

Supporting Information

Red-emissive Poly(phenylene vinylene)-derivated Semiconductors with Well-balanced Ambipolar Electrical Transporting Property

Yihan Zhang,^{ac} Jun Ye,^d Zheyuan Liu,^{bc} Qingqing Liu,^{ac} Xiaofei Guo,^{ab} Yanfeng Dang,^b Jianqi Zhang,^e Zhixiang Wei,^e Zhixiang Wang,^c Zhaohui Wang,^{af} Huanli Dong,^{*a} Wenping Hu^{ab}

^a Beijing National Laboratory for Molecular Sciences, Key Laboratory of Organic Solids, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China.

^b Tianjin Key Laboratory of Molecular Optoelectronic Sciences Department of Chemistry School of Science Tianjin University & Collaborative Innovation Center of Chemical Science and Engineering Tianjin 300072, China.

^c School of Chemical Sciences, University of Chinese Academy of Sciences, Beijing 100049, China.

^d Institute of High Performance Computing, Agency for Science, Technology and Research, Singapore 138632, Singapore.

^e Key Laboratory of Nanosystem and Hierarchical Fabrication, National Center for Nanoscience and Technology, Beijing 100190, China.

^f Department of Chemistry, Tsinghua University, Beijing 100084, China.

Content

1. GPC experiments

2. Thermal stability

3. Electrochemical properties

4. NMR experiments

5. Device fabrication

6. Transfer and output curves of PBPPV-based transistors constructed under different experimental conditions

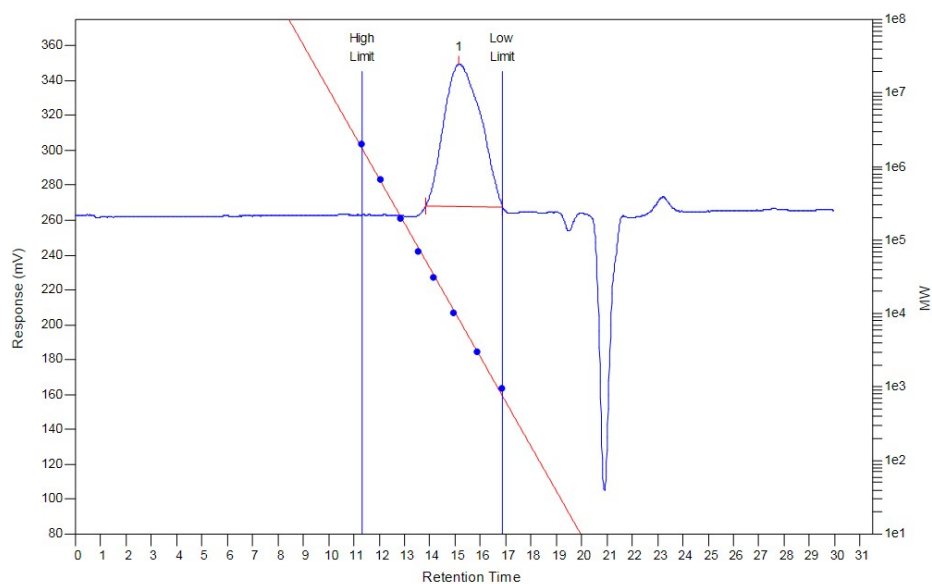
7. Table S1 A summary of charge carrier mobility for PPV-based conjugated polymers reported so far

8. Stability test for PBPPV-based devices

References

1. GPC experiments

(a)



(b)

MW Averages

Mp: 8180

Mn: 4554

Mv: 8238

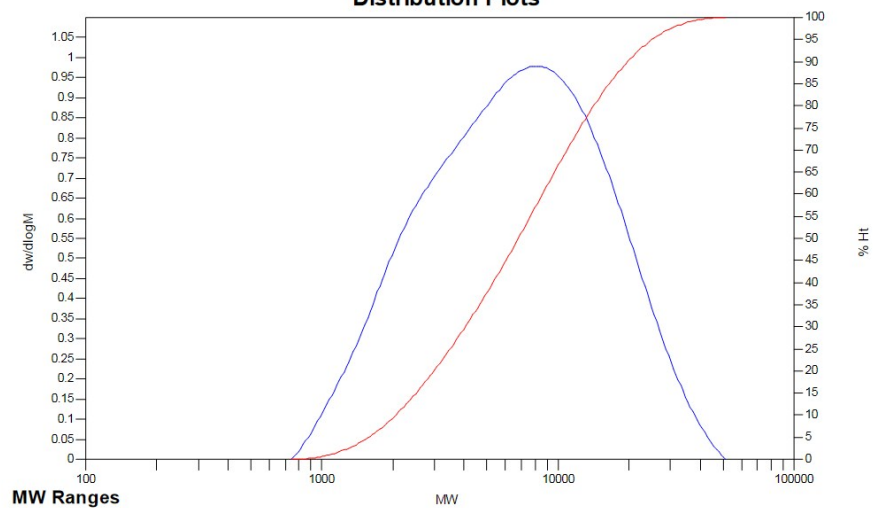
Mw: 9051

Mz: 15418

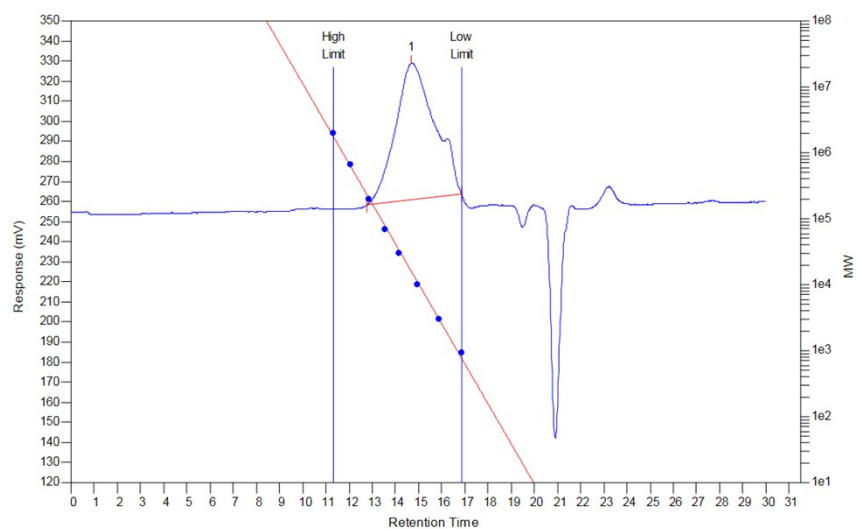
Mz+1: 21592

PD: 1.9875

Distribution Plots



(c)



