Polymer Solar Cells with Less/No Fullerene

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Conventional $PC_{61}BM$ demonstrates weak absorbance in the visible region, leading to inefficient photon harvest. Furthermore, the inherent tendency of fullerene to aggregation under elevated temperatures has been considered a key factor for deteriorated morphology and consequently reduced lifetime of polymer solar cells (PSCs). By adopting alkyl aromatic side-chains to both D/A comonomers on BDT-TPD backbone, a new D-A polymer PTP8 with enhanced thermal stability and packing order was synthesized and demonstrated a high V_{oc} (~1.0 V) and PCE (~6.0%) at a very low blend ratio of 1:0.5. The increased side-chain rigidity and bulkiness prevent the intercalation of fullerenes at molecular level. The enhanced packing and reduced π-π stacking distance further promote the polymer:fullerene demixing, leading to a large D/A ratio and highly ordered fullerene clusters which have been observed for the first time in amorphous polymer/fullerene blend film. In general, this "double aromatic side-chains" structure may become a universal designing approach for existing polymers to achieve high performance at low fullerene and additive concentration. We also used polymers as the electron acceptors to replace the conventional fullerene derivatives. We successfully designed and synthesized a series of BDT-Qx-T based polymers as the donor polymer used in all polymer solar cells (all-PSCs). Their properties were finely tuned by side-chain modification and the introduction of strong electron-withdrawing fluorine atoms to polymer acceptor unit. Then we systematically investigated the effect of molecular structure on the polymer morphology and photovoltaic properties in all-PSCs. We revealed that the fluorination can optimize polymer energy level and improve the polymer coplanarity, leading to enhanced intermolecular packing and balanced carrier transport. Meanwhile, the substitution of dodecyl for 2-ethylhexyl side chains can result in improved film morphology and hole transport. As a result of the synergistic effect between fluorination and side-chain modification, we achieved a high PCE over 6% for the optimized all-PSCs. More importantly, our approach may become a general and effective way to tailor the polymer molecular structure for achieving high performance all-PSCs