

The Role of Conjugated Side Chains in High Performance Photovoltaic Polymers

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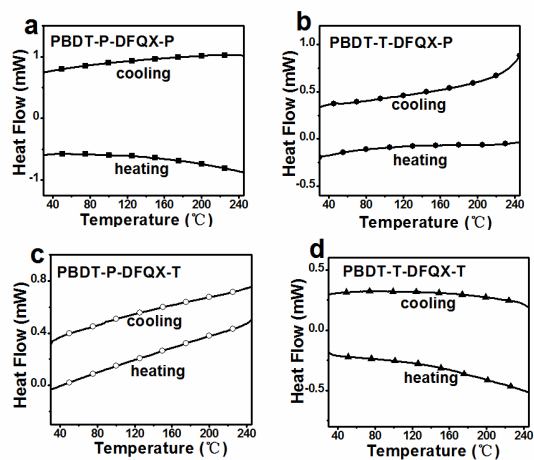


Figure S1. The differential scanning calorimetry (DSC) the thermograms of polymers under the protection of nitrogen (heating and cooling rate: 10 °C/ min)

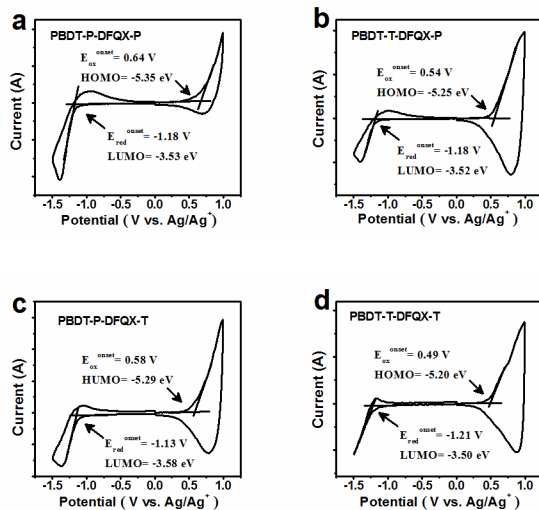


Figure S2. Thin film cyclic voltammograms of polymers in 0.1 M Bu₄NPF₆ acetonitrile solution at a scan rate of 100 mV · s⁻¹.

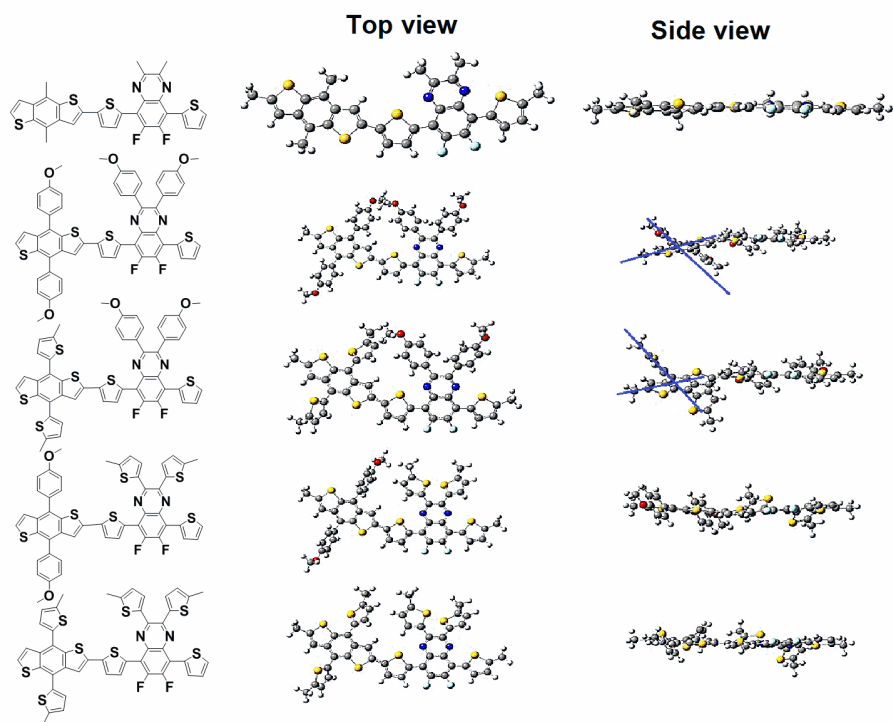


Figure S3. Top view and side view of optimized geometries of the four copolymers backbone units with a chain length $n=1$.