(d)

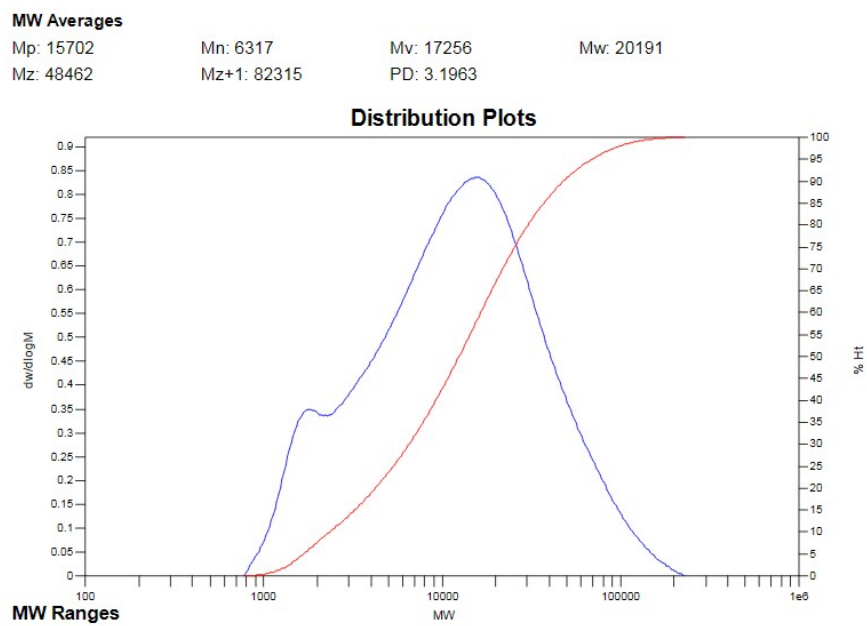


Figure S1. Gel Permeation Chromatography (GPC) trace of (a) PBPPV; (c) diPBPPV from refractive index (RI) detector. Molecular weight distribution plots of (b) PBPPV; (d) diPBPPV.

2. Thermal stability

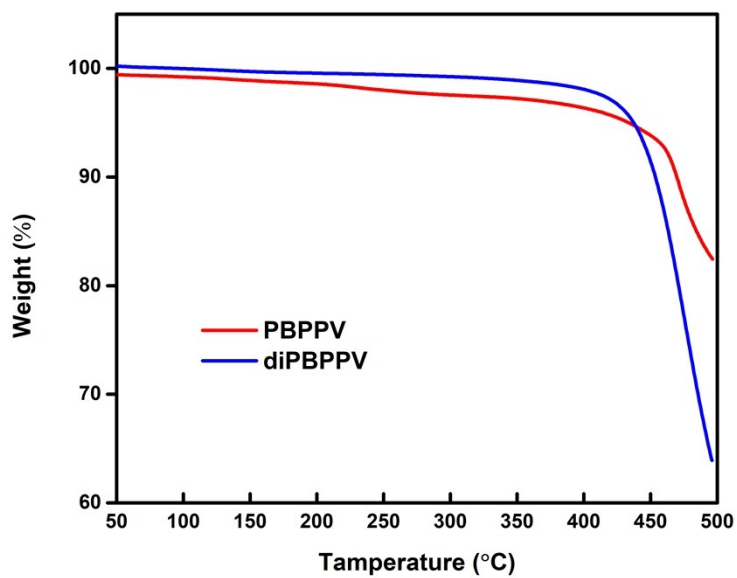


Figure S2. TGA plot of PBPPVs with a heating rate of $40\text{ }^{\circ}\text{C min}^{-1}$ under nitrogen atmosphere.

