Electronic Supplementary Information

A novel D-π-A blue fluorophore based on [1,2,4]triazolo[1,5-*a*]pyridine as electron acceptor and its application in organic light-emitting diodes

Chen Cao,[a,b] Wen-Cheng Chen,*[b] Shuang Tian,[b] Jia-Xiong Chen,[b] Zhong-Yi Wang,[a] Xu-Hui Zheng,[a] Chong-Wei Ding,[a] Jing-Hong Li,[a] Jie-Ji Zhu,[a] Ze-Lin Zhu,[b] Qing-Xiao Tong,*[a] and Chun-Sing Lee*[b]

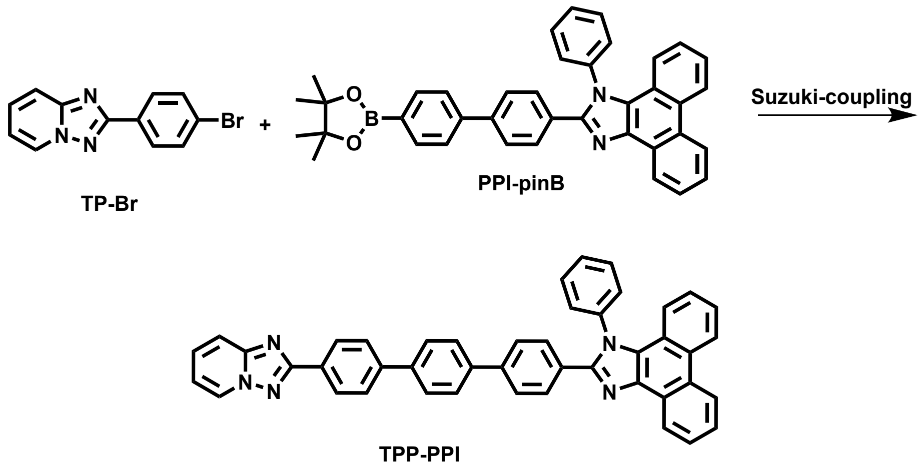
[a]*Department of Chemistry and Key Laboratory for Preparation and Application of Ordered Structural Materials of Guangdong Province, Shantou University, 243 University Road, Shantou, Guangdong, 515063, P. R. China. E-mail: qxtong@stu.edu.cn*

[b]*Center of Super-Diamond and Advanced Films (COSDAF) and Department of Chemistry, City University of Hong Kong, Hong Kong & City University of Hong Kong Shenzhen Research Institute, Shenzhen, Guangdong, P. R. China. E-mail: wenium@live.com, apcslee@cityu.edu.hk*

Synthesis

2-(4''-([1,2,4]triazolo[1,5-*a*]pyridin-2-yl)-[1,1':4',1''-terphenyl]-4-yl)-1-phenyl-1*H*-phenanthro[9,10-*d*]imidazole(TPP-PPI)

30 mL toluene, 15 mL ethanol and 15 mL 2 M Na_2CO_3 aq. were added to a mixture of 1-phenyl-2-(4'-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-[1,1'-biphenyl]-4-yl)-1*H*-phenanthro[9,10-*d*]imidazole (PPI-pinB, 1.6 g, 2.81 mmol), 2-(4-bromophenyl)-[1,2,4]triazolo[1,5-*a*]pyridine (TP-Br, 0.64 g, 2.34 mmol), and 0.20 g $Pd(PPh_3)_4$ (0.18 mmol) in a degassed three-necked flask. Then the suspension was heated to 90 °C with stirring under an argon atmosphere. After 24 h, the mixture was allowed to cool to room temperature, extracted with CH_2Cl_2 and dried over anhydrous $MgSO_4$ before removing the solvent. Finally, the product was purified by column chromatography on 200-300 mesh silica gel (eluent: petroleum ether/CH_2Cl_2 = 1/6) to give a white solid, with a yield of 73% (1.1 g). ^{1}H NMR (400 MHz, CD_2Cl_2) δ 8.80 (d, *J* = 8.4 Hz, 1H), 8.75 (d, *J* = 8.4 Hz, 1H), 8.64 (d, *J* = 6.8 Hz, 1H), 8.37 (d, *J* = 8.4 Hz, 2H), 7.87 – 7.50 (m, 21H), 7.30 (t, *J* = 7.5 Hz, 1H), 7.21 (d, *J* = 7.7 Hz, 1H), 7.04 (t, *J* = 6.9 Hz, 1H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 164.07, 152.28, 142.26, 140.20, 139.63, 130.82, 130.65, 130.37, 130.01, 129.53, 128.90, 128.13, 127.88, 127.83, 127.59, 127.04, 126.92, 125.28, 124.54, 123.64, 121.42, 116.72, 114.09. MS m/z: $[M + H]^+$ calcd for $C_{45}H_{29}N_5$, 639.76; found, 640.06. Anal. Calcd for $C_{45}H_{29}N_5$: C, 84.48; H, 4.57; N, 10.95; found: C, 84.55; H, 4.53; N, 10.89.



