

Project Summary 7

Interplay between microscopic structure and intermolecular charge transfer processes in polymer-fullerene bulk-heterojunctions

The successful development of a non-conventional spin sensitive technique and a depth resolved imaging method based on atomic force microscopy (AFM) in the previous funding period (Phase 2) allow us to probe the molecular excited states in the polymers and polymer-fullerene blends with respect to their origin (charge transfer (CT) state or triplet exciton), molecular orientation, and microstructure. These comprehensive studies were so far performed on the model systems P3HT and P3HT:PC60BM with the different degree of regio-regularity of the host polymer. With the optically detected magnetic resonance (ODMR) technique we were able to determine the orientation of P3HT monomers relative to the substrate surface and the parameters of triplet excitons formed upon photoexcitation. However, little contrast could be found in the low and high molecular weight, i.e. in amorphous and crystalline P3HT. In contrast, with depth-resolved AFM imaging we show that the entire surface of the highly regio-regular P3HT, including crystalline regions and crystalline fibers, is covered by an amorphous layer.

The complementarity of these two techniques and their applicability to the same sample encouraged us to elaborate a program of studies (Phase 3) on a highly performing donor-acceptor copolymer thieno[3,4-b]thiophene and benzodithiophene (PTB7) and its blends with PCBM and compare them with the behaviour of P3HT based blends. With PTB7 blends we are able to fabricate laboratory scale solar cells with power conversion efficiency of above 7%. The systematic investigations are aimed at clarifying the role of molecular orientation of PTB7 molecular units relative to substrate, which is claimed to be different to P3HT, and its influence on charge transfer and triplet exciton states generation yield.

To further improve the sensitivity and the resolution of our spin resonance set-up, we will increase the frequency range from 9 GHz to 34 GHz.

This will allow us to distinguish between amorphous and crystalline regions due to their influence on the structure of ESR signal from CT states. Finally, in combination with AFM subsurface imaging, the correlation between the complex hierarchical microstructure of this poorly investigated however highly performing donor-acceptor copolymer PTB7 and the charge transfer reactions will be established.