3. Electrochemical properties

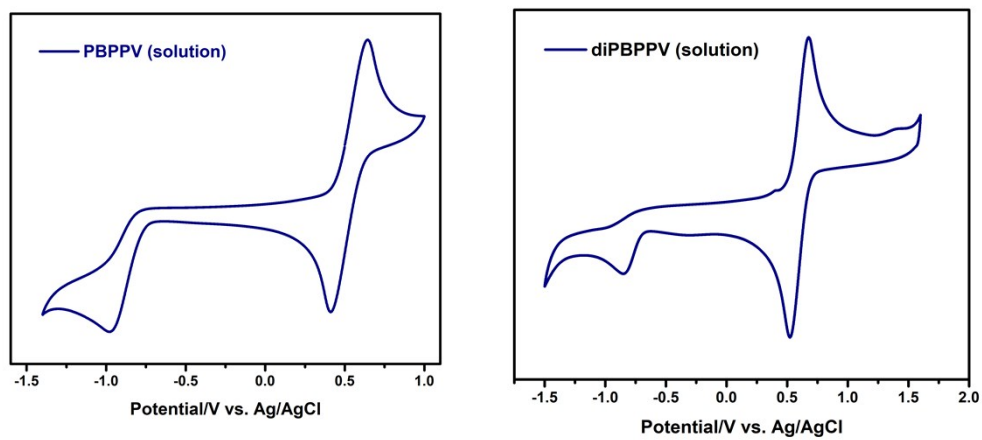
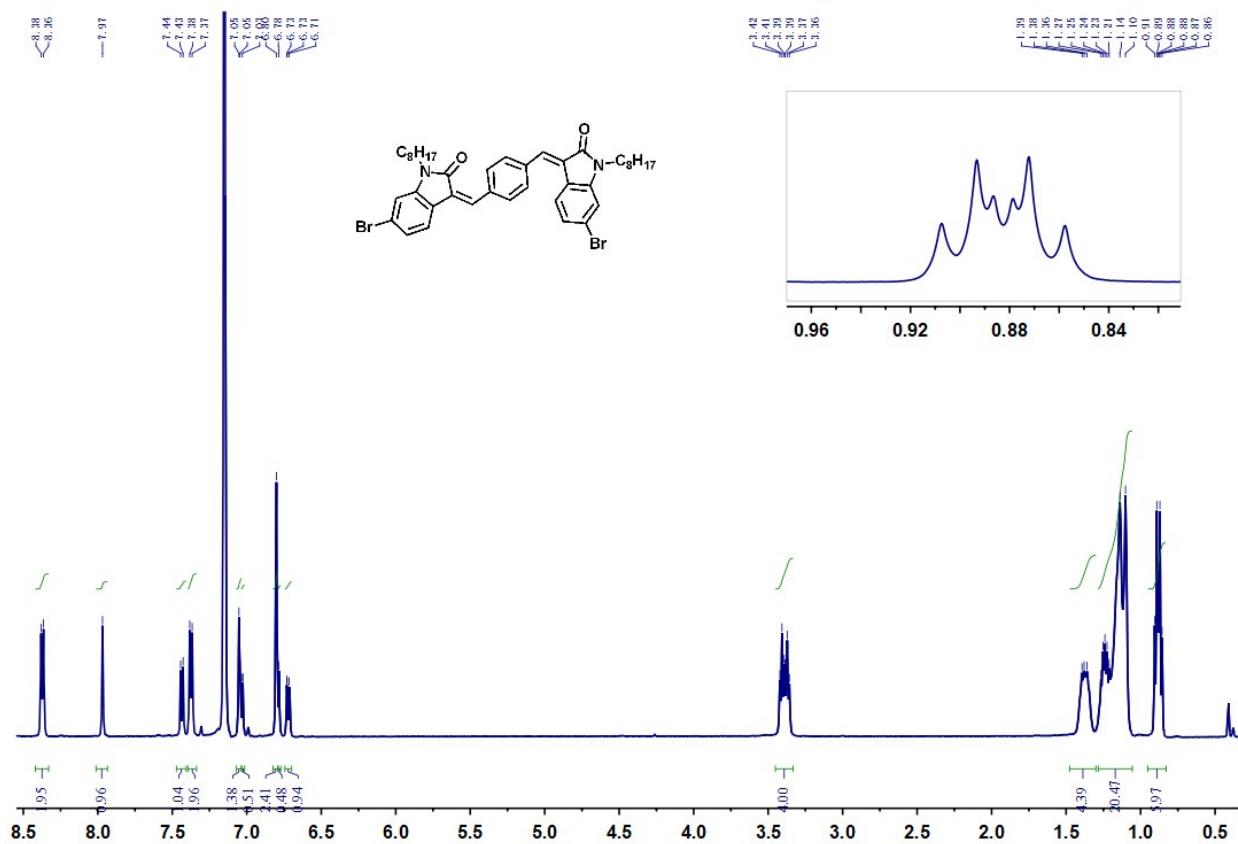


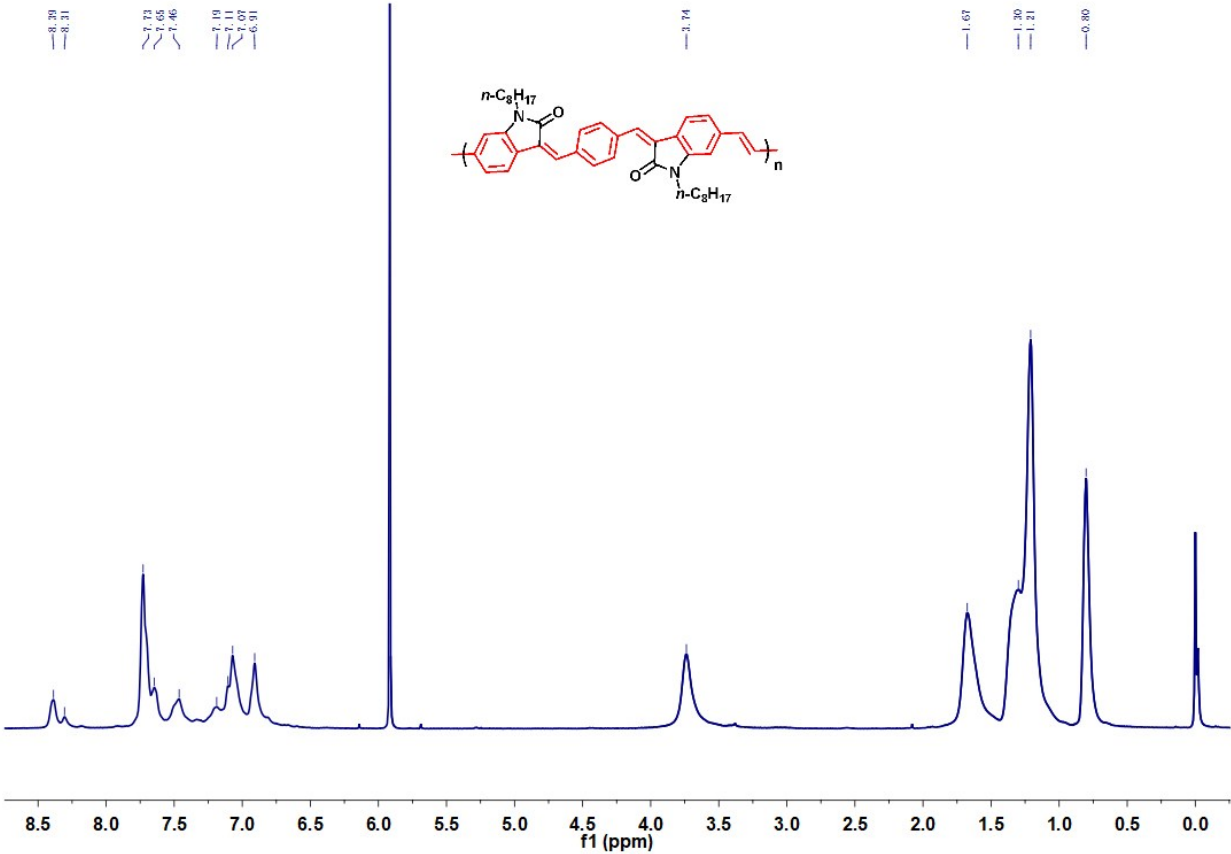
Figure S3. Cyclic voltammogram profile of PBPPVs. ($0.1\text{ M Bu}_4\text{NPF}_6/\text{CH}_2\text{Cl}_2$ with ferrocene at $v = 0.05\text{ V/s.}$)

