

**Constructing a Donor-Acceptor Linear-Conjugation Structure
for Heterologous Perylene Diimides to Greatly Improve the
Photovoltaic Performance**

Helin Wang, Lingcheng Chen* and Yi Xiao*

State Key Laboratory of Fine Chemicals, Dalian University of Technology, Dalian 116024,
China

*Email - lcchen@dlut.edu.cn; xiaoyi@dlut.edu.cn

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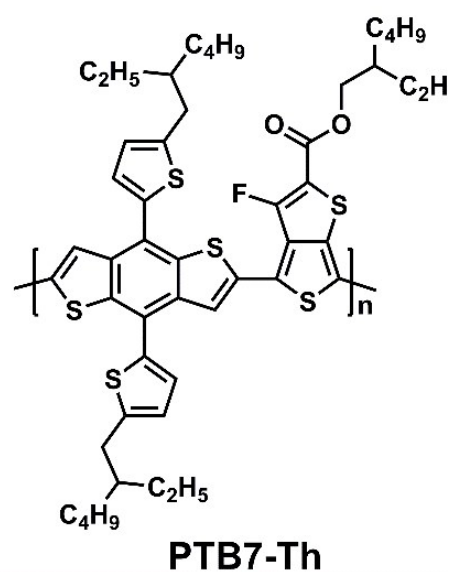
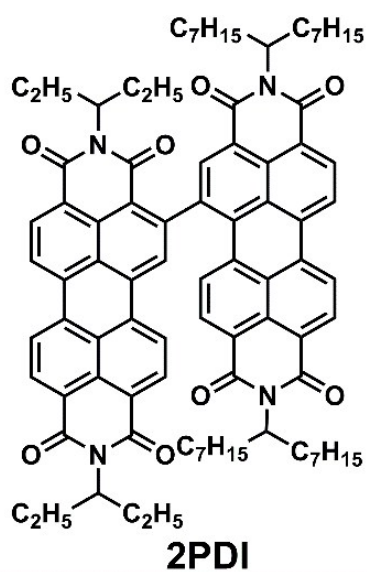


Fig. S1 The structures of the heterologous PDI dimer **2PDI** and the electron donor PTB7-Th

