

Supporting information

Efficient wide band gap photovoltaic polymers based on thiophene-thiazolothiazole units for high-performance polymer solar cells

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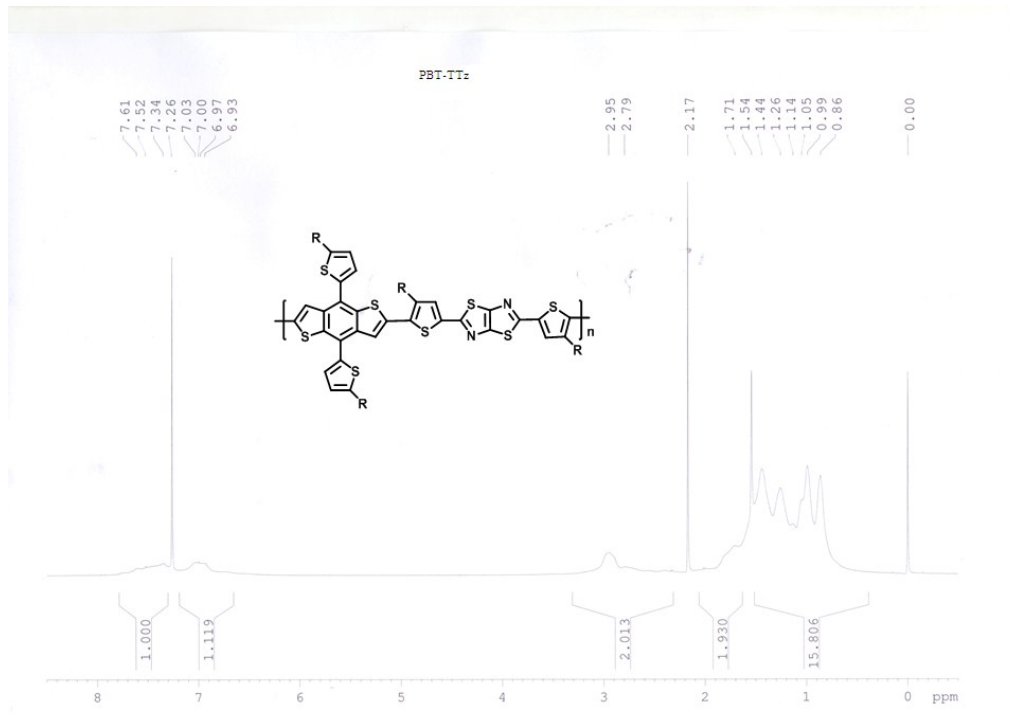


Fig. S1. ¹H NMR(400M, CDCl₃) spectra of PBT-TTz.

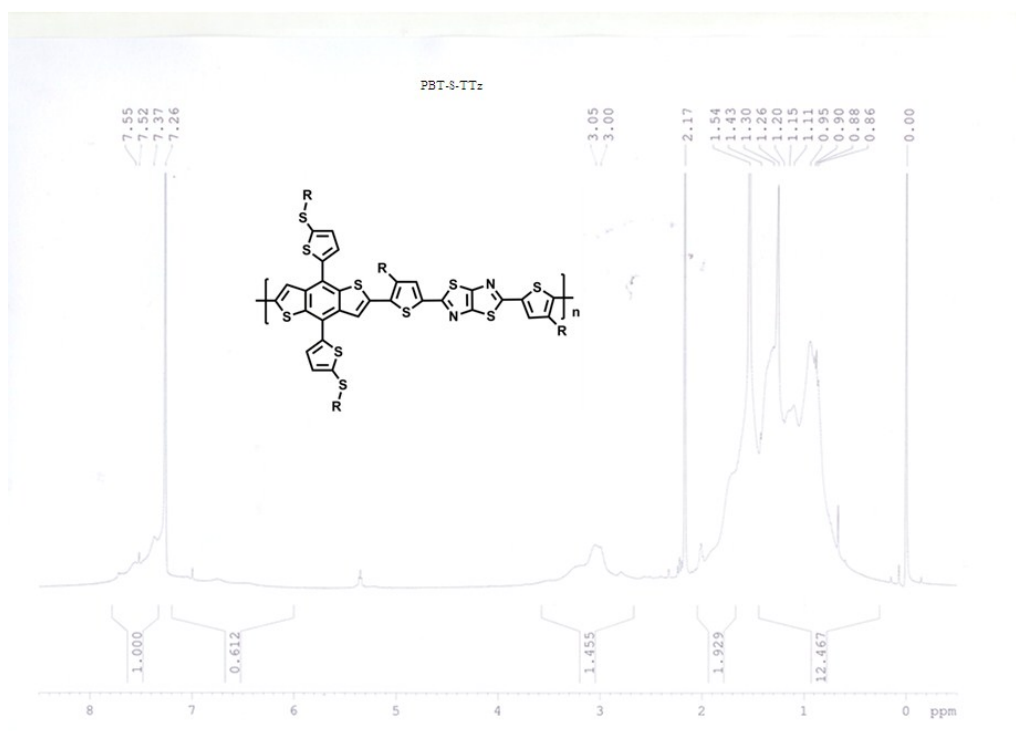


Fig. S2. ^1H NMR(400M, CDCl_3) spectra of PBT-S-TTz.