4. NMR experiments

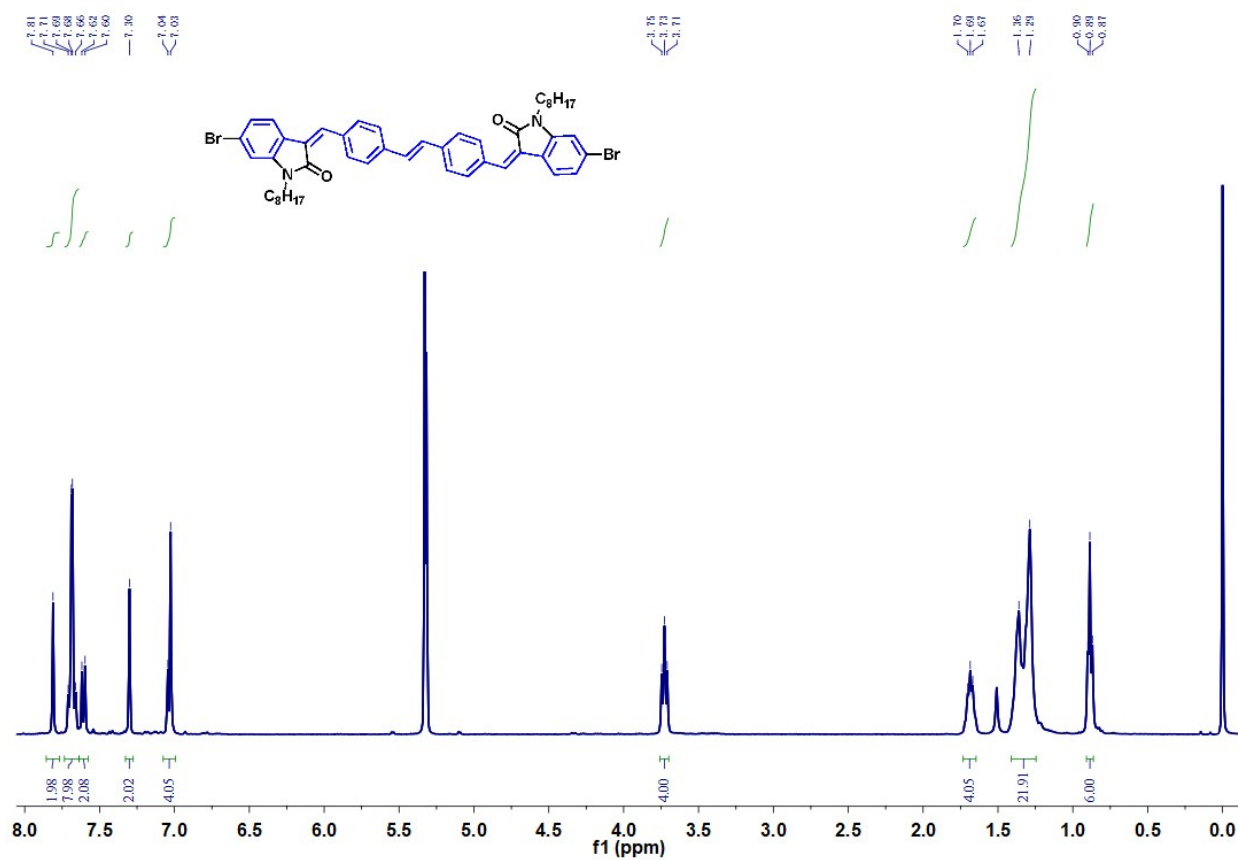
(a)



(b)



(c)



(d)

