Supporting Information

Perfluoroalkyl-Substituted Conjugated Polymers as Electron Acceptors for All-Polymer Solar Cells: the Effect of Diiodoperfluoroalkane Additives

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1. ^{1}H-NMR of the DPP polymers

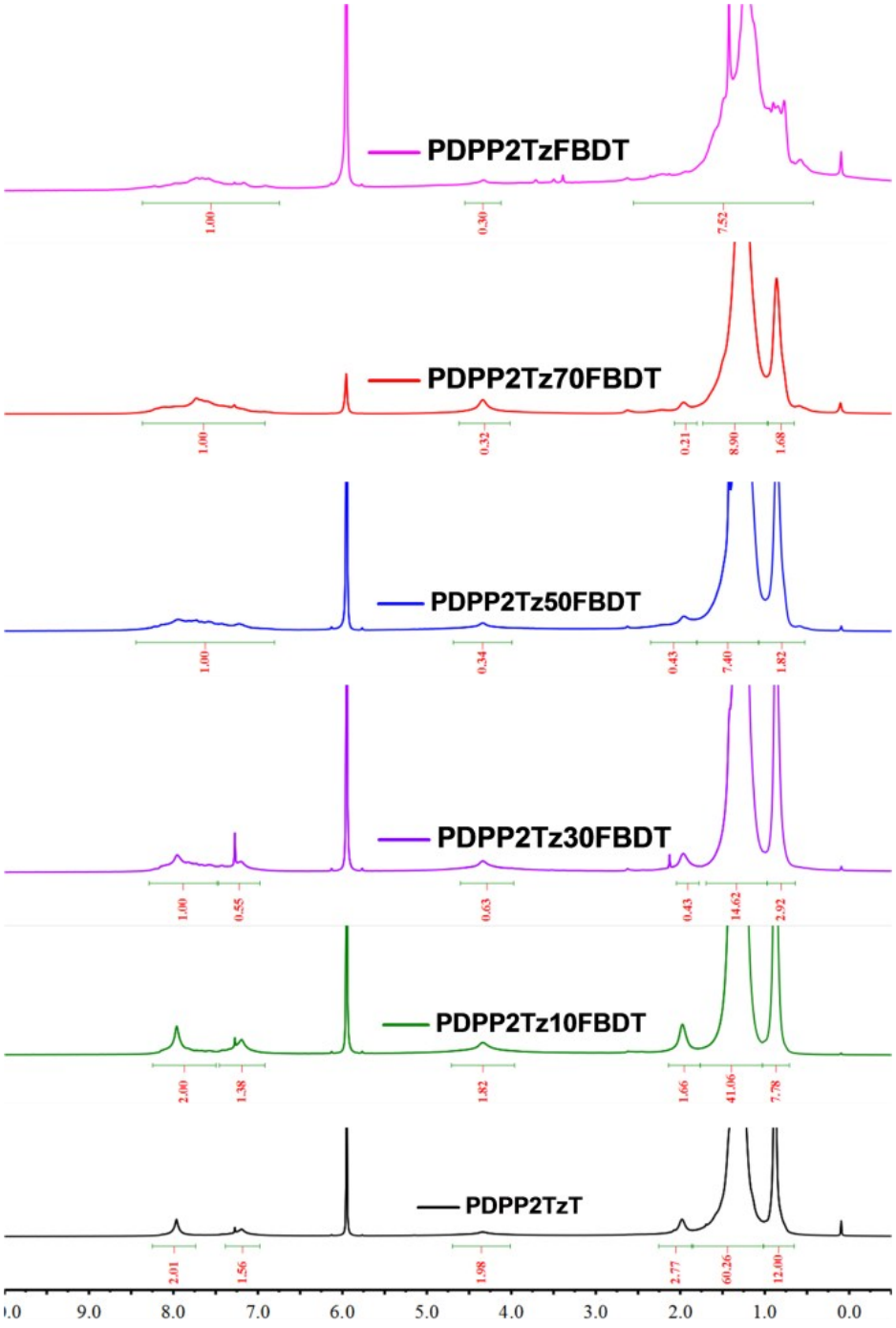

Fig. S1 ^{1}H-NMR spectra of the DPP polymers.