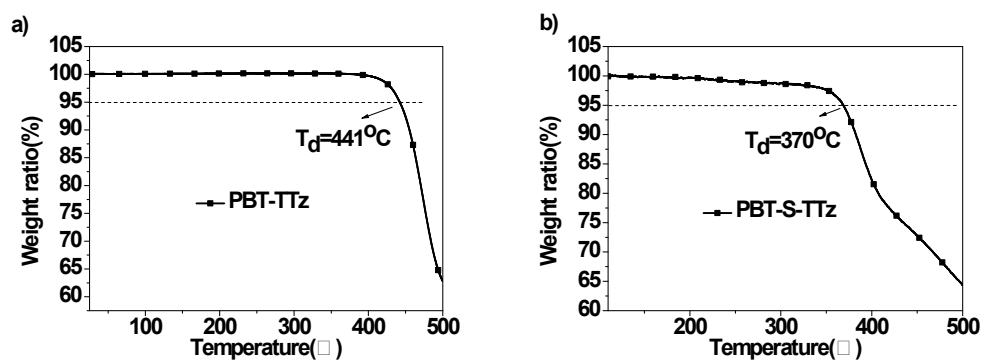
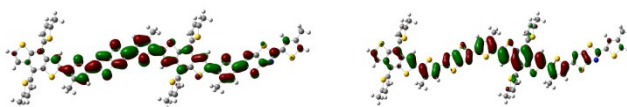


Fig. S3. Thermal Gravity Analysis (TGA) plots of the two polymers.

Thermal Gravity Analysis (TGA) was used to evaluate the thermal stability of the two polymers under Nitrogen atmosphere. As shown in the Fig. S3, after introducing sulphur atom into the side chain of the polymer, the thermal stability will decrease to 370°C due to the cleavage of Carbon-Sulphur single bond.

Polymer	LUMO	HOMO	$E_{\text{LUMO/HOMO}}$ (eV) ^a
PBT-S-TTz			-2.67/-5.00

PBT-TTz



-2.51/-4.88

Fig. S4. Density Functional Theory of the two polymers.

Density Functional Theory (DFT) at the B3LYP/6-31G(d, p) level was employed to study the difference of the two polymers. As shown in Fig. S4, the two polymers showed almost the same electric cloud distribution which matched well with the actual situation. The values of $E_{LUMO/HOMO}$ were stimulated by DFT, which quite fitted with the results calculated by cyclic voltammetry (CV).

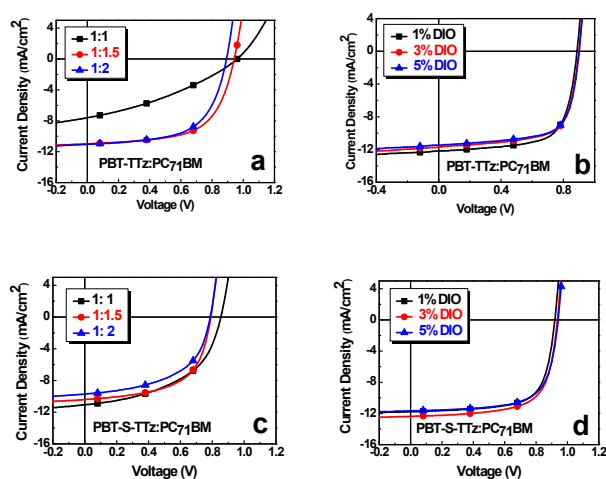


Fig.S5. J - V curves of PSC devices based on (a and b) PBT-TTz:PC₇₁BM and (c and d) PBT-S-TTz:PC₇₁BM active layer with different D/A ratio and different DIO concentrations.

Table S1. Photovoltaic data of the PSC devices based on PBT-TTz:PC₇₁BM and PBT-S-TTz:PC₇₁BM active layer under the illumination of AM 1.5G 100 mW/cm². The PCE values were averaged from five independent devices.

