

Abstract Submitted
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Charge transfer type excitons at donor/acceptor interfaces of organic solar cells AZUSA MURAOKA, KOICHI YAMASHITA, The Univ.of Tokyo, JST CREST — The conversion of excitons into charge within organic solar cells is complicated by bound electronhole pairs, or charge transfer states at donor/acceptor interfaces. The solar cell requires generating an efficient current. Thus it is necessary that charge transfer is further separated into free charge carriers to be transported to electrode. We focus on the improved the conversion efficiency of Bulk-heterojunction organic solar cells. We use dependent density functional theory with CAM-B3LYP/6-31G(d) to study the oscillator strengths, electronic structure, HOMO-LUMO band gap and energy level in several polymer (donor) : fullerene (acceptor) blends, such as MDMO-PPV, PCDTBT, PCPDTBT, PBB3, PTB7 and PTBF2 with PC70BM. To determine the effective physical factor in light energy conversion, we consider ,(i) charge transfer type excitation generated directly by photoinduced electron transition in the donor/acceptor interface (ii) the factors for controlling the conversion efficiency such as short-circuit current density and closed circuit voltage.

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