Scheme S1. Synthetic routes of TPP-PPI. Suzuki-coupling reaction: 2 M Na_2CO_3 aq., $Pd(PPh_3)_4$, toluene, EtOH, 90 °C.

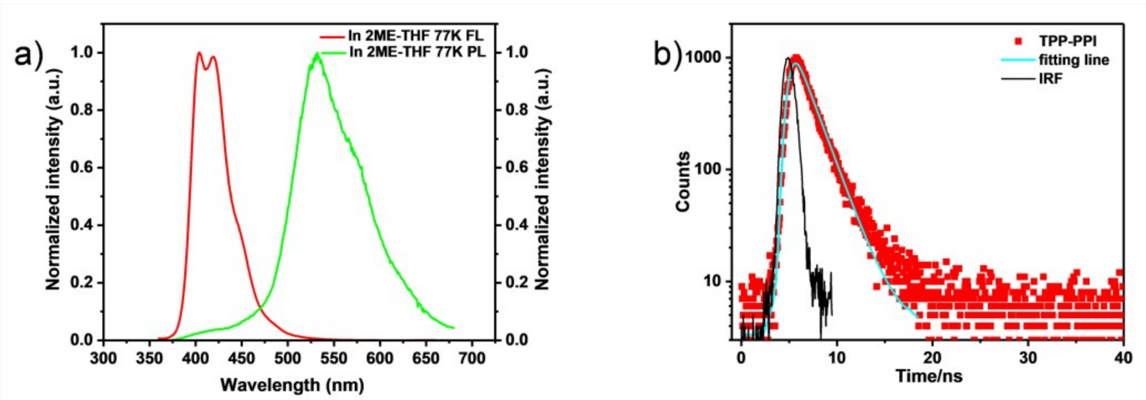


Fig. S1 a) Fluorescence and phosphorescence spectra in 2-methyltetrahydrofuran at 77 K; b) Transient PL decay of TPP-PPI's neat film.

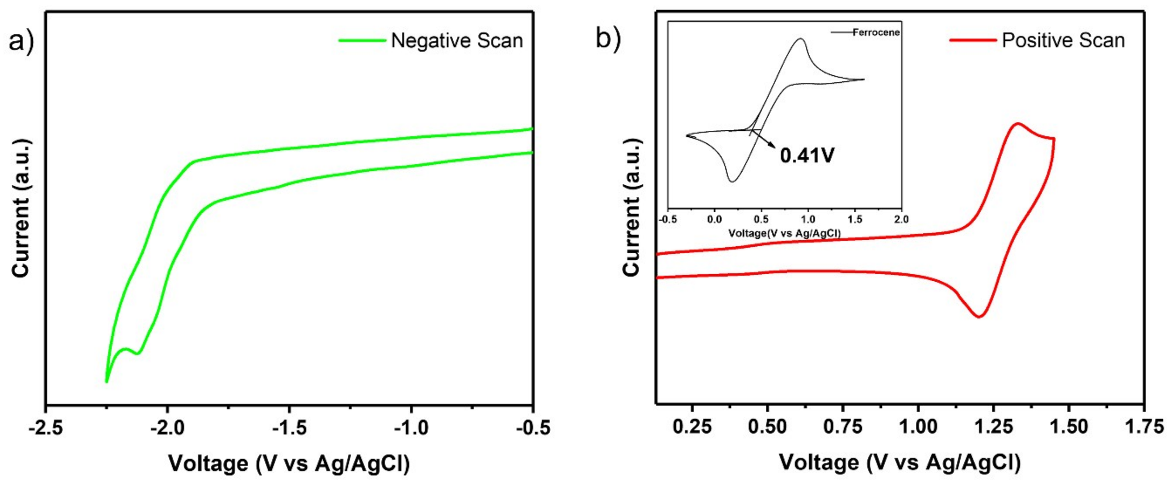


Fig. S2 Cyclic voltammogram of TPP-PPI a) negative scan in THF b) positive scan in DCM (inset: ferrocene).