2. GPC

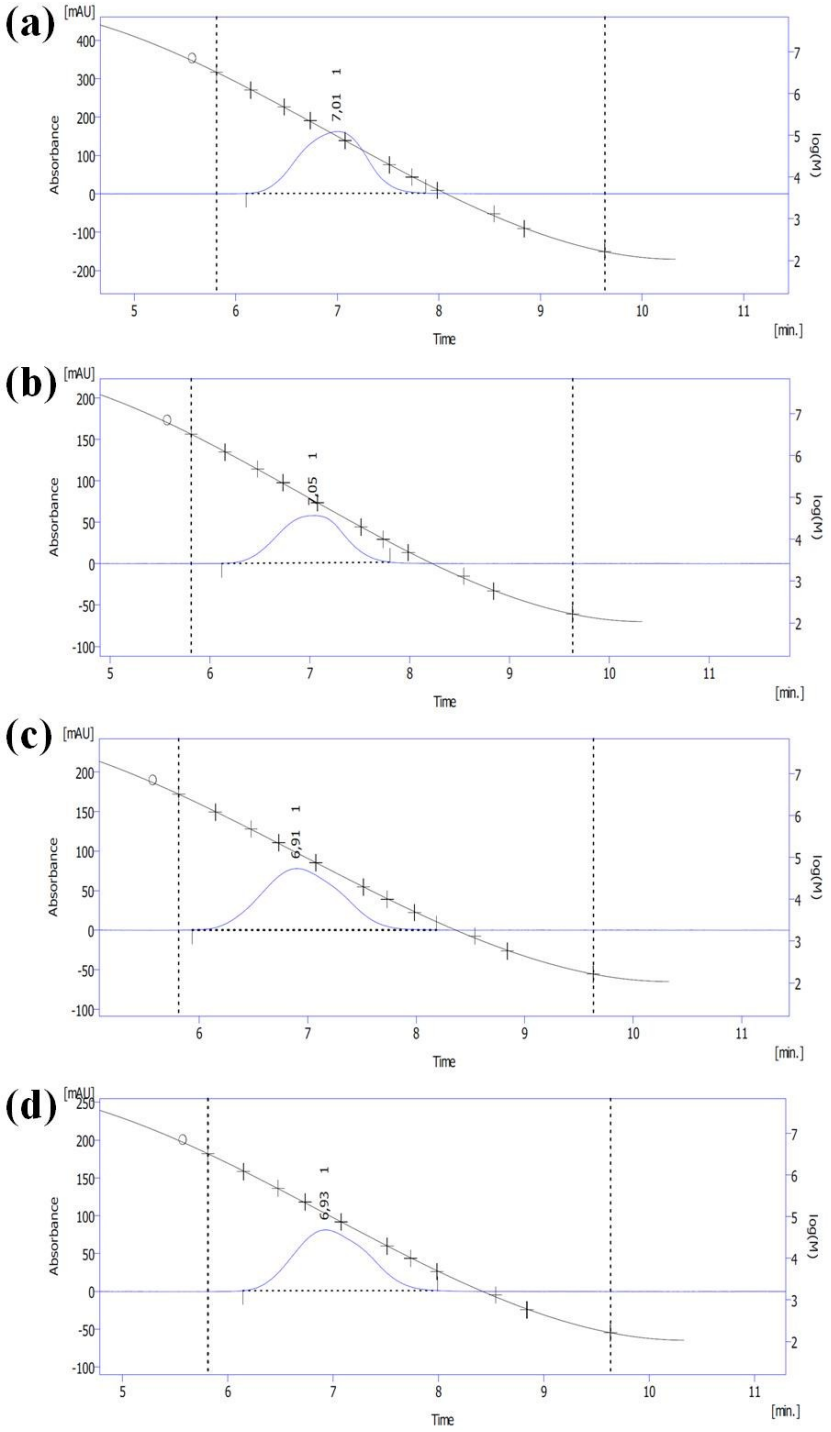

Fig. S2 GPC recorded at 140 °C with *o*-DCB as eluent for (a) PDPP2Tz10FBDT, (b) PDPP2Tz30FBDT, (c) PDPP2Tz50FBDT and (d) PDPP2Tz70FBDT.