Polymer Donor	D/A ratio	DIO additive	V_{oc} (V)	J_{sc} (mA/cm ²)	FF (%)	PCE/PCE _{max} (%)
PBT-TTz	1:1	w/o	0.961	7.21	34.0	2.22±0.10 / 2.36
	1:1.5	w/o	0.942	10.98	61.6	6.39±0.13 / 6.37
	1:2	w/o	0.892	11.05	60.4	5.74±0.17 / 5.95
	1:1	1%	0.887	11.49	68.5	6.87±0.23 / 6.98
	1:1.5	3%	0.899	11.69	68.6	7.16±0.09 / 7.21
	1:2	5%	0.902	11.46	69.1	7.14±0.13 / 7.14

PBT-S-TTz	1:1	w/o	0.854	10.48	49.7	4.18±0.27 / 4.45
	1:1.5	w/o	0.791	10.41	58.7	4.57±0.27 / 4.83
	1:2	w/o	0.787	9.21	53.3	3.57±0.25 / 3.86
	1:1	1%	0.92	11.78	69.7	7.39±0.16 / 7.55
	1:1.5	3%	0.936	12.39	68.3	7.45±0.17 / 7.92
	1:2	5%	0.941	11.67	68.9	7.35±0.11 / 7.57

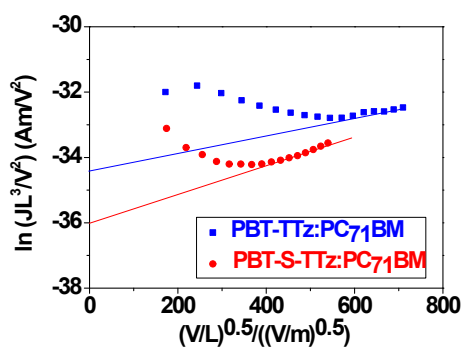


Fig. S6. $\ln(JL^3/V^2)$ versus $(V/L)^{0.5}$ plots of the polymers for the SCLC measurements.

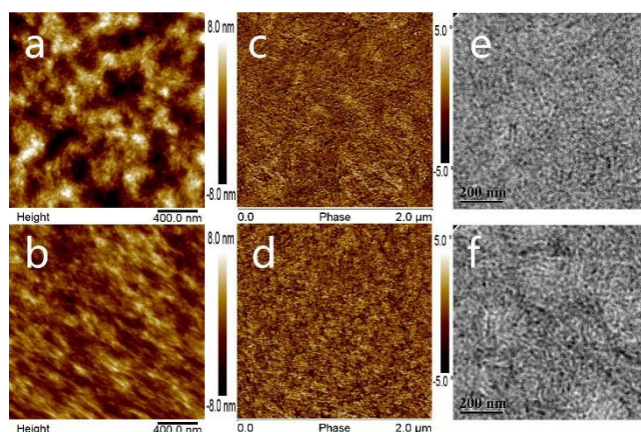


Fig. S7. AFM topography images (a and b), AFM phase images (c and d) and TEM images (e and f) of the polymer:ITIC active layers: (a, c and e) for the PBT-TTz:ITIC active layer; (b, d and f) for the PBT-S-TTz:ITIC active layer.

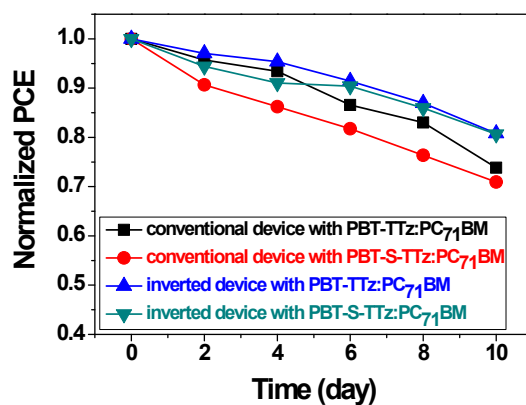


Fig. S8. Normalized PCEs as a function of time for fullerene-based devices stored for 10 days.

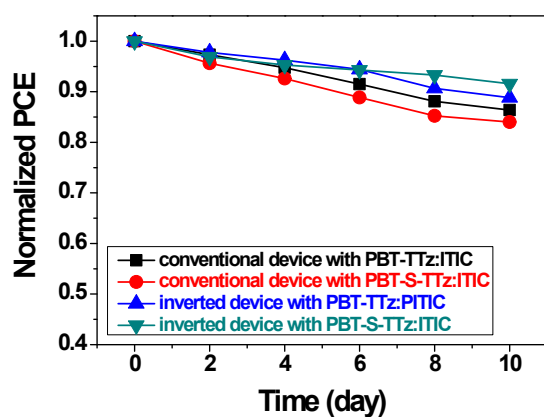


Fig. S9. Normalized PCEs as a function of time for fullerene-free devices stored for 10 days.

References

- [1] S. Zhang, M. A. Uddin, W. Zhao, L. Ye, H. Y. Woo, D. Liu, B. Yang, H. Yao, Y. Cui, J. Hou, *Polymer Chemistry* **2015**, 6, 2752.
- [2] S. Zhang, L. Ye, Q. Wang, Z. Li, X. Guo, L. Huo, H. Fan, J. Hou, *The Journal of Physical Chemistry C* **2013**, 117, 9550.