Predicting of Effective Intermolecular Complex of Donor-Acceptor by the Fluorine Position in Acceptor for the Non-fullerene Organic Solar Cell

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ITIC, which is composed of an IDTT core and DCI terminal groups, is non-fullerene molecule as the most representative acceptor for the organic solar cells(OSCs). Herein, we compared the isomeric ITIC, which have fluorine atoms on ortho and meta positions in the side chains, respectively, with PBDB-T donor on the power conversion efficiency(PCE) of OSCs via multiscale simulation method. First, the stacked structure was compared in PBDB-T:o-F-ITIC(i.e., PCE:11.11%) with PBDB-T:m-F-ITIC(i.e., PCE; 8.9%). The PBDB-T:o-F-ITIC structure showed closer stacking between DCI and benzodithiophene of PBDB-T, resulting the separation of LUMO and HOMO on donor and acceptor, respectively. It was due to curved structure in the backbone of o-F-ITIC, which was induced by repulsive force between neighboring ortho-fluorine atoms. Second, the PBDB-T:o-F-ITIC structure showed larger interfacial (i.e., contact) areas between donor and acceptor with planar and stretched structure of PBDB-T. To this end, we theoretically demonstrated that isomeric effect influences the intermolecular arrangement with the counterpart donor.