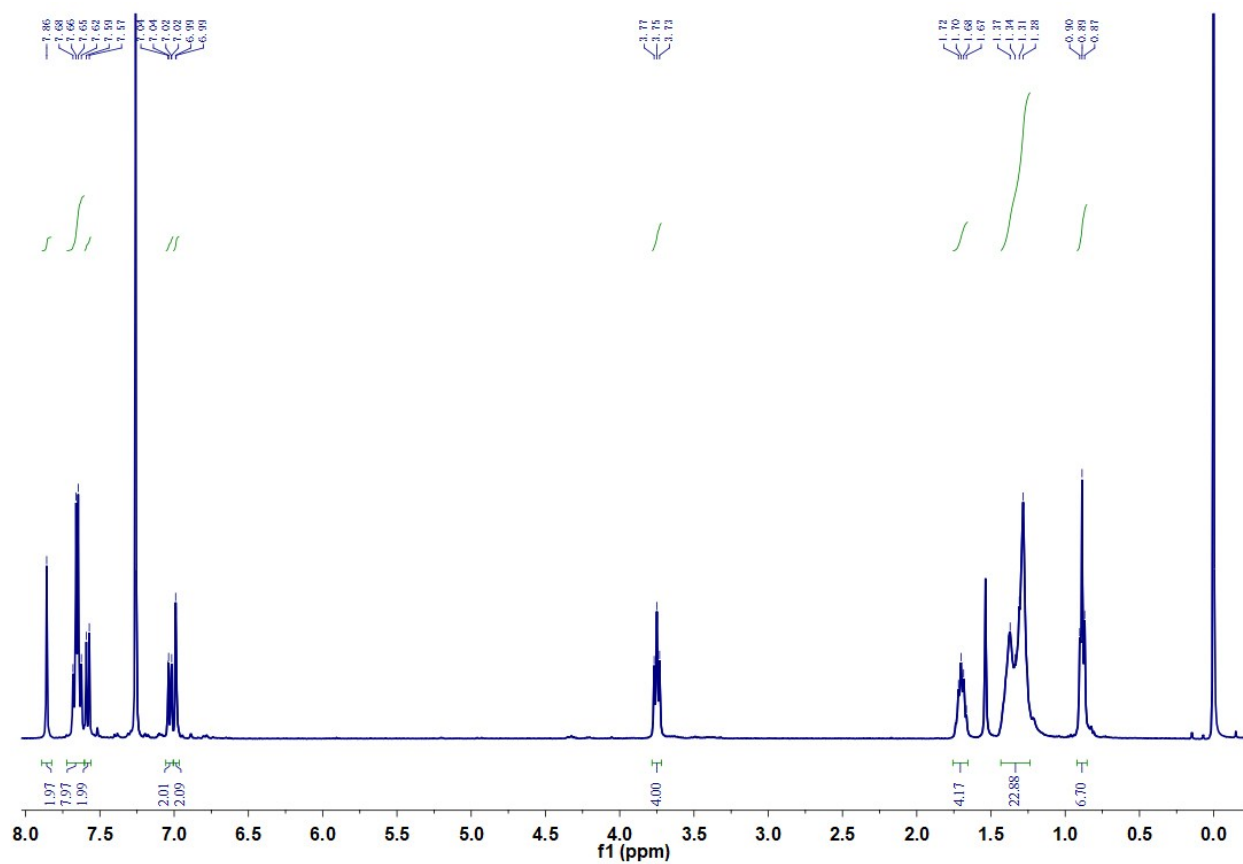


Figure S4. ^1H NMR spectra of (a) BPPV-2Br, (b) PBPPV, (c) diBPPV-2Br, (d) diPBPPV.

5. Device fabrication

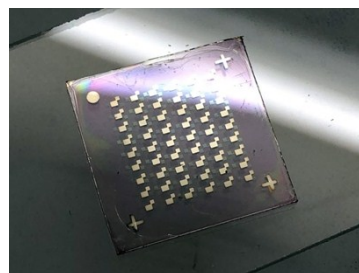
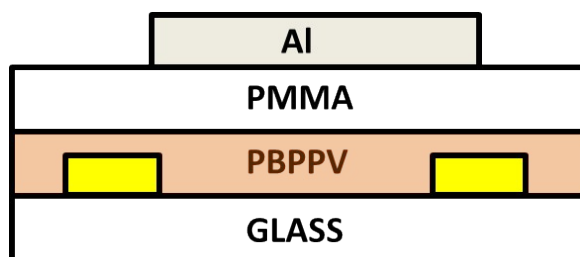


Figure S5. Diagram and photo of OFET devices.

