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

Supplementary Information

Enhancement of the thermoelectric performance for DTC-based polymer via *N*-octyl substitution

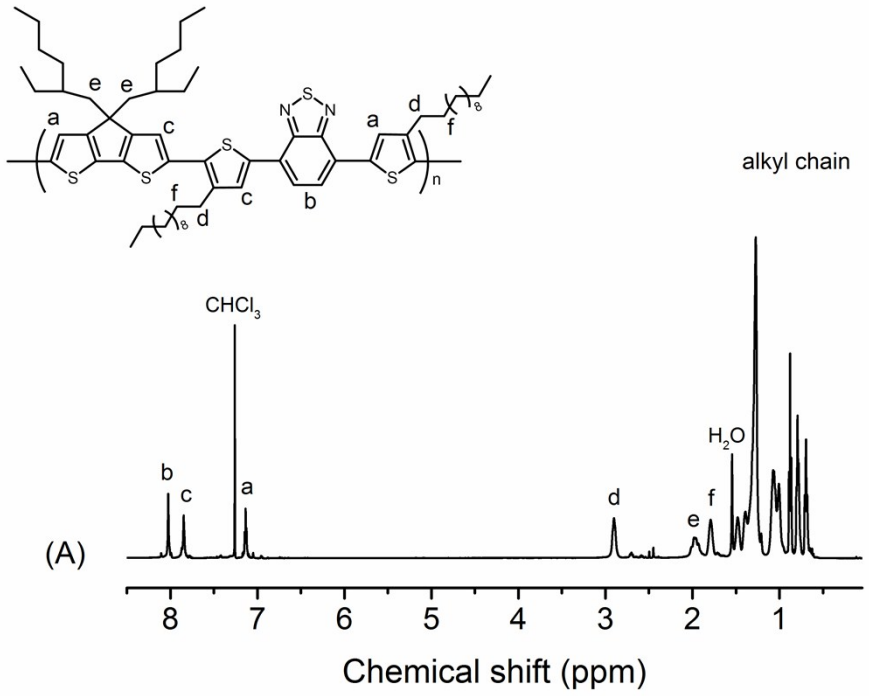
Houbo Zhou[a,b,c], Chunmei Gao[c], Tongchao Liu[a], Chengjun Pan[a] and Lei Wang[a,b,*]

[a]Shenzhen Key Laboratory of Polymer Science and Technology, College of Materials Science and Engineering, Shenzhen University, Shenzhen 518060, China.

[b]Key Laboratory of Optoelectronic Devices and Systems of Ministry of Education and Guangdong Province, College of Optoelectronic Engineering, Shenzhen University, Shenzhen 518060, China.

[c]College of Chemistry and Environmental Engineering, Shenzhen University, Shenzhen 518060, China.

* Corresponding author: L. Wang (Email: wl@szu.edu.cn).



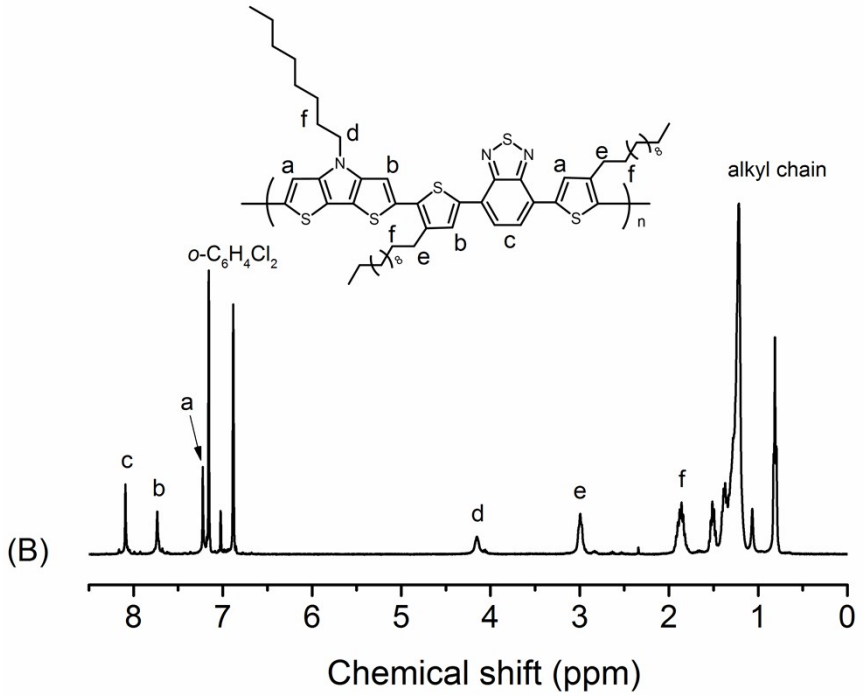


Figure S1. ^{1}H NMR spectra of P(DTCTBT) in $CDCl_3$ at room temperature (A) and P(DTPTBT) in *o*-$C_6D_4Cl_2$ at 110 °C (B).