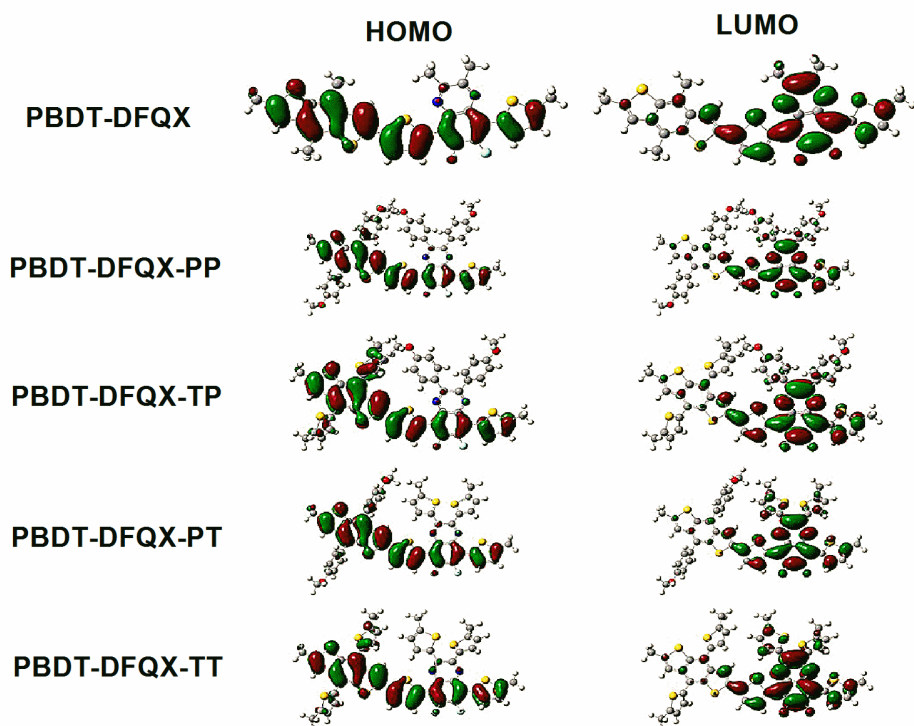


Figure S4. The frontier molecular orbital (LUMO, top; HOMO, bottom) obtained from DFT calculations on the polymers with a chain length $n=1$.

Table S1. The detailed photovoltaic data of the optimization process of the PSCs

Polymer	Ratio ^a	Treatment	V_{oc} (V)	J_{sc} (mA/cm ²)	FF (%)	PCE (%)	Thickness (nm)
PBDD-DFQX-PP	1:1	None	0.89	6.04	54.87	2.95	97
	1:2	None	0.80	8.11	45.60	2.96	83
	1:3	None	0.81	8.67	38.04	2.67	75
	1:2	3%DIO	0.86	7.63	43.47	2.85	79
	1:2	3% CN	0.87	7.89	34.80	2.39	77
	1:2	CH ₃ OH	0.89	8.66	51.38	3.96	87
PBDD-DFQX-TP	1:1	None	0.82	12.34	60.12	6.08	95
	1:2	None	0.84	10.68	55.94	5.02	67
	1:3	None	0.82	7.60	39.99	2.49	49
	1:1	3%DIO	0.78	10.42	54.36	4.42	88
	1:1	3% CN	0.80	9.46	49.87	3.77	84
	1:1	CH ₃ OH	0.87	11.31	60.44	5.95	91
PBDD-DFQX-PT	1:1	None	0.85	12.13	63.46	6.54	76
	1:2	None	0.85	10.87	60.91	5.63	58
	1:3	None	0.79	5.97	59.25	2.73	64
	1:1	3%DIO	0.78	12.06	59.30	5.58	82
	1:1	3% CN	0.84	9.95	63.13	5.28	78
	1:1	CH ₃ OH	0.84	11.51	63.28	6.11	87
PBDD-DFQX-TT	1:1	None	0.79	13.11	69.15	7.16	85
	1:1.2	None	0.85	12.53	68.51	7.29	98
	1:1.5	None	0.83	12.67	67.63	7.11	92
	1:2	None	0.83	11.92	69.92	6.92	72
	1:3	None	0.81	10.05	69.07	5.62	61
	1:1.2	3%DIO	0.78	12.33	69.44	6.68	80
	1:1.2	3% CN	0.84	12.31	65.96	6.82	86
	1:1	CH ₃ OH	0.86	13.95	62.18	7.46	81
	1:1.2	CH ₃ OH	0.86	12.77	69.93	7.68	95
	1:1.5	CH ₃ OH	0.83	12.60	70.79	7.41	101

[a] Polymer/PC₇₁BM weight ratio.

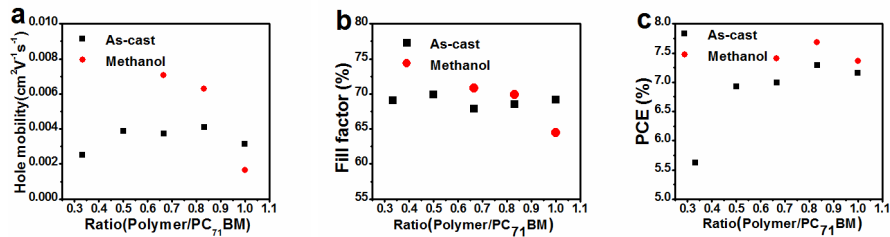


Figure S5. Photovoltaic properties of PBDD-DFQX-TT-based PSCs under different processing conditions

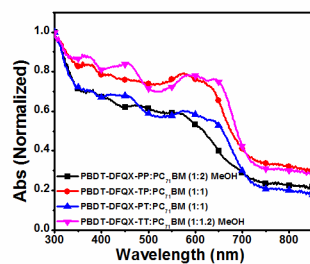


Figure S6. UV/Vis absorption spectra of blend films under the optimal conditions.

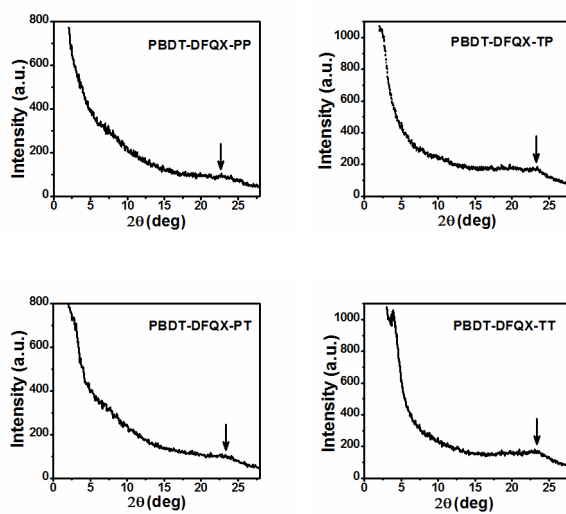


Figure S7. XRD patterns of the pristine polymer films.