6. Device performances on other conditions

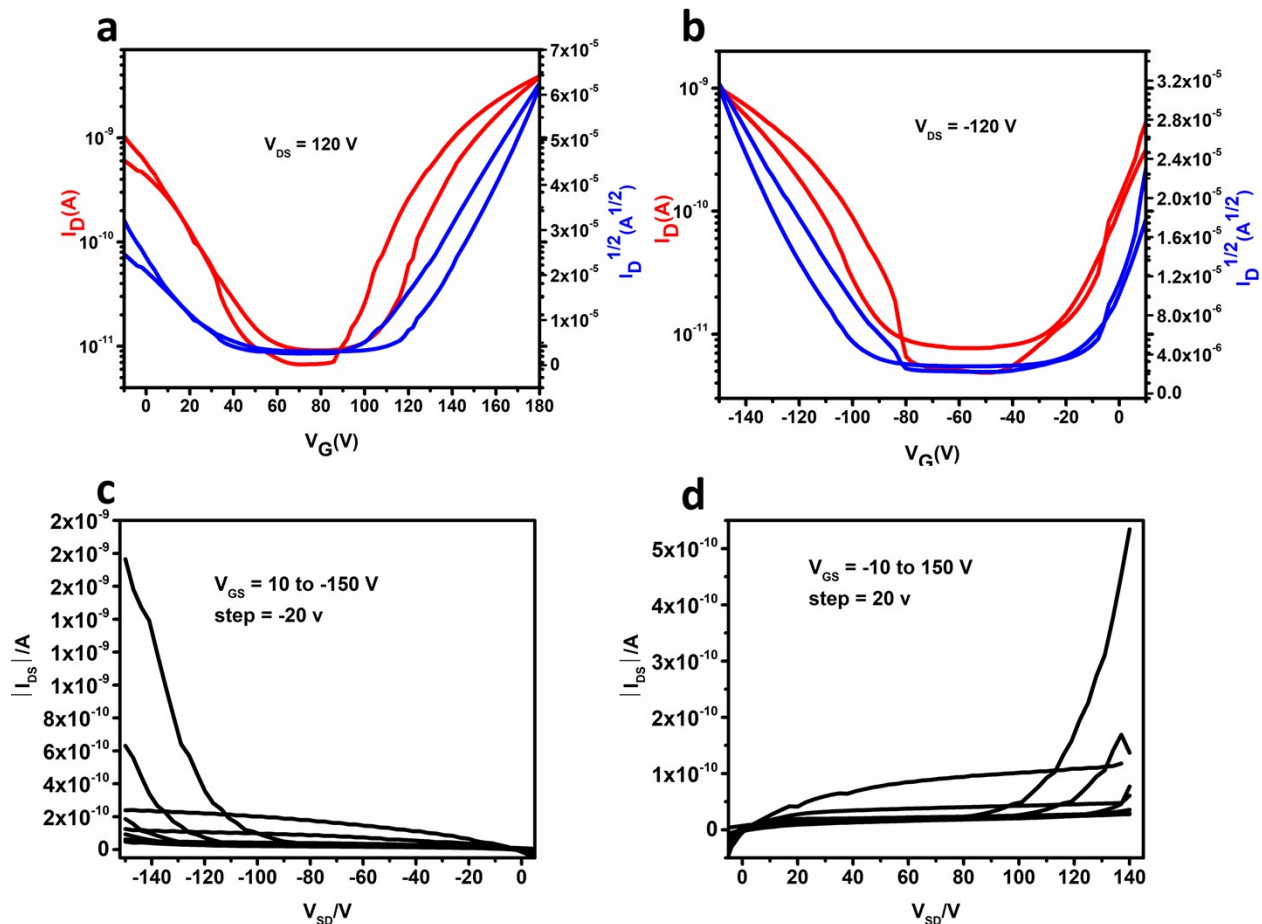


Figure S6. Transfer (top) and output (bottom) curves of TG/BC OFET devices based diPBPPV thin film (annealed at 150 °C). Device parameters: channel width/length (W/L) = 10, $C_i = 3.9 \text{ nF cm}^{-2}$.

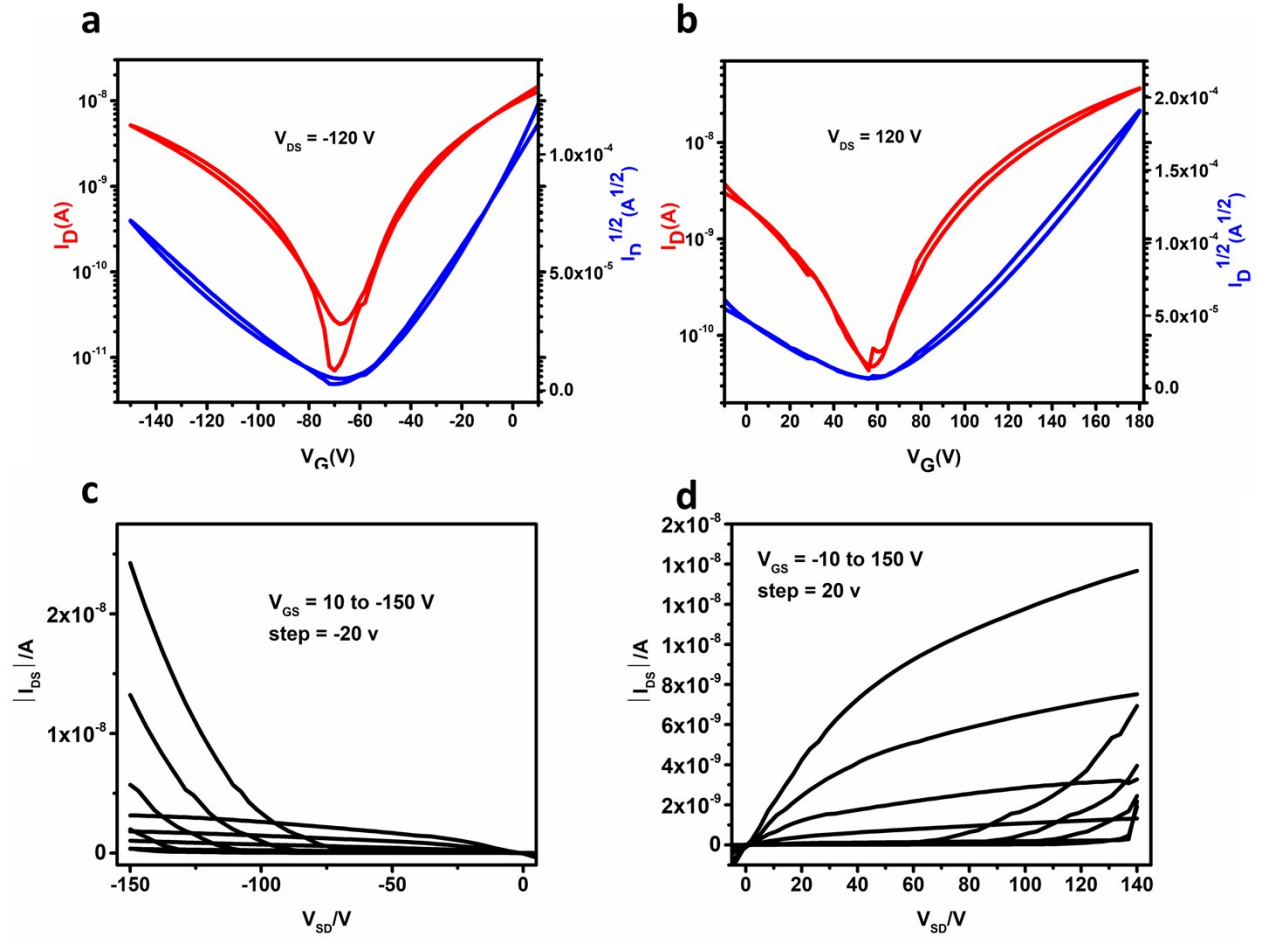


Figure S7. Transfer (top) and output (bottom) curves of TG/BC OFET devices based diBPPV thin film (annealed at 200 °C). Device parameters: channel width/length (W/L) = 10, $C_i = 3.9 \text{ nF cm}^{-2}$.