3. Optical absorption spectra of pure polymers

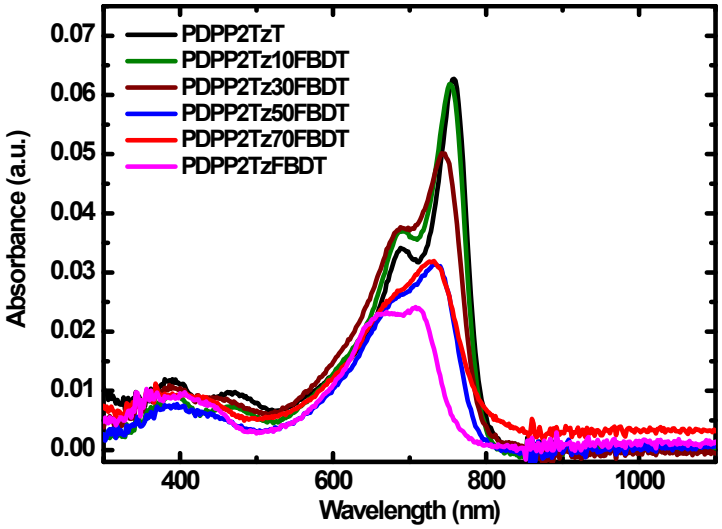

Fig. S3 Optical absorption spectra of the DPP polymers in $CHCl_3$ solution. The concentration is 0.001 g L^{-1}.

4. Cyclic voltammetry

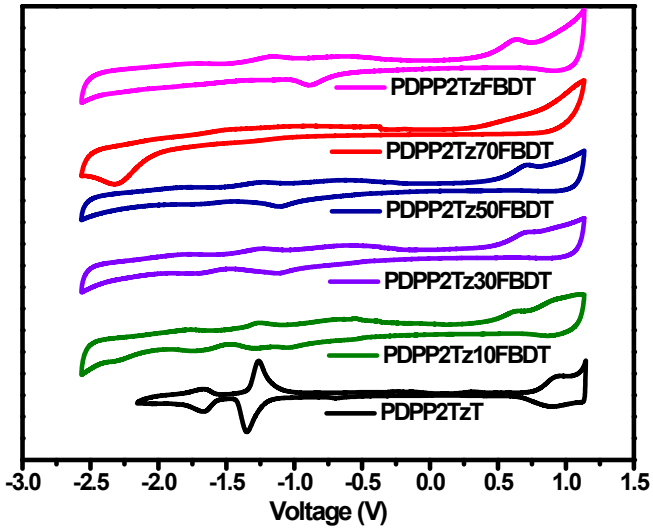

Fig. S4 Cyclic voltammograms of the DPP polymers in this work. Potential vs. Fc/Fc^{+}.

5. DFT calculations

Density function theory (DFT) calculations were performed at the B3LYP/6-31G* level of theory by using the Gaussian 09 program package.

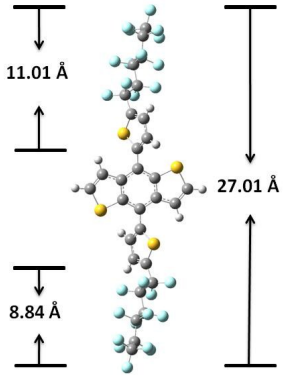

Fig. S5 Computed molecular structure of FBDT.

