Plenary Talk PV IV Tue 9:15 B Audimax

The dimer-approach to characterize opto-electronic properties of organic semiconductors — •Bernd Engels — Institut für Physikalische und Theoretische Chemie, Universität Würzburg

Spectroscopic approaches are essential for an understanding of the electronic structure and properties of organic semi-conductors but the information are often ambiguous. Hence, for the assignment of the spectra theory is necessary but depending on the underlying approach, the simulations are contradictory too. In this talk, we will describe the so-called dimer-approach [1] and provide a few examples in which this approach could successfully assign absorption as well as emission spectra [2,3] and could delivered an atomistic picture of photo-induced relaxation effects in perylene-based materials. The model Hamiltonians of standard monomer-based approaches are also briefly discussed to reveal the differences between both methods and to shed some light on their strengths and shortcomings. Finally, we will compare both approaches in their description of amorphous materials.[4]

[1] B. Engels, V. Engel PCCP 2017, 19, 12604-12619.

[2] D. Bellinger, J. Pflaum, C. Brüning, V. Engel, B. Engels PCCP 2017 19, 2434

[3] V. Settels, A. Schubert, M. Tafipolski, W. Liu, V. Stehr, A. K. Topczak, J. Pflaum, C. Deibel, R. F. Fink, V. Engel, B. Engels J. Am. Chem. Soc. 2014, 136, 9327-9337

[4] C. Brückner, M. Stolte F. Würthner, J. Pflaum, B. Engels J. Phys. Org. Chem. 2017; 30; e3740