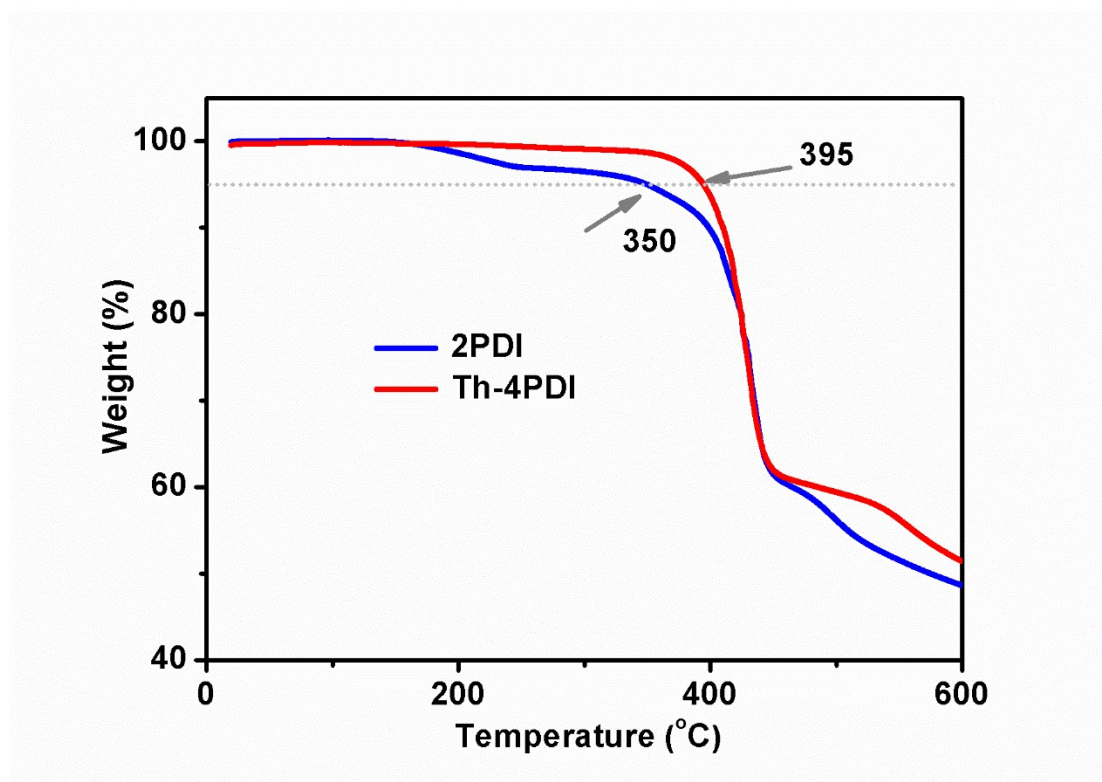


Fig. S2 TGA curves of **2PDI** and **Th-4PDI**.

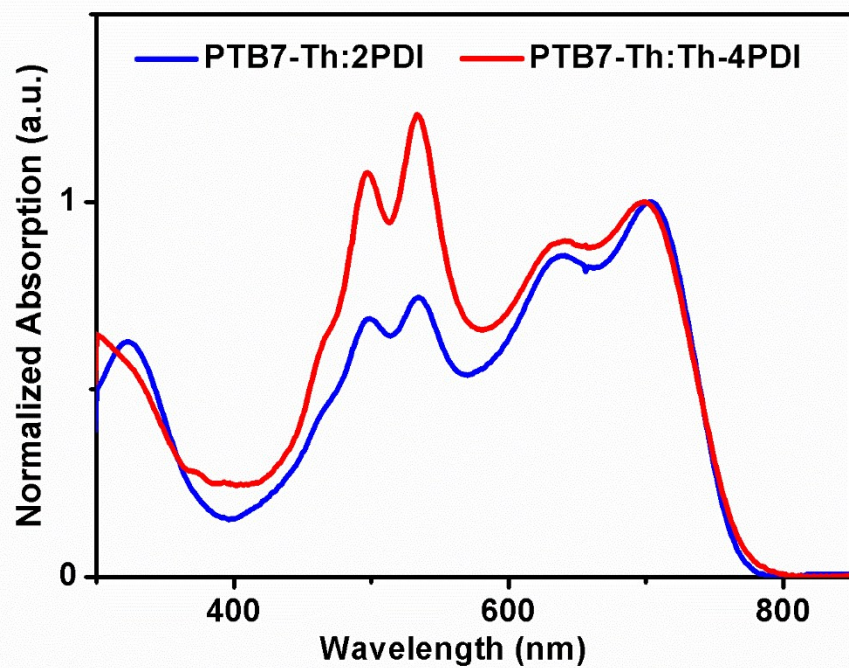


Fig. S3 The absorption spectra of blend films based on PTB7-Th-**2PDI** and PTB7-Th-**Th-4PDI**.

Table S1. Summary of device parameters of PTB7-Th:**Th-4PDI** solar cells with different additives

