Charge Transfer and Charge Separation Dynamics in Efficient Non-fullerene Solar Cells

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Abstract

Recently, Non-fullerene organic solar cells (OSCs) has been making rapid progress and reaching record breaking efficiency [1]. In the conventional idea for the fullerene based OSCs, one need a large donor-acceptor (D/A) offsets to cause rapid (i.e., <1ps) and effective charge separation from exciton at the D/A heterojunction [2]. However, recent work showed that non-fullerene OSC with small D/A offset can also achieved very high power conversion efficiency (PCE) [1,3-4]. The explanation for this is that charge separation occurs over hundreds of ps from thermalized charge transfer exciton (CTEs) at the D/A heterojunction for the non-fullerene system [5], thus charge separation in efficient non-fullerene OSC with small D/A offset is an endothermic process.

Here we will present our recent transient absorption (TA) spectroscopy studies to further elucidate the temperature dependence of charge transfer and charge separation dynamics in a number of non-fullerene OSC model systems with negligible D/A LUMO offset but variable HOMO offsets. We selectively create acceptor excitons and showed that acceptor excitons dissociate into CTEs at a similar rate (~100ps) as donor excitons despite the significantly large driving force provided by the HOMO offset. In contrast, by tracing the electro-absorption signal, it was demonstrated the generation of free charges after hole transfer required additional thermal excitation. Our result show the charge separation is indeed an endothermic behavior in non-fullerene OSCs, but charge transfer is not. Our result give a deeper understanding of the working mechanism of non-fullerene OSCs, which will have important fundamental implications on the development of OSCs.

Keywords: Ultrafast spectroscopy, organic solar cells, charge generation and separation.

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