SIMULATION OF PHOTO-INDUCED PROCESSES AT ORGANIC-ORGANIC INTERFACES

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In the present work we focus on investigations about photo-induced processes in thin organic films and at the organic-organic interfaces. Their accurate description and understanding are prerequisites for the design opto-electronic devices such as organic solar cells or light emitting diodes. In organic solar cells, separation of optically excited electron-hole pairs and long-range charge transport play an important role for the efficiency. Both are largely influenced by the film structure and the molecular orientation at interfaces between electron donor (D) and acceptor (A) molecules. In our presentation we briefly mention the dimer approach which successfully delivered atomistic pictures for photo-induced relaxation effects in aggregates and allowed a correct description of the energy disorder in the vicinity of amorphous interfaces.[1,2] Furthermore, we focus on our simulations about the individual steps of the light to energy conversion process in the vicinity of the interfaces of organic solar cells [3] and describe recent works about the interpretation of femtosecond (fs) time-resolved second harmonic generation (TR-SHG) in DIP-PDIR-CN_2 interfaces.[4]

[1] B. Engels, V. Engel **PCCP** (2017), *19*, 12604-12619
[2] C. Brueckner t al. https//doi.org/10.1002/poc.3740
[3] C. Brueckner et al. J. Phys. Chem C (2017), *121*, 4-25; *ibid* J. Phys. Chem C (2017), *121*, 26-51
[4] S. Wirsing, M. Hänsel, V. Belova, F. Maass, F. Schreiber, K. Broch, B. Engels, P. Tegeder in preparation.

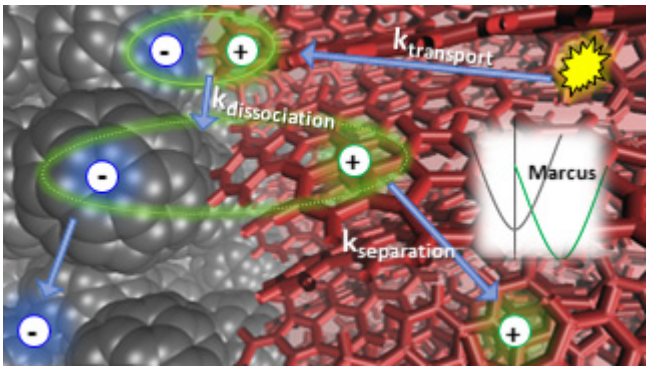

Figure 1: Various processes at organic-organic interfaces