6. 2D-GIWAXS pattern of PDPP5T thin film

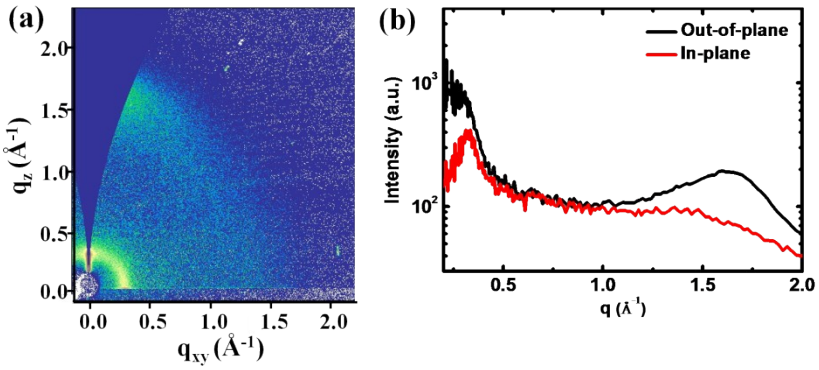

Fig. S6 Characteristics of PDPP5T thin film spin coated from $CHCl_3$. (a) 2D-GIWAXS pattern and (b) the out-of-plane and in-plane cuts of the corresponding 2D-GIWAXS patterns. The crystallographic parameter of PDPP5T is calculated: q_{xy} = 0.33 Å^{-1} and d = 19.0 Å for lamellar stacking peak (100); q_z = 1.64 Å^{-1} and d = 3.83 Å for π-π stacking peak (010).

7. All-polymer solar cells fabricated from $CHCl_3$ solution without additives

In this part we summarize the results on solar cell fabricated from pure $CHCl_3$ solution without additives, report the hole and electron mobility from SCLC measurements, and analyze the morphology by AFM.

Table S1 Characteristics of PDPP5T:DPP-polymer (1:1) solar cells fabricated from $CHCl_3$ solution.

Acceptor	Thickness [nm]	J_{sc} [mA cm^{-2}]	V_{oc} [V]	FF	PCE [%]
PDPP2TzT	100	0.51	0.75	0.36	0.13
PDPP2Tz10FBDT	100	0.46	0.79	0.31	0.11
PDPP2Tz30FBDT	80	0.60	0.81	0.34	0.17
PDPP2Tz50FBDT	85	1.16	0.77	0.39	0.39
PDPP2Tz70FBDT	80	0.72	0.79	0.42	0.24
PDPP2TzFBDT	90	0.66	0.75	0.40	0.20

Table S2 Hole and electron mobility in all-PSCs by SCLC measurement. The thin films were fabricated from $CHCl_3$ solution.

Polymer	μ_h (cm^2 V^{-1} s^{-1})	μ_e (cm^2 V^{-1} s^{-1})	μ_h/μ_e
PDPP2TzT	2.7×10^{-4}	8.7×10^{-6}	31
PDPP2Tz10FBDT	1.3×10^{-4}	3.0×10^{-6}	43
PDPP2Tz30FBDT	9.1×10^{-5}	7.0×10^{-6}	13
PDPP2Tz50FBDT	2.4×10^{-4}	8.7×10^{-6}	28
PDPP2Tz70FBDT	9.5×10^{-5}	3.2×10^{-6}	30
PDPP2TzFBDT	2.3×10^{-4}	2.0×10^{-7}	1150

