Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

High Performance Conjugated Terpolymers as Electron Donors in Near Infrared Nonfullerene Organic Solar Cells

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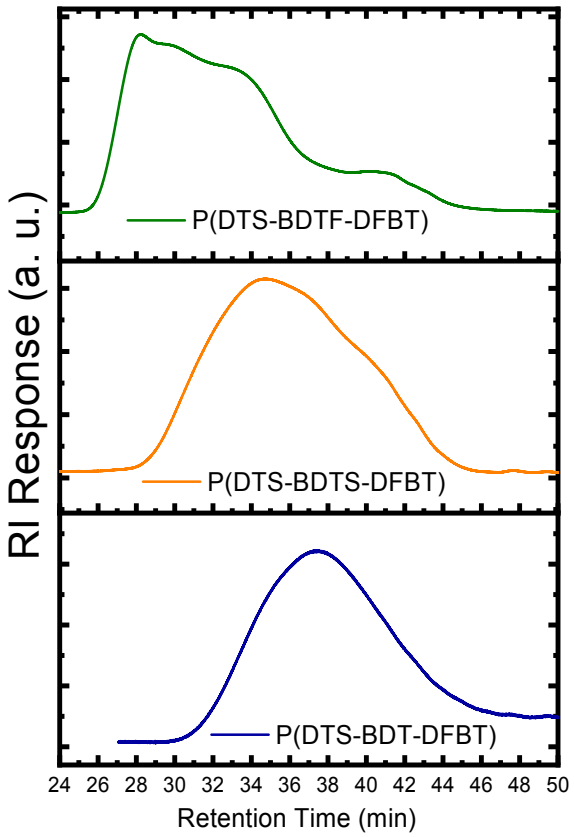

Figure S1. Gel permeation chromatography (GPC) profiles of the synthesized terpolymers

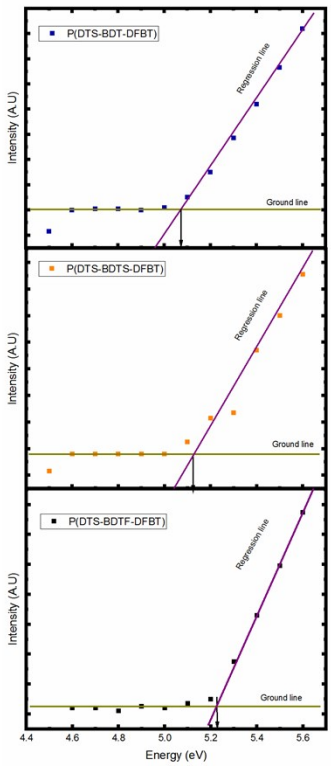

Figure S2. Photoelectron Emission Spectra in air of P(DTS-BDT-DFBT), P(DTS-BDTS-DFBT) and P(DTS-BDTF-DFBT).

