DOCTORAL THESIS

Understanding Fundamental Physical Properties of Non-fullerene Acceptors for High Performance Organic Photovoltaics

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Abstract

The development of non-fullerene acceptors (NFAs) promoted the progress of bulk heterojunction (BHJ) organic solar cells (OSCs) with remarkable power conversion efficiencies (PCEs) over 18%, push the OSCs field to a new phase. This thesis focuses on the emerging "Y-series" NFAs, presents the optical and electrical characterization of these high-performance OSCs materials and correlated the fundamental solid state properties with their molecule structure and OSCs performance.

We first focus two A-DA'D-A type "Y" acceptors incorporating the same backbone skeleton and end groups but without (Y3) or with (Y18) alkyl side chains, and examine the alkyl side chains effects on their charge transport properties and device performance. We probe investigation into the fundamental interplay between their chemical structures and opto-electronic properties including the (i) charge transport, (ii) heat transfer, and (iii) electronic disorder. We found that the BHJ with Y18 possesses more efficient phonon transfer and charge transport as well as suppressed electronic disorder. Among these properties, the extremely low Urbach energy (E_U) of 23 meV in Y18 stands out because it is even under the thermal energy (~26 meV) which sets the electronic disorder limit at room temperature. With all the contrasting results, a simple molecular model has rationalized in which the extra alkyl chains in Y18 help suppress the formation of rotamers, endowing it with a disorder-free molecular conformation and remarkable solid state properties.

With the knowledge of the conformational effects of the molecules on the thermal properties, we further focused on the heat energy transfer of the organic materials relevant to organic semiconductor applications. Here, we probe heat diffusion properties of Y-series non-fullerene acceptors processing different DA'D framework,

named BZ4F-5, BZ4F-6, and BZ4F-7, we found that backbone rings extension from five- to six- and seven-membered-fused rings trigger longer phonon mean free path and higher thermal diffusivities (D) in their pristine solid films and bulk heterojunction blends. Particularly, the correlation between the thermal transport properties in Y-series acceptors and their backbone geometry, molecule stacking, and thin-film crystallinity is demonstrated. More importantly, both organic thin-film transistors (OTFTs) and OSCs confirm that thermal durability of organic semiconductor devices correlated with the thermal properties of their active layer. Although BZ5F-6 and BZ4F-7 based devices possess similar device performance at room temperature, superior heat dissipation in BZ4F-7 molecule endows it with enhanced device lifetime.