Ratio	Additives [volume]	J _{sc} [mA/cm ²]	V _{oc} [V]	FF [%]	PCE [%]
wt/wt					
1.5:1	NULL	13.49 (13.38±0.12)	0.745 (0.743±0.002)	48.5 (48.1±0.4)	4.87 (4.74±0.13)
1:1		13.49 (13.37±0.13)	0.765 (0.759±0.006)	52.5 (52.3±0.2)	5.42 (5.30±0.12)
1:1.5		13.85 (13.71±0.15)	0.741 (0.738±0.003)	47.2 (47.1±0.2)	4.84 (4.69±0.15)
1:1	1% CN	16.78 (16.67±0.11)	0.755 (0.751±0.005)	50.0 (49.6±0.4)	6.33 (6.17±0.16)
	2% CN	13.46 (13.32±0.14)	0.776 (0.771±0.006)	58.5 (57.9±0.6)	6.11 (5.94±0.17)
	3% CN	12.63 (12.49±0.14)	0.773 (0.771±0.004)	58.3 (57.7±0.6)	5.69 (5.69±0.15)
	1% DPE	15.47 (15.35±0.12)	0.765 (0.763±0.002)	50.2 (49.9±0.3)	5.94 (5.80±0.14)
	2% DPE	15.18 (15.06±0.12)	0.776 (0.772±0.004)	55.4 (55.1±0.4)	6.53 (6.41±0.12)
	4% DPE	15.41 (15.28±0.13)	0.751 (0.745±0.006)	47.5 (47.1±0.6)	5.50 (5.34±0.16)
	0.5% DIO	18.02 (17.91±0.12)	0.764 (0.758±0.006)	49.3 (48.8±0.5)	6.79 (6.66±0.13)
	1% DIO	16.65 (16.53±0.12)	0.772 (0.768±0.004)	55.8 (55.6±0.3)	7.17 (7.06±0.11)
	1.5% DIO	17.28 (17.13±0.15)	0.759 (0.754±0.005)	49.8 (49.4±0.4)	6.53 (6.38±0.15)
	2% DIO	17.31 (17.17±0.14)	0.765 (0.763±0.002)	49.5 (49.2±0.3)	6.56 (6.43±0.13)

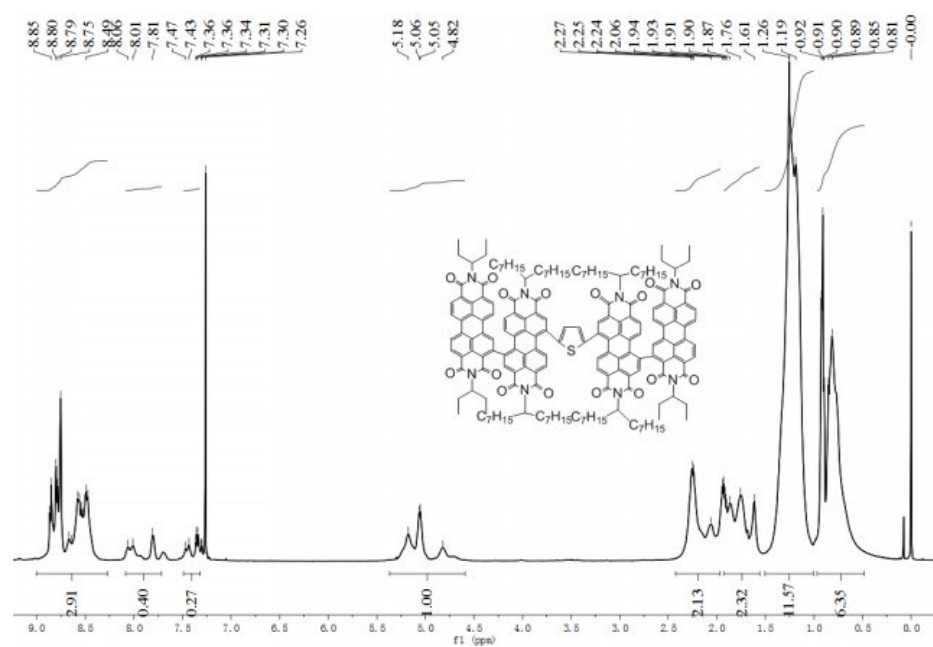


Fig. S4 ¹H NMR spectrum of compound Th-4PDI.