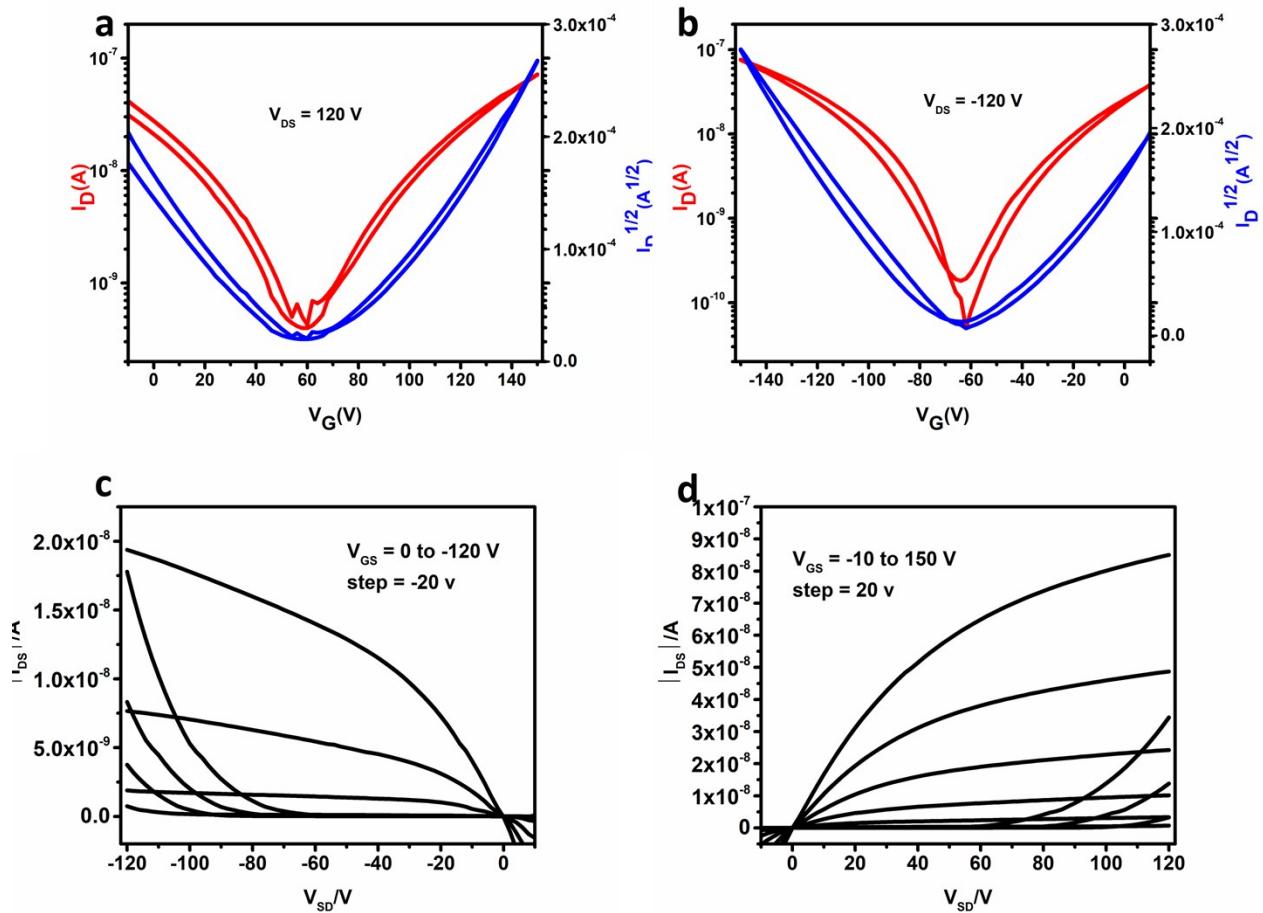
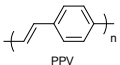
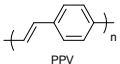
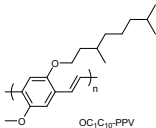
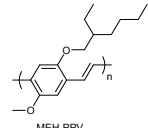
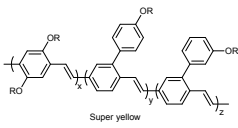
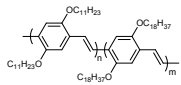
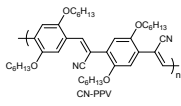
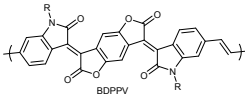
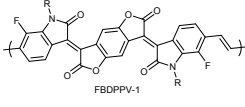
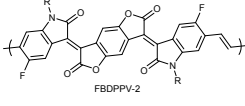
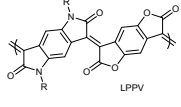
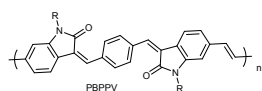


Figure S8. Transfer (top) and output (bottom) curves of TG/BC OFET devices based diBPPV thin film (annealed at 280 °C). Device parameters: channel width/length (W/L) = 10, $C_i = 3.9 \text{ nF cm}^{-2}$.

7. Table S1 A summary of charge carrier mobility for PPV-based conjugated polymers reported so far

Polymer	Energy level	Charge Transfer property			Refs.
	HOMO/LUMO/band gap (eV)	μ_e (cm ² V ⁻¹ s ⁻¹)	μ_h (cm ² V ⁻¹ s ⁻¹)	Device structure	
 PPV	-5.2/-2.7/2.5	-	5.0×10^{-7}	SCLC	1
 PPV	-5.2/-2.7/2.5	10^{-4}	-	BG-TC, Ca/Ca	2
 OC ₁ -C ₁₀ -PPV	-5.0/-2.8/2.2	3.0×10^{-3}	6.0×10^{-4}	Top contact, Au/Ca	3
 MEH-PPV	-5.0/-2.8/2.2	-	10^{-4}	Bottom contact, Au-on-Cr/Au-on-Al	4
 Super yellow	-4.8/-2.4/2.4	6.0×10^{-5}	3.0×10^{-4}	Top contact, Ag/Ca	5
 C ₁₁ H ₂₃ O, C ₁₈ H ₃₇ O	-	-	1.0×10^{-2}	BG-BC, Au/Au	6
 CN-PPV	-5.4/-3.2/2.2	4.0×10^{-5}	-	BG-TC, Ca/Ca	2, 7
 BDPPV	-5.83/-4.41/1.42	0.84	-	TG-BC, Au/Au, on SiO ₂	8
 FBDPPV-1	-6.19/-4.26/1.46	1.39	-	TG-BC, Au/Au, on SiO ₂	9
 FBDPPV-2	-6.22/-4.30/1.39	0.62	-	TG-BC, Au/Au, on SiO ₂	
 LPPV	-5.99/-4.49/1.50	0.16	-	TG-BC, Au/Au, on SiO ₂	10

