Interplay of Charge-Transfer Exciton and Effective Band Gap in Organic Donor-Acceptor Blends

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Abstract. In organic photovoltaic blends an appropriate adjusting of HOMO/LUMO energy levels at donor-acceptor interface is essential for charge separation of light induced excitons and photovoltaic current extraction. However, chosen combinations of promising organic semiconductors does not always result in efficient charge separation and expected high power conversion efficiency. We argue that this can happen when the effective band gap of the donor–acceptor blend is considerably higher than charge transfer exciton binding energy. Here, we examine the band gap structure and charge transfer exciton binding energy of two donor-acceptor material combinations using energy resolved-electrochemical impedance spectroscopy (ER-EIS) and photoluminescence. The ER-EIS method allows to observe otherwise obscured effective band gap between HOMO onset of the donor and the LUMO onset of the acceptor as determined directly in the blend. The experimental results for well-known P3HT:$PC_{61}BM$ blend confirmed the favorable relation between electronic bandgap and charge transfer exciton energy. On the other hand, the PCDTBT:Y6 blend shows considerably wider effective bandgap than the expected one from difference between $LUMO_{Y6}$ and $HOMO_{PCDTBT}$, which implies large barrier for exciton dissociation. We assume therefore that this combination of materials is not suitable for photovoltaic application.