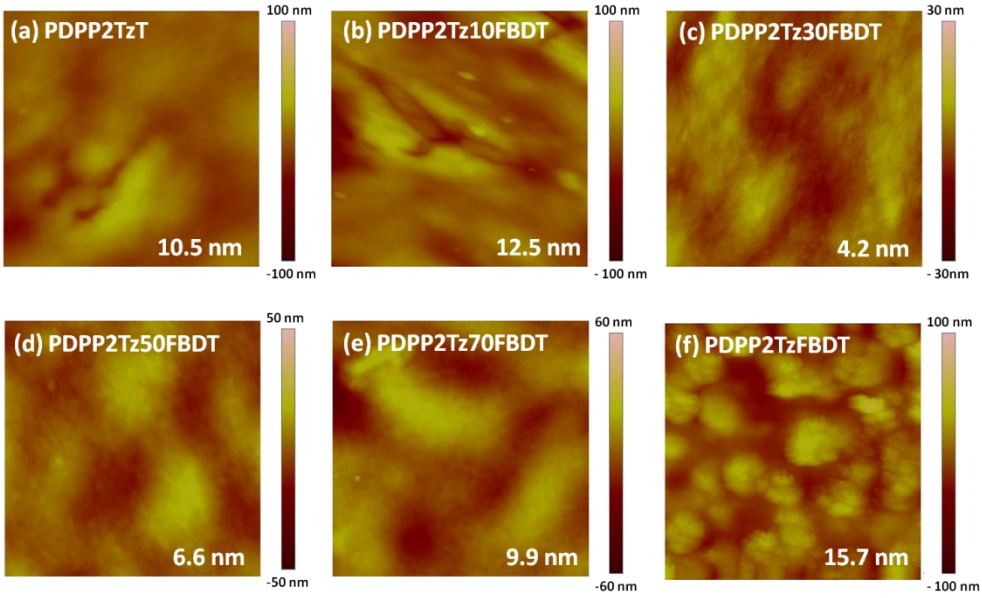

Fig. S7 AFM height images (3×3 μm^2) of PDPP5T:DPP-polymer (1:1) blends spin coated from $CHCl_3$ solution. The root mean square (RMS) roughness is also included in the panels.

8. All-polymer solar cells fabricated from $CHCl_3$ solution containing additives

Table S3 Characteristics of PDPP5T:PDPP2TzFBDT solar cells for different solvent with additives and different layer thickness.

Solvent	Thickness [nm]	J_{sc} [mA cm^{-2}]	V_{oc} [V]	FF	PCE [%]
$CHCl_3$:IC_4F_8I 5%	70	2.4	0.65	0.37	0.56
$CHCl_3$:IC_4F_8I 10%	70	6.4	0.68	0.37	1.6
$CHCl_3$:IC_4F_8I 20%	65	6.5	0.68	0.40	1.8
$CHCl_3$:$IC_6F_{12}I$ 5%	70	7.4	0.69	0.42	2.1
$CHCl_3$:$IC_6F_{12}I$ 10%	60	6.9	0.67	0.46	2.1
$CHCl_3$:$IC_6F_{12}I$ 10%	75	6.9	0.67	0.45	2.1
$CHCl_3$:$IC_6F_{12}I$ 10%	110	5.6	0.65	0.36	1.3
$CHCl_3$:$IC_6F_{12}I$ 20%	70	7.2	0.67	0.44	2.1
$CHCl_3$:1-CN:$IC_6F_{12}I$ 3%/10%	70	0.82	0.69	0.42	0.24

9. PTB7-Th:PDPP2TzFBDT and PDPP2T-DTP:PDPP2TzFBDT cells

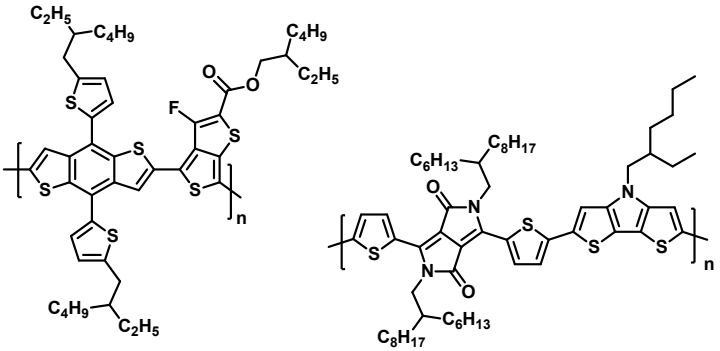

Fig. S8 Chemical structures of the donor polymers PTB7-Th and PDPP2T-DTP.

Table S4 Characteristics of donor (PTB7-Th or PDPP2T-DTP):PDPP2TzFBDT solar cells for different solvent with additives and different layer thickness. The thickness of active layers is around 65 nm.

