range of perylene based dyes, e.g. perylene-tetracarboxylic-dianhydride (PTCDA) or diindeno-perylene (DIP). It was found that the trapping is due to the characteristics of the perylene itself. This is supported by the fact that the potential energy curves and the character of the excited states are very similar for all considered dye molecules. Nevertheless, for DIP a much more efficient EET was measured than for PTCDA [2]. This can be explained by modeling the exciton diffusion within a simple hopping approach. The results give a hint that EET in pi-stacked aggregates is highly affected by exciton trapping due to the mechanism mentioned above. [1] H. M. Zhao, et al., J. Am. Chem. Soc. 131 (2009), 15660. [2] D. Kurrle, J. Pflaum, J. Appl. Phys. Lett. 92 (2008), 133306; R. R. Lunt, et al., Adv. Mat. 22 (2010), 1233.

MO 27.2 Thu 16:00 P1

Charge and exciton transport in organic crystals — •Vera Stehr[1], Johannes Pfister[2], Reinhold F. Fink[2], Carsten Deibel[1], and Bernd Engels[2] — [1]Physikalisches Institut, Universität Würzburg, 97074 Würzburg — [2]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, 97074 Würzburg

Organic solar cells become more and more interesting for applications due to their low production costs and easy processability. In order to increase their efficiency it is very important to understand the basic principles of charge and exciton transport in these materials. The charge carrier mobility and the exciton diffusion have been studied theoretically by means of quantum chemical methods and a hopping approach using Marcus theory along with the master equation. The implementation of the approach presented here is straightforward and it is shown to provide qualitatively good results concerning the directional and morphological dependency of the transport parameters. We demonstrate that quantitatively good agreement for the exciton transport properties is obtained in several organic crystals while charge carrier transport properties turn out to be generally more demanding. Results for promising organic semiconductors such as fluorinated perylene bisimides are presented.