Development of Nonfullerene Acceptors with Spiro-substituted Fluorene Units

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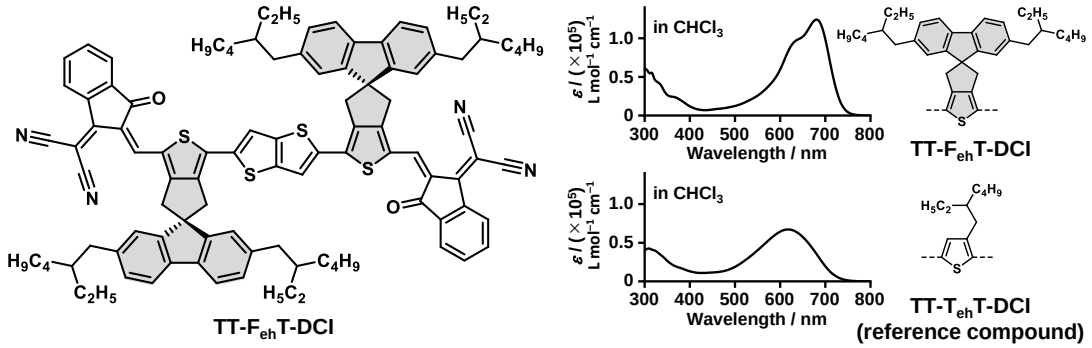
As the candidate of acceptor materials in organic photovoltaics (OPVs), considerable efforts have been devoted to developing new electron-accepting π-conjugated molecules. Most of high-performance nonfullerene acceptors possess planar fused structures with bulky substituents on the central part. We have reported a series of oligothiophenes having orthogonally fused fluorene units for insulated molecular wires.[1-3] In this molecule, the presence of cyclopentene-annelation is important to achieve planar π-conjugated backbone, and orthogonally fused fluorene unit can suppress the intermolecular interactions. In this study, to utilize the advantages of this unit, we developed new nonfullerene acceptor (**TT-F$_{eh}$T-DCI**).

The physical properties of **TT-F$_{eh}$T-DCI** were investigated by electrochemical and photophysical measurements. Cyclic voltammetry measurements showed a reduction wave with the half-wave reduction potential ($E_{red}^{1/2}$) of –0.95 V vs. Fc/Fc$^+$. Based on $E_{red}^{1/2}$, the lowest unoccupied molecular orbital (LUMO) energy level of **TT-F$_{eh}$T-DCI** was estimated to be –3.85 eV. On UV-vis absorption measurements, **TT-F$_{eh}$T-DCI** showed narrower absorption bands at around 600-720 nm with higher molar extinction coefficient, compared to that of the reference compound (**TT-T$_{eh}$-DCI**). This phenomenon indicates that the planarity of π-conjugated backbone was improved by the introduction of cyclopentene-annelation. From the absorption edge of 735 nm (1.69 eV) and the LUMO energy level, the highest occupied molecular orbital (HOMO) energy level was determined to be –5.54 eV.

The photovoltaic characteristics of **TT-F$_{eh}$T-DCI** were investigated in OPVs with an inverted configuration of [ITO/ZnO/PBDB-T (CAS No. 1415929-80-4): **TT-F$_{eh}$T-DCI** /MoO_x/Ag]. **TT-F$_{eh}$T-DCI** showed higher power conversion efficiency (PCE) than reference compound, and the maximum PCE value of 6.12% was observed.



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