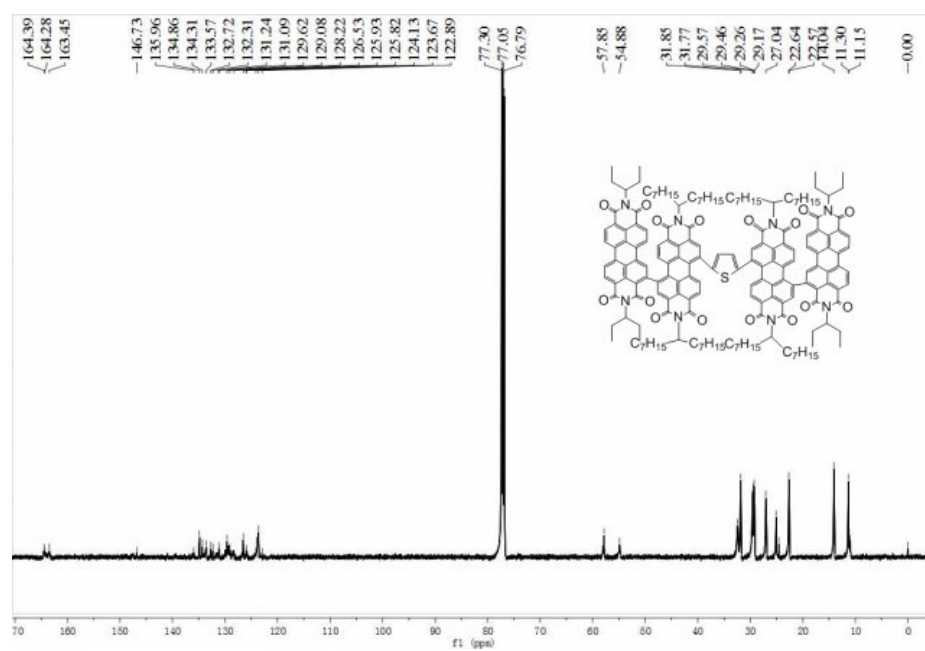


Fig. S5 ^{13}C NMR spectrum of compound Th-4PDI.

WHL-6(CHCA)

16070714 74 (2.465)

TOF LD-
5.84e3

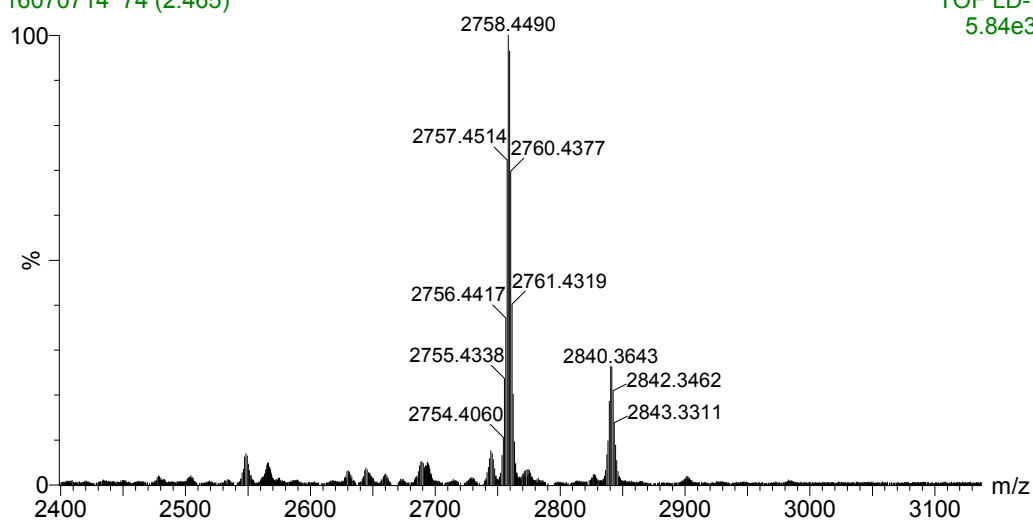


Fig. S6 MALDI-TOF/TOF-HRMS mass spectrometry of compound **Th-4PDI**.