KPFM study of model donor-acceptor self-assemblies for organic photovoltaics

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The Kelvin probe force microscope (KPFM) constitutes an extremely powerful tool of characterization in the field of organic photovoltaics. In ultra-high vacuum (UHV) and in non-contact mode (nc-mode) it is possible to record simultaneously the topography and the contact potential difference (CPD) with an exceptional level of resolution. For donor-acceptor bulk-heterojunction blends it has been demonstrated that KPFM enables the investigation of the charge carrier generation on the sub-10nm scale [1]. However, to further enhance the understanding of these processes it is advantageous to study model molecular systems that possess better defined electronic and structural properties than the one found in bulk heterojunctions.
In this communication, KPFM and scanning tunneling microscopy (STM) investigations of model donor-acceptor self-assemblies on highly oriented pyrolytic graphite (HOPG) will be presented. First, the characteristics of a mixed monolayer of evaporated C_{60} and the semiconducting polymer P3DDT will be discussed. In a second step, a new generation of donor-acceptor dyads will be introduced that has been synthesised following the concept developed by W. Li *et al.* [2]. Scanning probe microcsopy measurements proof the auto-organization of this model system in the form of periodic lamella on HOPG. The scanning probe microscopy data will be compared to the results of molecular mechanics (MM) and molecular dynamics (MD) simulations. Finally, the nature of the CPD contrasts [3] will be examined and a comparison of CPD measurements in dark and under illumination will be discussed. The results affirm the value of these new donor-acceptor model-systems for organic photovoltaics.

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