Morphology impact on the performance of polymer-fullerene solar cells

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The goal of the joint project is to gain synthetic control over the π-π backbone-backbone interchain distance $D_{\pi-\pi}$ of low band gap poly(*p*-arylene-ethynylene)-*alt*-poly(-*p*-arylene-vinyl-ene)s based copolymers. We investigate the influence of $D_{\pi-\pi}$ on the nanoscale morphology of the polymer-fullerene bulk heterojunction and its implications on the photovoltaic performance of solar cells. Grafting solubilizing alkoxy side chains guarantees a good contact between polymer and fullerene and offers a possibility to control the π-π stacking distance.

The photophysical and photovoltaic properties are strongly affected by $D_{\pi-\pi}$ and by the extent of donor-acceptor interfacial area formation which in turn can be controlled by selective modification of the polymer architecture. A detailed knowledge of the structural properties and structure formation in the pure conjugated polymer materials as well as in the active layers is essential for a better understanding of how targeted modification of the polymer architecture can improve the performance of the materials in solar cell applications. Our investigations cover a broad range of length scales.

The expertise of the MPIP lies in a combination of scattering methods (light, x-rays and neutrons), atomic force microscopy (AFM) and microscopy. These methods allow the determination of the structural properties of the materials over a broad range of length scales starting from the π-π interchain distances up to domain sizes. By application of conductive AFM and Kelvin probe force microscopy we can relate the position resolved electronic properties to the topological structure of the thin films and the photovoltaic performance of the solar cell.

Knowledge of the structure formation in the bulk samples, in solution and finally in the thin film as a function of temperature is essential to distinguish the impact of the polymer architecture from the impact which certain film preparation methods and tempering might have. Time-resolved and stroboscopic x-ray scattering experiments allow to follow the structure formation during the film fabrication process and tempering. This includes e.g. the dynamics of the structure formation from a single droplet (as confining geometry), over its evaporation on the substrate to the final structure of the thin films.

Process properties and, thus in turn the final structure of the film, are also strongly affected by the mechanical properties of the materials in bulk and solution. Hence our structural investigations will be accompanied by comprehensive rheological measurements. Insitu-rheology in combination with scattering methods allows to monitor the structural changes in the presence of an external shear field.