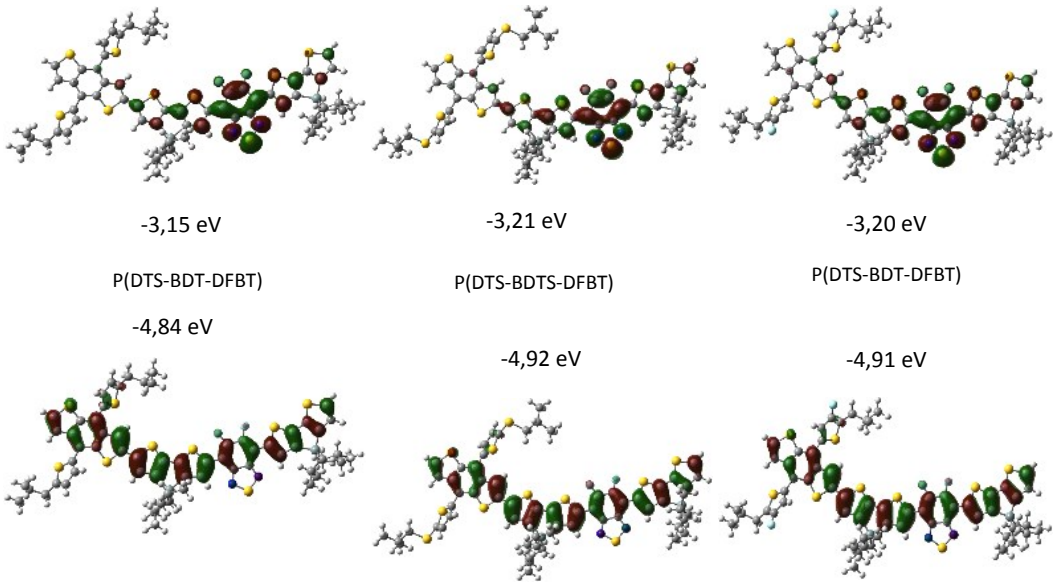

Figure S3. Molecular structure and calculated E_{HOMO} E_{LUMO} levels of P(DTS-BDT-DFBT) (left), P(DTS-BDTS-DFBT) (middle) and P(DTS-BDTF-DFBT) (right) simulated using density functional theory (DFT).