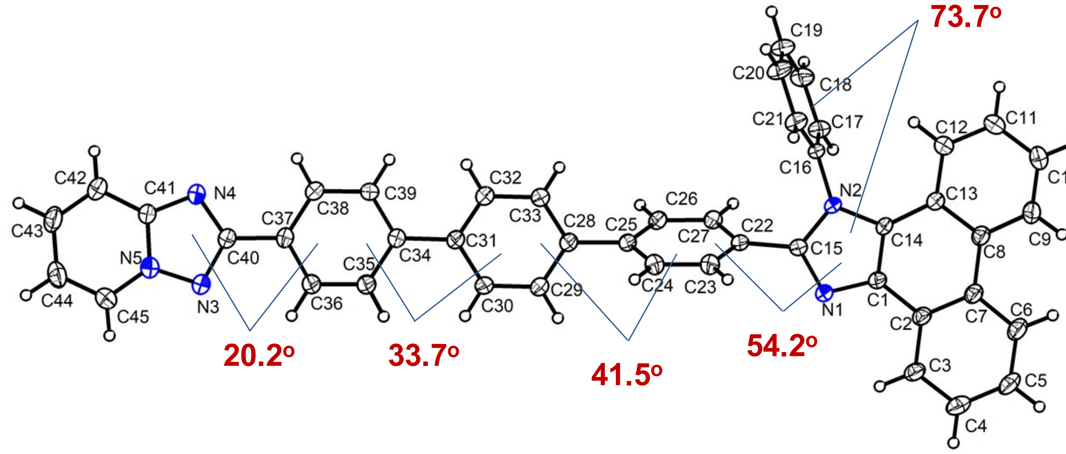


Fig. S3 Molecular Oak Ridge Thermal Ellipsoid Plot Program (ORTEP) structure

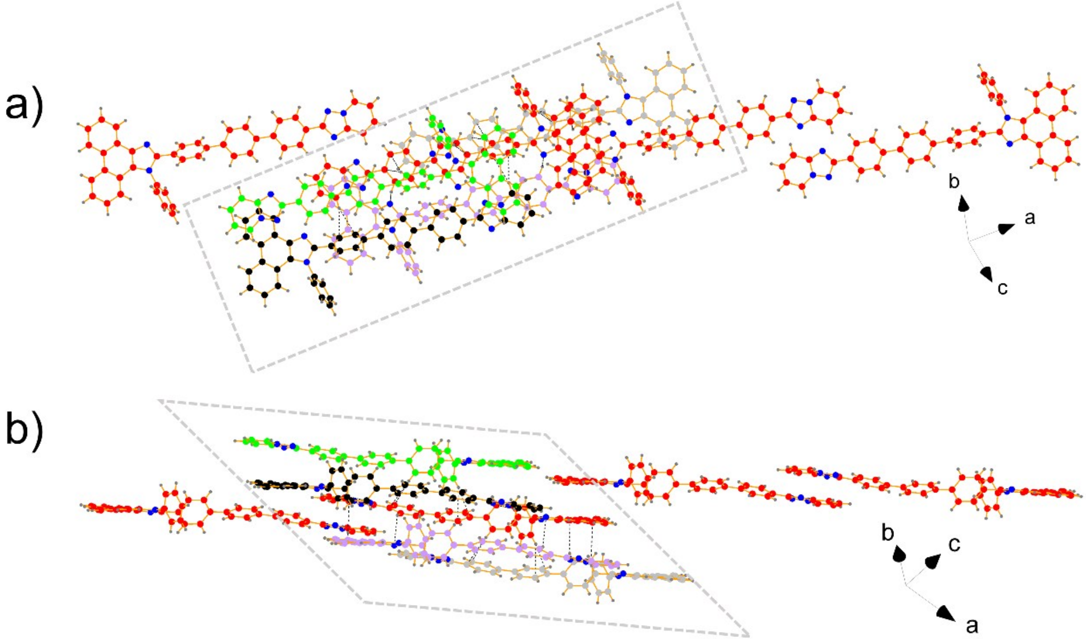


Fig. S4 Another similar chains around red chain: a) top view b) side view

