Supporting Information

for

Molecular Symmetry Effect on Morphology and Self-aggregation of Semiconducting Polymers

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1. Experimental section

Materials

All reagents and chemicals were purchased from commercial sources Sigma-Aldrich and Suna Tech Inc. unless specified. (E)-1,2-bis(5-(trimethylstannyl)thiophen-2-yl)ethene (TVT), (E)-(4-fluoro-5-(2-(5-(trimethylstannyl)thiophen-2-yl)vinyl)thiophen-2-yl)trimethylstannane (asy-1FTVT), and (E)-1,2-bis(3-fluoro-5-(trimethylstannyl)thiophen-2-yl)ethane (2FTVT) are synthesized by following the methods and reported literatures.¹

Device fabrication

Organic solar cells were fabricated with inverted structure (ITO/ZnO/active layer/MoO₃/Ag). The ITO substrate was cleaned with ultra sonication with acetone and IPA for 10 min each and dried in a hot oven. Then, the cleaned ITO substrate was treated by UV ozone for 30 min. ZnO precursor was spin coated on ITO substrates and annealed at 200°C for 10 min. A blend of PTB7-Th:NDI-based copolymers was dissolved in CF (1:1.5 w:w) with concentration of 18 mg/ml. Then, this blend solution with 0.5% CN was spin coated on ZnO layer in N₂-filled glove box. The MoO₃ and Ag was deposited by thermal evaporation on the active layer under 2*10⁻⁶ Torr.
$^1$H-NMR spectrum of (2)
$^1$H-NMR spectrum of (3)
$^1$H and $^{13}$C-NMR spectra of (4)
$^1$H and $^{13}$C-NMR spectra of (5)
$^1$H, $^{13}$C, and $^{19}$F-NMR spectra of asy-IFTVT
Figure S1. $^1$H, $^{13}$C, and $^{19}$F nuclear magnetic resonance (NMR) spectroscopy of all the compounds.
Figure S2. Cyclic voltammograms (CV) of the second reduction cycles of (a) PNDI TVT, (b) asy-PNDI1FTVT, and (c) PNDI2FTVT.
Figure S3. Space charge limited current (SCLC) mobility plots of three acceptor polymers.
Figure S4. Gel permeation chromatographs of PNDITVT, asy-PNDI1FTVT and PNDI2FTVT.
Figure S5. Differential Scanning Calorimeter thermograms of three copolymers.
Figure S6. Optimized four model compounds (a) NDITVT (b) ND11FTVT-3,3 containing fluorine atoms at 3,3 positions, (c) ND11FTVT-3,8 containing fluorine atoms at 3,8 positions, and (d) ND12FTVT.
Figure S7. Jablonski diagram of asy-PNDI1FTVT.
Figure S8. Contact angle measurement of PTB7-Th, PNDITVT, asy-PNDI1FTVT, and PNDI2FTVT (average value of 5 drops of each solvent).
References