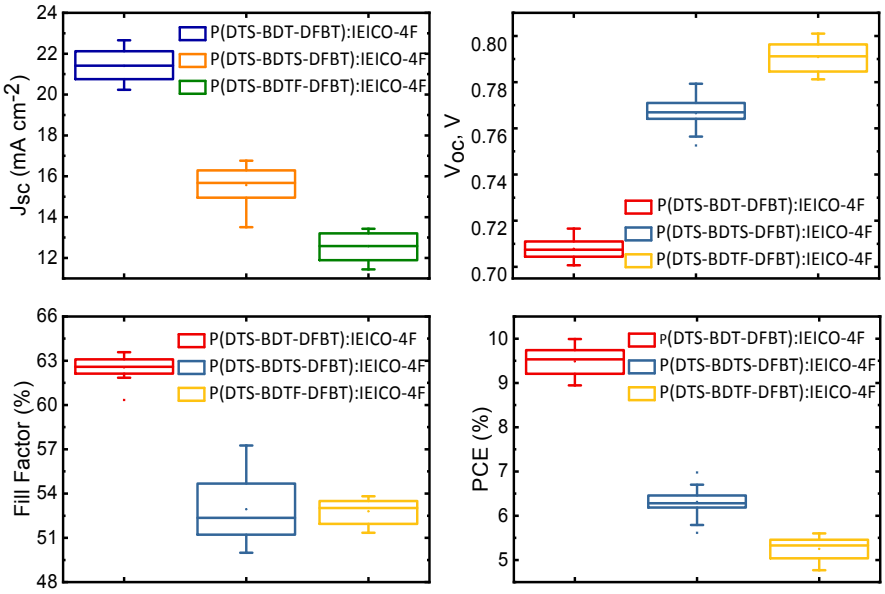

Figure S4. Photovoltaic parameters of the 18 OSCs

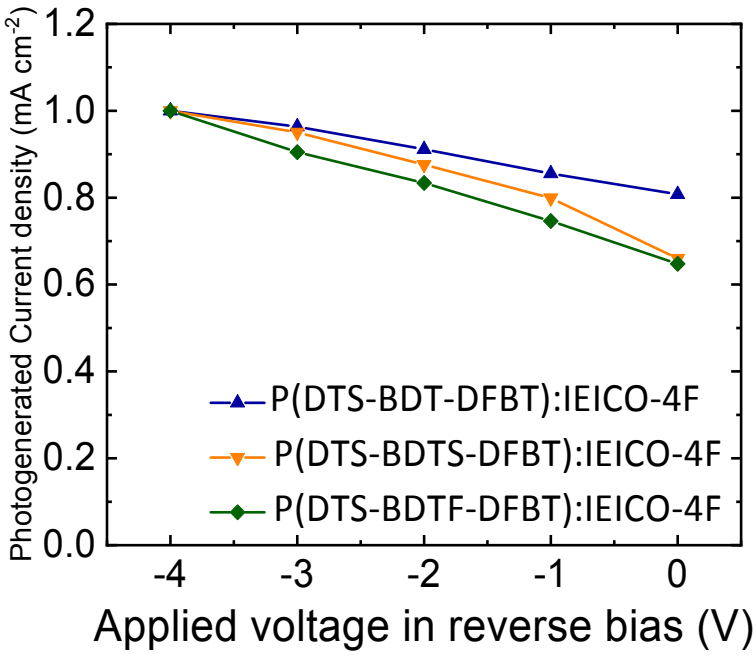

Figure S5. Photogenerated current density as function of applied voltage. Photogenerated current density was measured by integrating the current density from EQE spectra under different voltage bias.

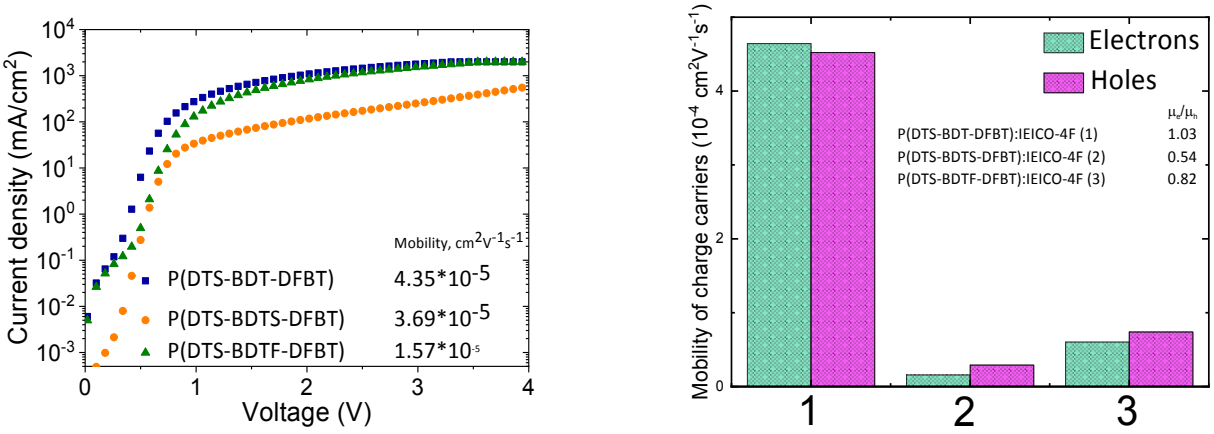

Figure S6. Experimental dark current densities as a function of effective voltage for a) hole-only diodes of the pristine film and b) ratio of hole to electron mobility in the P(DTS-BDT-DFBT):IEICO-4F, P(DTS-BDTS-DFBT):IEICO-4F and P(DTS-BDTF-DFBT):IEICO-4F devices. Hole mobility and electron mobility was determined by making hole and electron only devices.