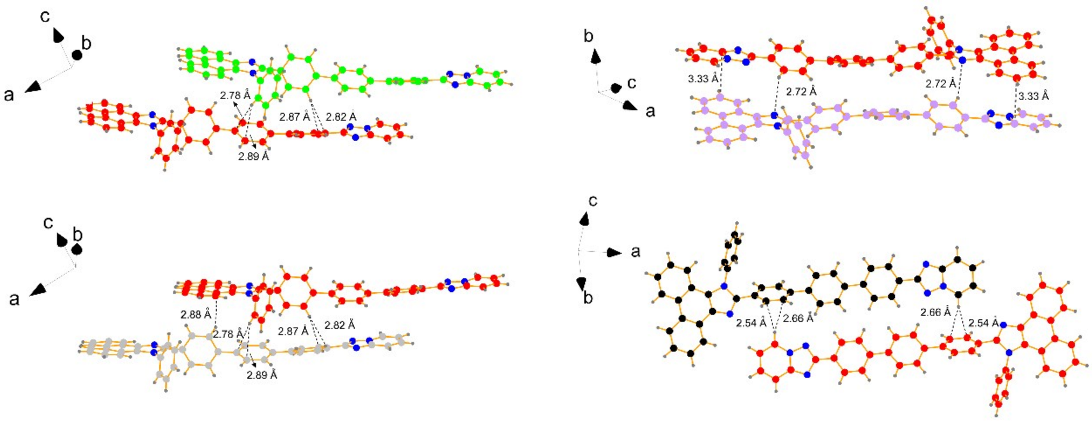


Fig. S5 The detail interaction between the adjacent chains

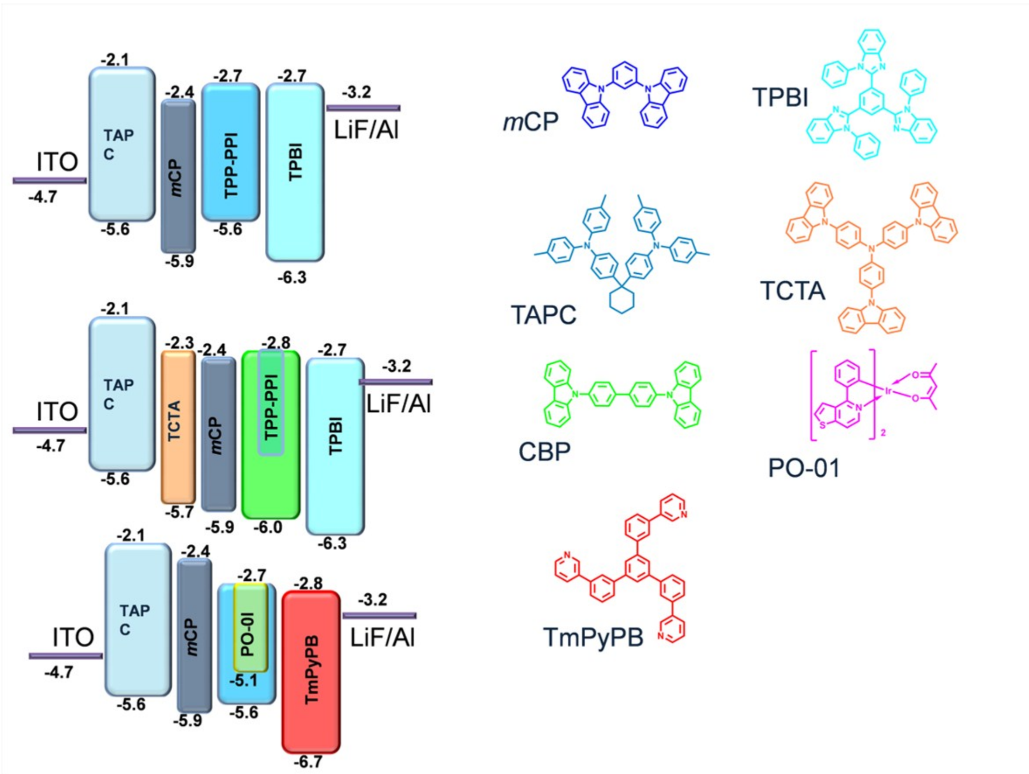


Fig. S6 Energy level diagram of the non-doped OLEDs, doped OLEDs, yellow OLEDs and the chemical structures of the used materials.

