## Sub-Bandgap Absorption in Organic Solar Cells: Experiment and Theory

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Most high-performance organic solar cells involve bulk-heterojunctions in order to increase the active donor-acceptor interface. The power conversion efficiency depends critically on the nano-morphology of the blend and the interface. Spectroscopy of the sub-bandgap region, i.e., below the bulk absorption of the individual components, provides unique opportunities to study interface-related properties. We present absorption measurements in the sub-bandgap region of bulk hetero junctions made of poly(3-hexylthiophene-2,5-diyl) as electron donor and [6,6]-phenylC61-butyric acid methyl ester (P3HT:PCBM) as electron acceptor and compare them with quantum-chemical calculations and recently published [1] data on the external quantum efficiency (EQE). The very weak absorption of the deep sub-bandgap region measured by the ultra-sensitive Photothermal Deflection Spectroscopy (PDS) features Urbach tails, polaronic transitions, conventional excitons, and possibly charge-transfer states. The quantum-chemical calculations allow characterizing some of the unsettled spectral features, in particular the charge-transfer states and excitons in the subband-gap region by visualizing the charge difference and transition densities.



Charge transfer state of a oligothiophene–fullerene complex in the subbandgap region as calculated by TD-DFT and visualized by the charge difference density (red=hole, blue=electron)

[1] M. Presselt, M. Bärenklau, R. Rösch, W. J. D. Beenken, E. Runge, S. Shokhovets, H. Hoppe and G. Gobsch (**2010**) *Applied Physics Letters*, *97*, 253302.