Donor	Solvent	J_{sc} [mA cm^{-2}]	V_{oc} [V]	FF	PCE [%]
PTB7-Th	$CHCl_3$:1-CN 3%	5.7	0.83	0.45	2.1
	$CHCl_3$:$IC_6F_{12}I$ 10%	6.9	0.77	0.46	2.5

PDPP2T-DTP	$CHCl_3$:1-CN 3%	2.7	0.52	0.42	0.6
	$CHCl_3$:$IC_6F_{12}I$ 10%	4.8	0.50	0.43	1.0

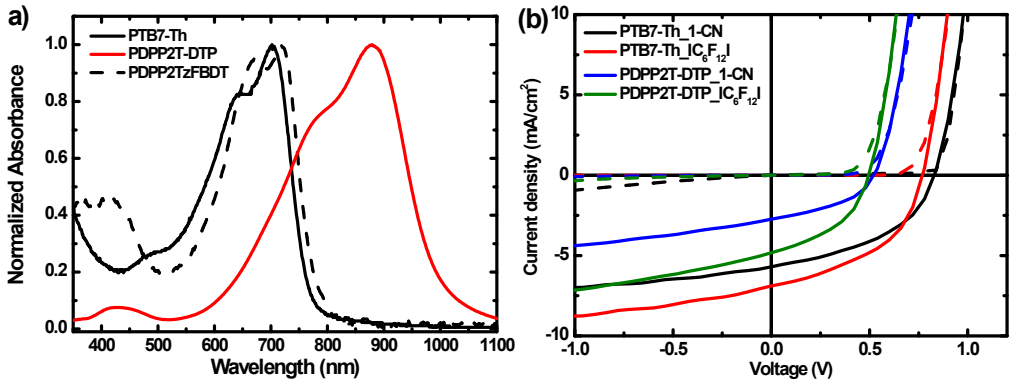

Fig. S9 (a) Optical absorption spectra of PTB7-Th, PDPP2T-DTP and PDPP2TzFBDT. (b) *J-V* characteristics in dark (dashed lines) and under white light illumination (solid lines) of the donor:PDPP2TzFBDT cells fabricated from $CHCl_3$ solution with 3% 1-CN or 10% $IC_6F_{12}I$.

10. Calibration of PL intensity by absorption spectra

The PL intensity in Fig. 6 was calibrated by absorption spectra of the same thin films. PDPP5T was set as the standard sample and the intensity of other PL spectra was calibrated by using the following equation:

I_{PL} (sample) = I_{PL} (measured) × $I_{abs}^{760\ nm}$ (PDPP5T) / $I_{abs}^{760\ nm}$ (sample)

in which $I_{abs} = 1 - 10^{-OD}$, where OD is the absorbance intensity.

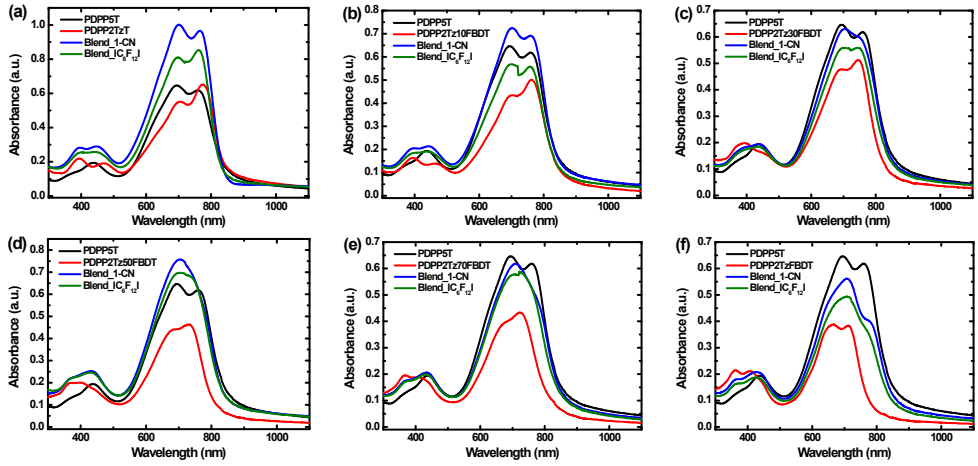

Fig. S10 Absorption spectra of the pure DPP polymers and PDPP5T:DPP-polymer (1:1) thin films. These thin films were further used to perform PL measurement as shown in Fig. 6.