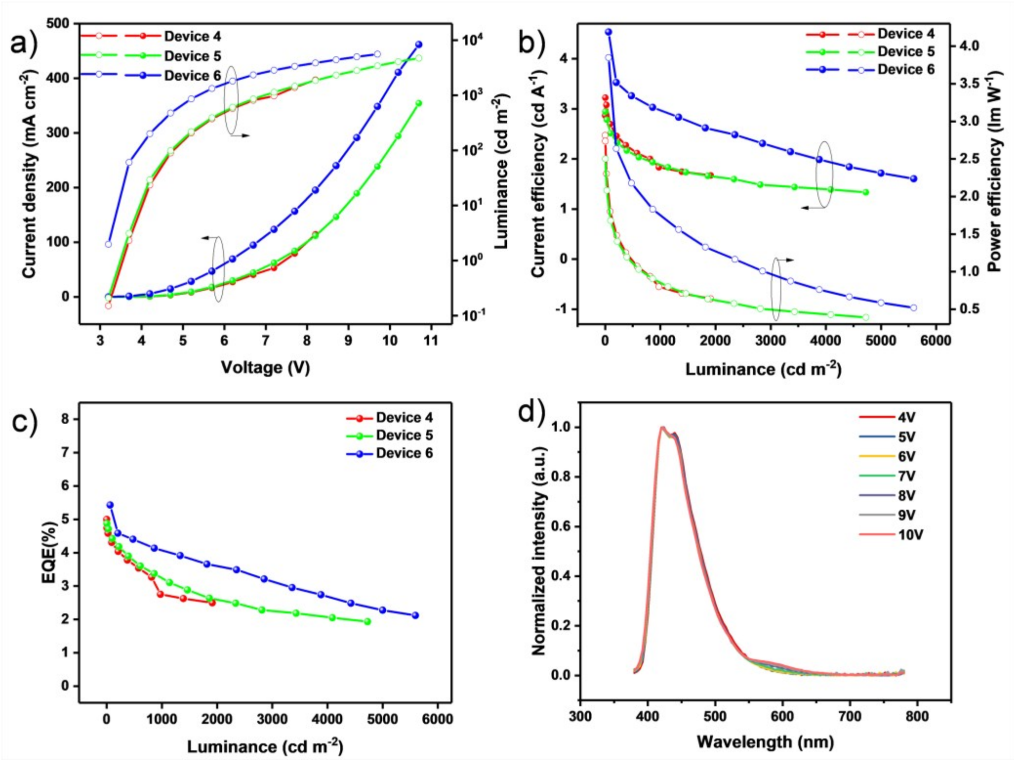


Fig. S7 a) Current density-voltage-luminescence characteristic curves, b) plots of current efficiency-luminance-power efficiency, c) luminance-EQE plots and d) EL spectra at different voltage of device 6.