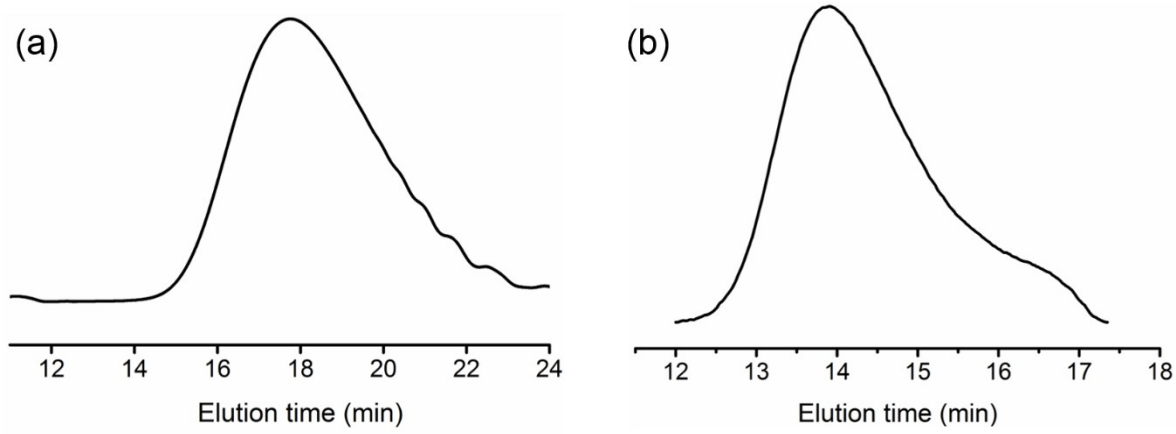


Figure S2. GPC curves of P(DTCTBT) with THF as eluent at 40 °C (a) and P(DTPTBT) with 1,2,4-trichlorobenzene as eluent at 150 °C (b).

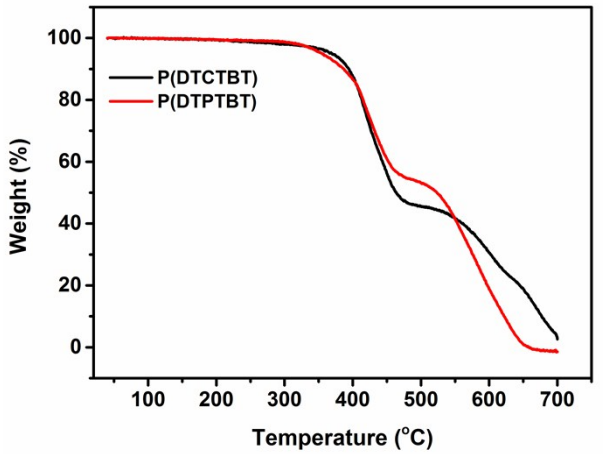


Figure S3. TGA analysis of P(DTCTBT) and P(DTPTBT)

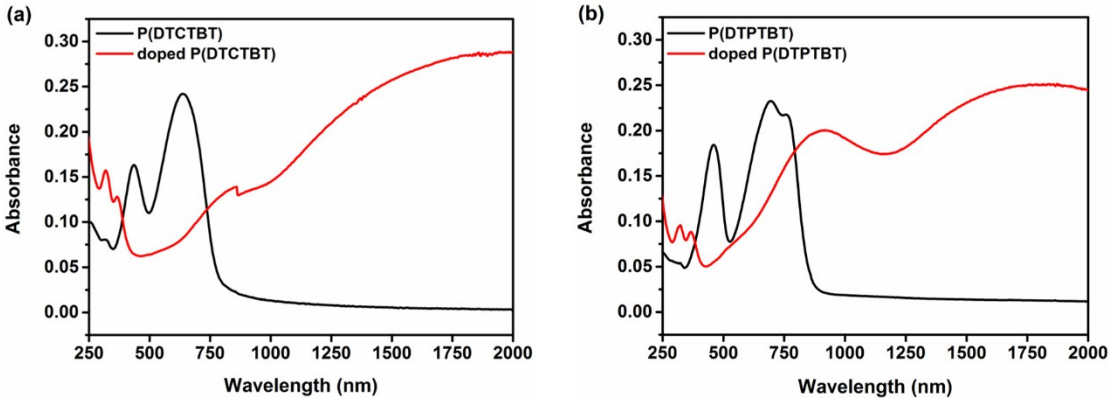


Figure S4. UV-vis-NIR spectra of P(DTCTBT) before and after doping by $FeCl_3$ (a) and P(DTPTBT) before and after doping by $FeCl_3$ (b).

