Molecular Design and Property Relationship for Ideal Polymeric Solar Cells

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A series of semi-crystalline, low band gap (LBG) polymers were designed, synthesized and characterized for polymer solar cells (PSCs). The devices achieve power conversion efficiency (PCE) of over 7% without any post treatment (annealing, solvent additive, *etc*.) and outstanding long-term thermal stability for 200 h at 130 °C. These excellent characteristics are closely related to the molecular structures where 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 9.39% 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 $mA \cdot cm^{-2}$.[1-3] 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, leading to commercially viable PSCs. These new polymers provide a great possibility to overcome the efficiency barrier of 10% and accelerate the real application of plastic solar cells.

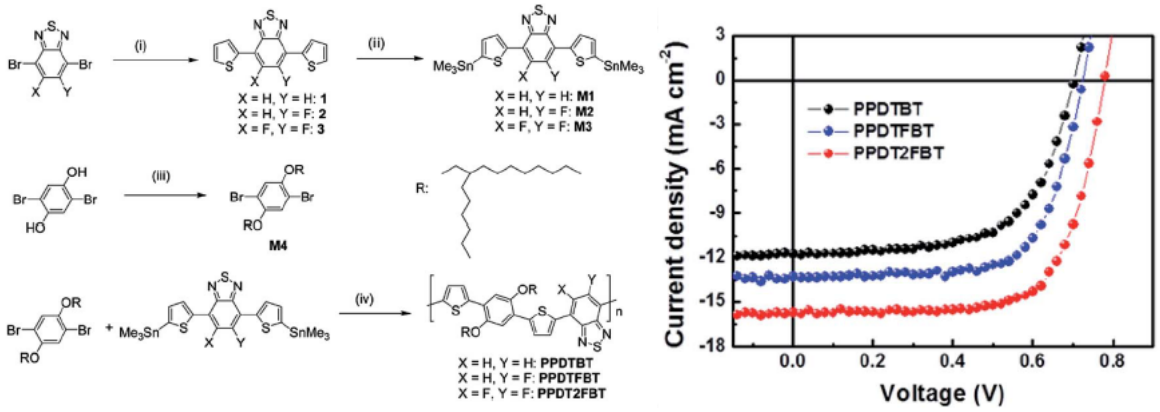

Fig. 1. Synthetic scheme to a series of semi-crystalline polymers and J-V characteristics

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