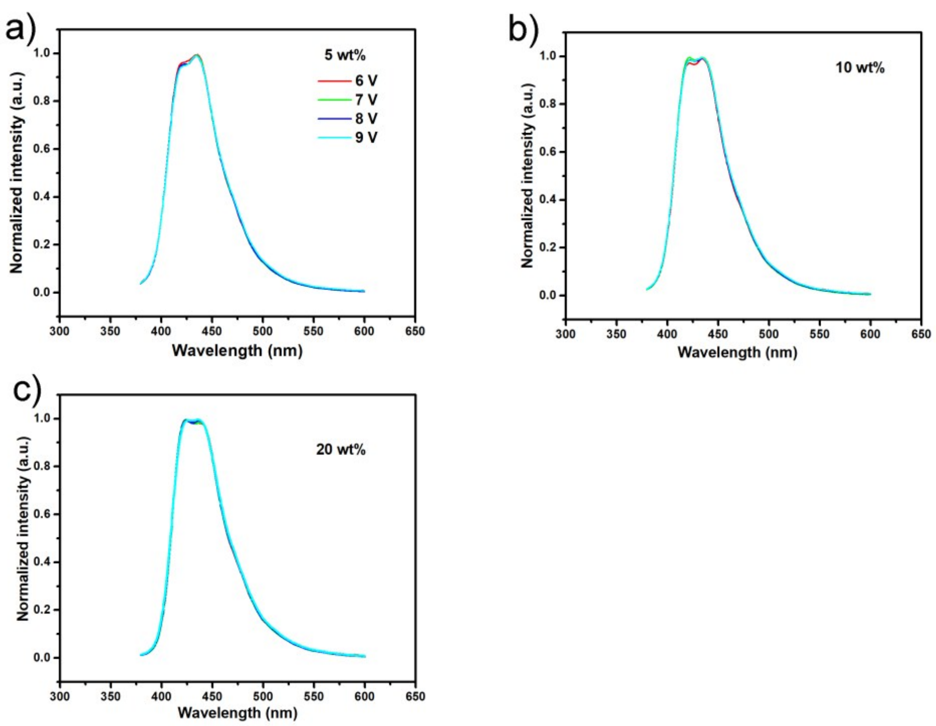


Fig. S8 Voltage-dependent EL spectra for device a) 7, b) 8 and c) 9.