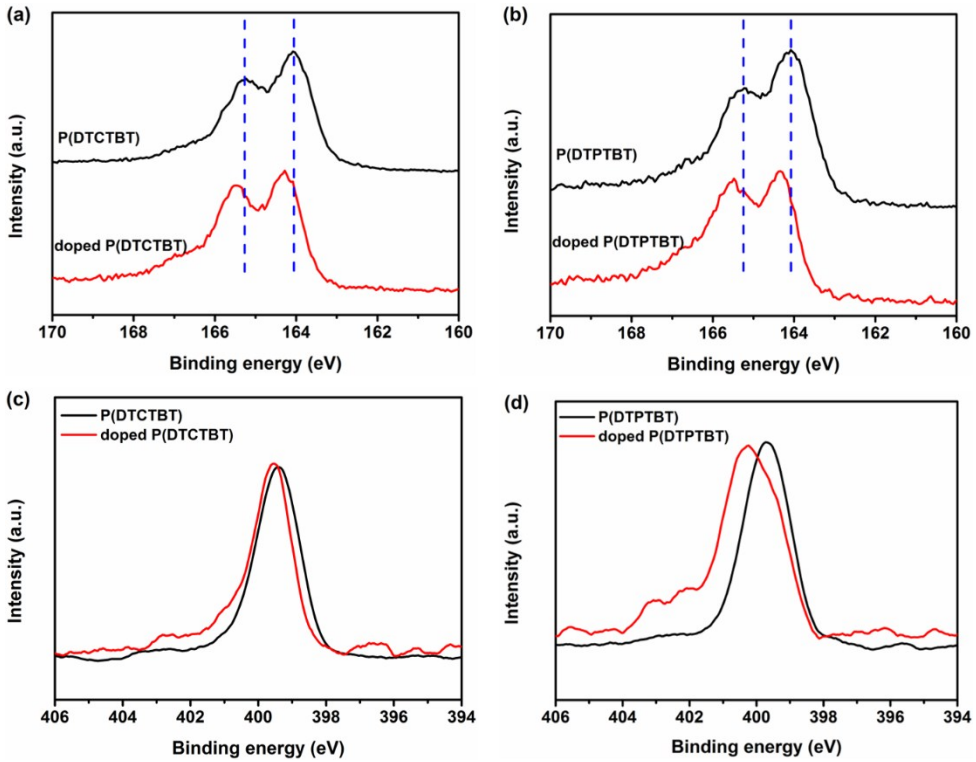


Figure S5. XPS spectra of S2p for P(DTCTBT) (a), P(DTPTBT) (b) and N1s for P(DTCTBT) (c), P(DTPTBT) (d) before and after doping.

Table S1. The high resolution XPS results of S2p (binding energy and area) for polymers in different conditions[1].

	P(DTCTBT)		**doped P(DTCTBT)**		**P(DTPTBT)**		**doped P(DTPTBT)**	
	T units	BT units	T units	BT units	T units	BT units	T units	BT units
$S2p_{3/2}$ (eV)	**164.05**	**165.65**	**164.27**	**165.87**	**164.05**	**165.65**	**164.35**	**165.95**
$S2p_{1/2}$ (eV)	**165.20**	**166.70**	**165.45**	**166.92**	**165.20**	**166.75**	**165.52**	**167.08**
Area of $S2p_{3/2}$	**9200**	**2200**	**6250**	**2050**	**7400**	**1850**	**4000**	**1500**
Area of $S2p_{1/2}$	**4550**	**1050**	**3500**	**950**	**3650**	**870**	**2400**	**750**

Intensity ratio[2]:

P(DTCTBT): $\frac{S2p(BT)}{S2p(T)} = \frac{2200 + 1050}{9200 + 4550} = 0.236$

doped P(DTCTBT): $\frac{S2p(BT)}{S2p(T)} = \frac{2050 + 950}{6250 + 3500} = 0.308$

P(DTPTBT): $\frac{S2p(BT)}{S2p(T)} = \frac{1850 + 870}{7400 + 3650} = 0.246$

doped P(DTPTBT): $\frac{S2p(BT)}{S2p(T)} = \frac{1500 + 750}{4000 + 2400} = 0.352$

References:

[1] Y. Vaynzof, T. J. K. Brenner, D. Kabra, H. Sirringhaus and R. H. Friend, *Adv. Funct. Mater.*, 2012, **22**, 2418–2424.

[2] J. Tan, Z. Chen, D. Wang, S. Qin, X. Xiao, D. Xie, D. Liu and L. Wang, *J. Mater. Chem. A*, 2019, **7**, 24982–24991.