Interface Engineering in Organic Semiconducting Materials for Solar Cells

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Abstract

This work presents the synthesis of various organic polymers and copolymers with the intention to study the effect of chiral substituents on the packing and morphology of such materials in the solid state for their potential use in bulk heterojunction solar cells. Conjugated alternating copolymer designed solar cells have the advantageous characteristics of highly tuneable optical band gaps. Additionally, selection of different polymer units and side chains can allow fine-tuning of the active layer morphology possibly resulting in increased efficiency. [1a][1b] Polymer based solar cells are produced by physical mixing of the 2 components and their efficiencies not only rely on the ability of the components to create interpenetrating domains throughout the active layer but many other factors such as the size of the optical band gap, absorption coefficient, charge carrier mobility, crystallinity, solubility and surface morphology.

Various units are under investigation with the core unit being diketopyrrolopyrrole (DPP), as its photochemical and thermal stability are now seen as vital properties for making stable and efficient solar cells. The core unit contains a planar bicyclic structure, which increases the possibility of strong π - π stacking interactions, [2] and polar carbonyl functionalities able to induce intermolecular hydrogen bonding. These factors can lead to close packing of the molecules in the solid state and well defined domains. The DPP unit is attractive as it presents a multitude of opportunities to modify and enhance the core structure. Thiophene DPP based polymers have been reported to feature high charge carrier mobilies and these species are electron donors so there is potential to control the size of the optical band gap by copolymerisation with electron withdrawing moieties. [3] Furthermore, the lactam N atom provides a site for addition of alkyl groups therefore allowing variation of the solubility of a resulting polymer or when left unalkylated, a site for hydrogen bonding interactions. [4]

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