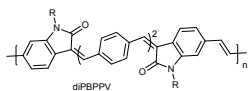


-5.56/-3.58/1.98

2.6×10^{-5}

2.0×10^{-5}

TG-BC,
Au/Au, on
glass



-5.59/-3.55/2.04

4.5×10^{-4}

3.0×10^{-4}

TG-BC,
Au/Au, on
glass

This
work

8. Stability test for PBPPV-based devices

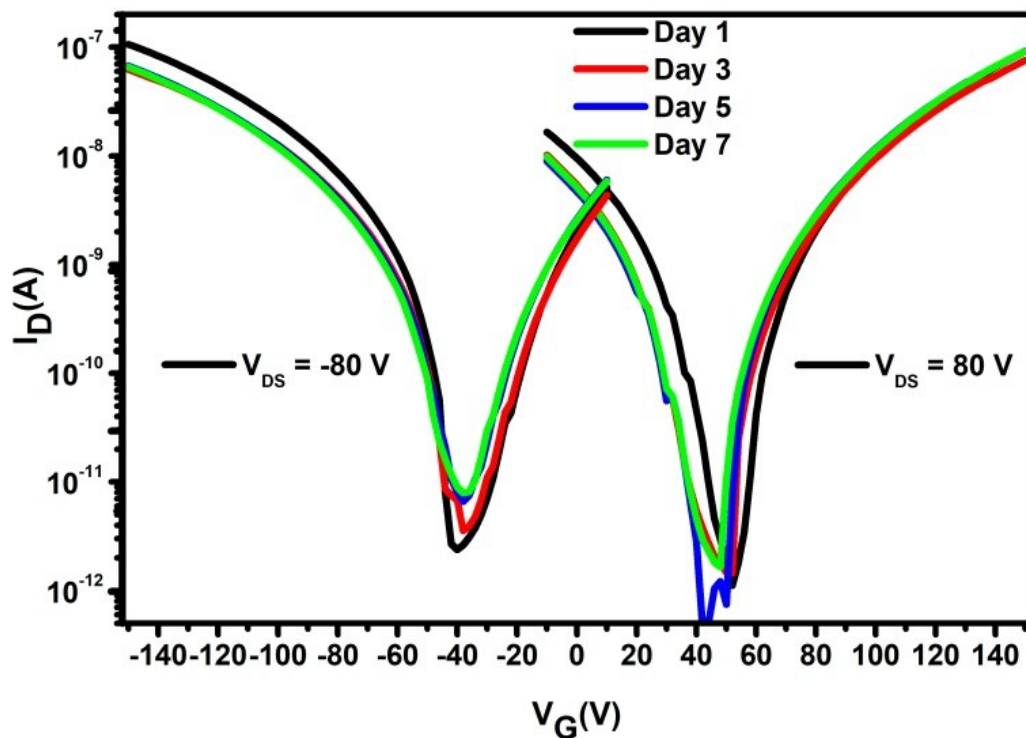


Figure S9. Stability test within one week for diPBPPV-based devices (device stored in air, humidity less than 30%, device parameters: channel width/length (W/L) = 10, C_i = 6.8 nF cm⁻², annealed at 280 °C)

References

- 1 Blom, P. W. M., Jong, M. J. M. d. and Vleggaar, J. J. M., *Appl. Phys. Lett.*, 1996, **68**, 3308.
- 2 Chua, L.-L., Zaumseil, J., Chang, J.-F., Ou, E. C. W., Ho, P. K. H., Sirringhaus, H. and Friend, R. H., *Nature*, 2005, **434**, 194.
- 3 Zaumseil, J., Friend, R. H. and Sirringhaus, H., *Nat. Mater.*, 2006, **5**, 69.

- 4 Sakanoue, T., Fujiwara, E., Yamada, R. and Tada, H., *Appl. Phys. Lett.*, 2004, **84**, 3037.
- 5 Swensen, J. S., Soci, C. and Heeger, A. J., *Appl. Phys. Lett.*, 2005, **87**, 253511.
- 6 van Breemen, A., Herwig, P. T., Chlon, C. H. T., Sweelssen, J., Schoo, H. F. M., Benito, E. M., de Leeuw, D. M., Tanase, C., Wildeman, J. and Blom, P. W. M., *Adv. Funct. Mater.*, 2005, **15**, 872.
- 7 Greenham, N. C.; Moratti, S. C.; Bradley, D. D. C.; Friend, R. H.; Holmes, A. B. *Nature* 1993, **365**, 628.
- 8 Lei, T., Dou, J.-H., Cao, X.-Y., Wang, J.-Y. and Pei, J., *J. Am. Chem. Soc.*, 2013, **135**, 12168.
- 9 Lei, T., Xia, X., Wang, J.-Y., Liu, C.-J. and Pei, J., *J. Am. Chem. Soc.*, 2014, **136**, 2135.
- 10 Lu, Y., Yu, Z.-D., Zhang, R.-Z., Yao, Z.-F., You, H.-Y., Jiang, L., Un, H.-I., Dong, B.-W., Xiong, M., Wang, J.-Y. and Pei, J., *Angew. Chem. Int. Ed.*, 2019, **58**, 11390.