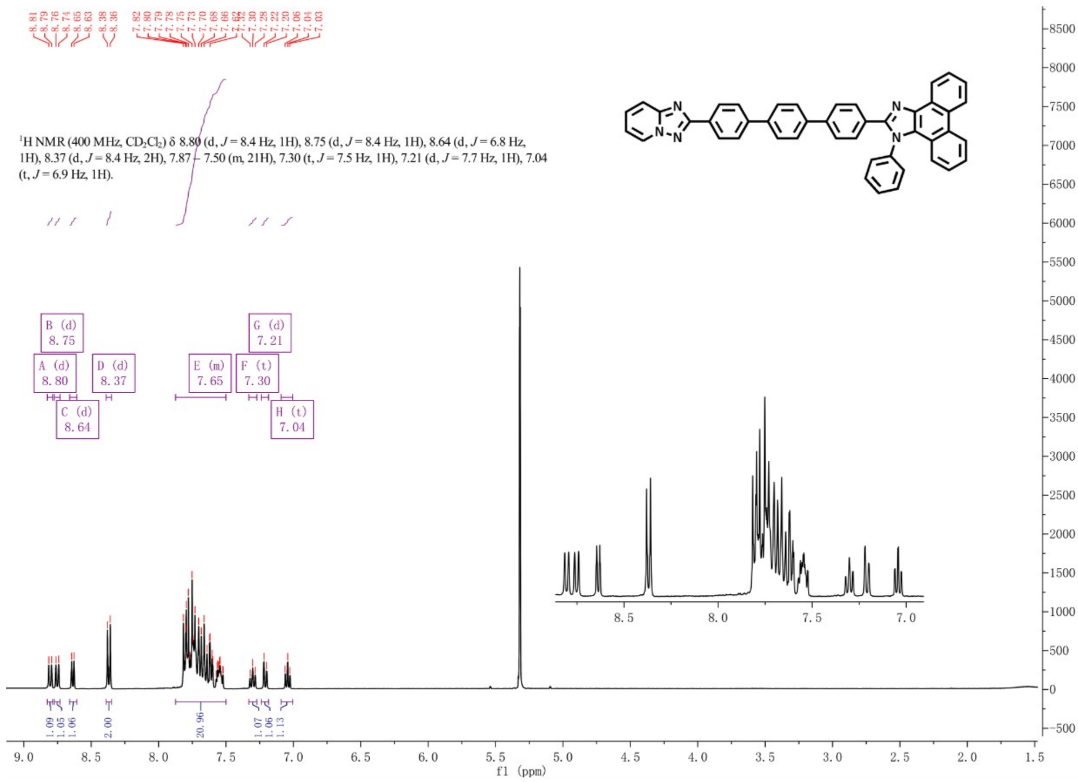


Fig. S9 ^{1}H-NMR of TPP-PPI in CD_2Cl_2

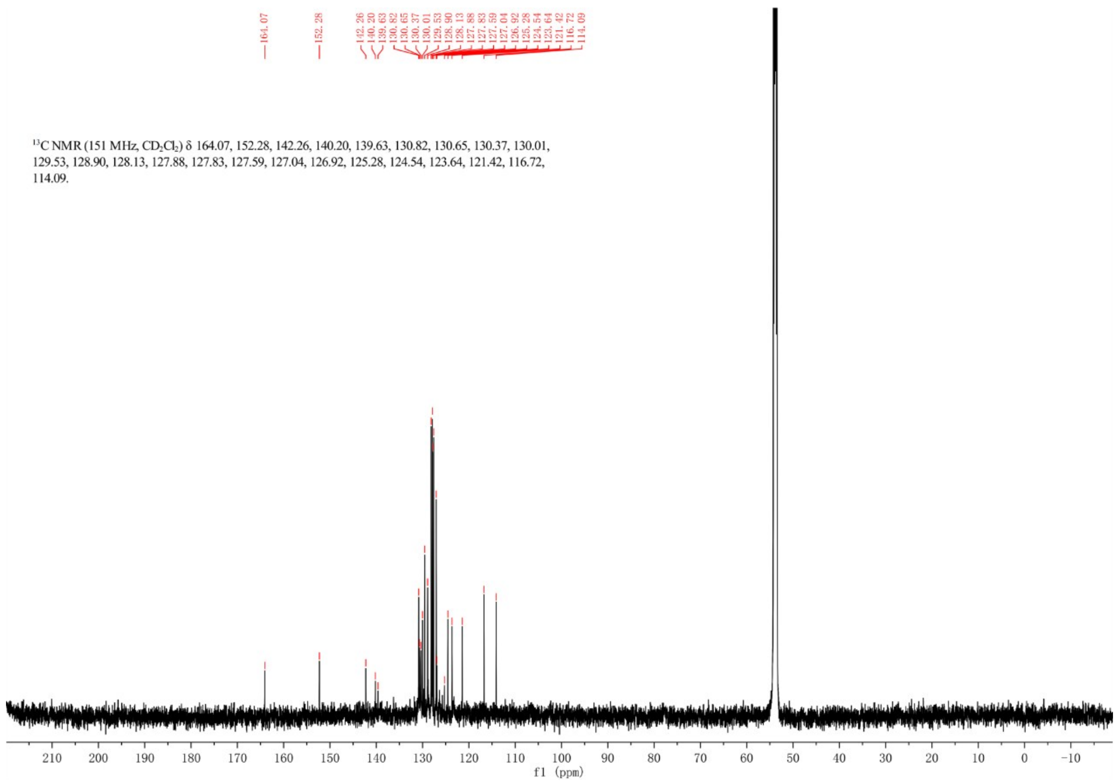


Fig. S10 ^{13}C-NMR of TPP-PPI in CD_2Cl_2

Table S1 Summary of the photophysical data of TPP-PPI in different solvents

	λ_{abs} (ε) [10^5 M^{-1} cm^{-1}]	λ_{fl} (nm)	PLQY(%)
n-hexane	260 (0.095),330(0.093)	398, 422	69.6
THF	260(0.94), 330(0.92)	433	~100
DCM	260(0.90), 330(0.80)	439	~100
ACN	260(0.52), 330(0.50)	445	93.5

Table S2 Summary of the recent orange device data

CE (cd A^{-1})	**PE (lm W^{-1})**	**EQE (%)**	**Ref.**
Max/@1000 cd m^{-2}	Max/@1000 cd m^{-2}	Max/@1000 cd m^{-2}	
56.94/56.39	64.61/42.11	24.7/20.9	This work
-/-	64.5/57.3	24.5/24.2	1
-/-	73.1/-	27.0/-	2
57.3/54.1	60.0/53.4	18.9/17.8	3
69.3/65.8	89.0/44.5	22.6/21.4	4

References.

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