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A theoretical study on charge transfer type excitons at donor/acceptor interfaces of organic solar cells. AZUSA MURAOKA, Japan Women's Univ-Facul Sci, JST CREST, REINA TACHIBANA, Japan Women's Univ-Facul Sci, MIKIYA FUJII, KENJI MISHIMA, KOICHI YAMASHITA, Univ. of Tokyo, JST CREST, JAPAN WOMEN'S UNIV. TEAM, UNIV. OF TOKYO TEAM, CREST, JST TEAM — The conversion of excitons into charges within organic solar cells is complicated by bound electron-hole pairs, or charge transfer states at donor/acceptor interfaces. It is necessary that charge transfer is further separated into free charge carriers to be transported to electrodes. It was experimentally verified that the hot process is more dominant than the energy-gradient-driven intermolecular hopping for charge separation of an electron and a hole after the exciton generation in efficient photoconversion systems. We analyze the conversion efficiency of bulk-heterojunction organic solar cells in several polymer (donor):fullerene (acceptor) blends, such as, PCPDTBT, PTB2, PTB7 and PTBF2 with PC70BM using density functional theory and time-dependent density functional theory, and compare the numerical results with the experimental data. We discuss on the followings: (i) the charge transfer distance may be a good descriptor to design donor materials of high charge carrier separation, (ii) to examine whether the direct optical generation of CT states takes place in the charge separation process of the D/A complex, and (iii) the CS process takes place by the hot or cool process by examining an electron coupling of the D/A complex.

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