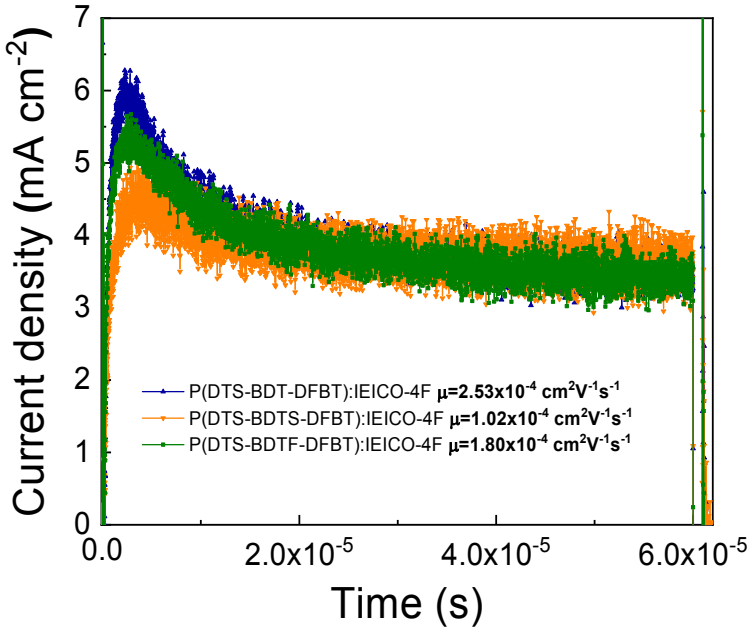

Figure S7. Photo-CELIV traces of P(DTS-BDT-DFBT), P(DTS-BDTS-DFBT) and P(DTS-BDTF-DFBT)-based solar cells at a fixed delay time.

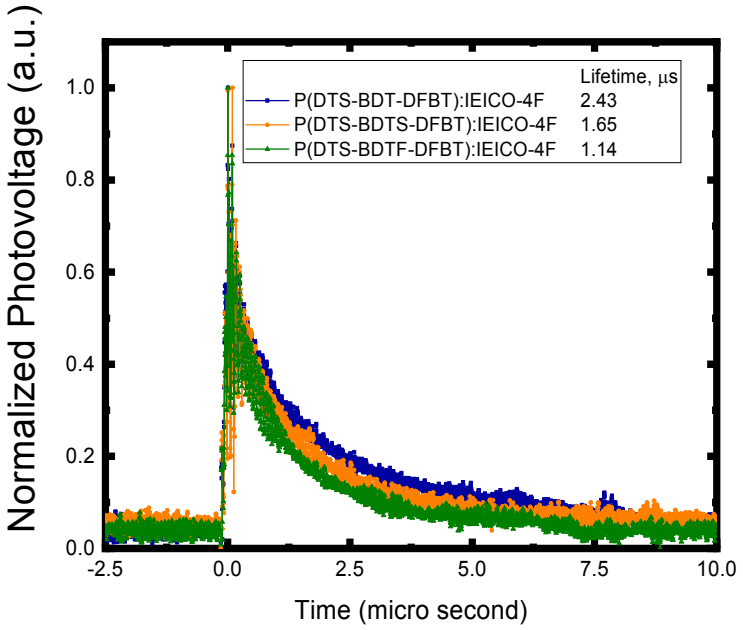

Figure S8. TPV traces of P(DTS-BDT-DFBT), P(DTS-BDTS-DFBT) and P(DTS-BDTF-DFBT)-based solar cells at open-circuit voltage conditions.

Table S1: Molecular weight characteristics of the synthesized polymers

Polymer	Average Molecular Weight per Number [$\bar{M}_n$] (g/mol)	Average Molecular Weight per Weight [$\bar{M}_w$] (g/mol)	Polydispersity Index [$Đ$]
P(DTS-BDT-DFBT)	15350	38300	2.5
P(DTS-BDTS-DFBT)	25050	78050	3.1
P(DTS-BDTF-DFBT)	183200	675500	3.7

Table S2. Optimization parameters of the active layer blends

Active Layer	D:A ratio	J_{sc}, mA/cm^2	V_{oc}, V	FF, %	PCE, %
P(DTS-BDT-DFBT):IEICO-4F	1:1	17.4	0.74	58.6	7.6
	1:1.5	17.4	0.74	58.5	7.5
	1:2	15.9	0.75	58.5	7.0
Annealing 100 ^{o}C, 10min.	1:1	16.7	0.72	58.9	7.1
P(DTS-BDTS-DFBT):IEICO-4F	1:1	10.6	0.85	56.6	5.2
	1:1.5	10.0	0.85	58.8	5.0
	1:2	9.3	0.85	58.9	4.7
Annealing 100 ^{o}C, 10min.	1:1	10.1	0.85	55.5	4.8
P(DTS-BDTF-DFBT):IEICO-4F	1:1	14.2	0.79	49.1	5.5
	1:1.5	13.3	0.78	50.5	5.2
	1:2	13.2	0.78	51.9	5.3
Annealing 100 ^{o}C, 10min.	1:1	12.7	0.77	44.3	4.3