Semi-Crystalline Photovoltaic Polymers for Binary and Ternary Blend Polymer Solar Cells

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A series of semi-crystalline, low band gap (LBG) polymers were designed and synthesized by considering non-covalent Coulomb interactions in a polymeric backbone and characterized for polymer solar cells (PSCs). Intra- and/or intermolecular noncovalent hydrogen bonds and dipole-dipole interactions assure strong interchain interactions without losing solution processability. The semi-crystalline polymers form a well-distributed nano-fibrillar networked morphology with $PC_{70}BM$ with balanced hole and electron mobilities (h/e mobility ratio of 1~2) and tight interchain packing (π-π stacking distance of 3.57-3.59 Å) in the blend films. Furthermore, the device optimization with a processing additive and methanol treatment improves efficiencies up to 8~9% in a ~300 nm thick conventional single-cell device structure. The thick active layer in the PPDT2FBT:$PC_{70}BM$ device attenuates incident light almost completely without damages in fill factor (0.71~0.73), showing a high short-circuit current density of 15.7~16.3 $mA \cdot cm^{-2}$. PPDT2FBT closely tracks theoretical photocurrent production while maintaining a high fill factor in remarkably thick films. The unique behavior arises from high vertical carrier mobility, an isotropic morphology with strong, vertical π-π stacking and a suitable energy band structure. The ability of PPDT2FBT to function efficiently in thick cells allows devices to fully absorb the incident sunlight while providing a pathway to defect-free, large area film processing by industrial solution casting techniques.[1-3]

We also demonstrated high-performance, ternary-blend polymer solar cells by modifying a high efficiency binary blend bulk heterojunction (PPDT2FBT:$PC_{71}BM$) with addition of a low bandgap, nitrile-substituted PPDT2CNBT as a ternary component. PPDT2CNBT was designed to have a complementary absorption and the deeper frontier energy levels based on the same polymeric backbone with PPDT2FBT. The structural similarity of PPDT2CNBT with PPDT2FBT enhanced the compatibility for two donor polymers and minimized the disruption of the crystalline morphology of the binary PPDT2FBT:$PC_{71}BM$ blend. The detailed morphological and photovoltaic properties will be discussed in detail.

References

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