Electronic Supplementary Information

Blue pyrene-based AIEgens: the inhibited intermolecular π-π stacking through the introduction of substituents with controllable intramolecular conjugation, and high external quantum efficiencies up to 3.46% in nondoped OLED

*Jie Yang [#a], Le Li [#b], Yun Yu [a], Zichun Ren[a], Qian Peng [c], Shanghui Ye *[b], Qianqian Li [a], Zhen Li *[a]*

[a] Department of Chemistry, Hubei Key Laboratory on Organic and Polymeric Opto-Electronic Materials Wuhan University, Wuhan 430072 (P.R. China), Fax: (+86)27-68756757.

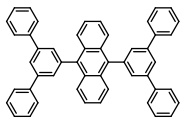
E-mail: lizhen@whu.edu.cn; lichemlab@163.com

[b] Key Laboratory for Organic Electronics and Information Displays (KLOEID) Institute of Advanced Materials (IAM) Nanjing University of Posts and Telecommunications

Nanjing 210046 (P.R. China), E-mail: yeshh@iccas.ac.cn

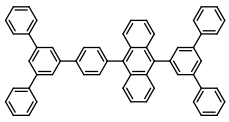
[c] Key Laboratory of Organic Solids, Beijing National Laboratory for Molecular Science (BNLMS), Institute of Chemistry, Chinese Academy of Sciences, 100190 Beijing, China.

[#] These authors contributed equally to this work.



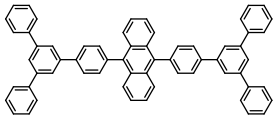
MAM

CE 2.94 cd/A, EQE 3.9%, λ_{EL} 444 nm, CIE (0.16,0.12)



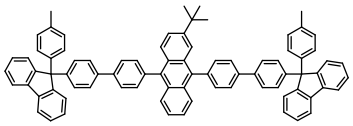
MAT

CE 2.97 cd/A, EQE 6.14%, λ_{EL} 438 nm, CIE (0.16,0.09)



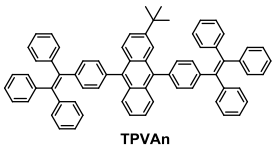
TAT

CE 3.64 cd/A, EQE 7.18%, λ_{EL} 444 nm, CIE (0.16,0.09)



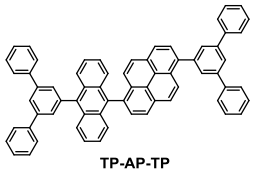
BFAn

CE 5.6 cd/A, EQE 5.1%, λ_{EL} 450 nm, CIE (0.15,0.12)



TPVAn

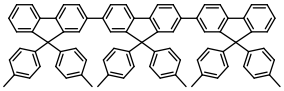
CE 5.3 cd/A, EQE 5.3%, λ_{EL} 456 nm, CIE (0.14,0.12)



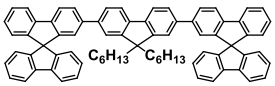
TP-AP-TP

CE 5.63 cd/A, EQE 7.51%, λ_{EL} 456 nm, CIE (0.15,0.13)

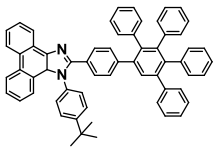
CE 1.10 cd/A, EQE 4.1%, CIE (0.16,0.04)



CE 1.53 cd/A, EQE 5.3%, CIE (0.16,0.04)

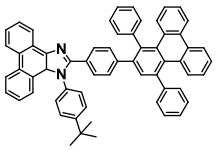


CE 1.52 cd/A, EQE 2.7%, CIE (0.17,0.07)



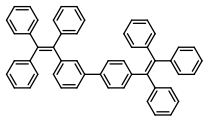
TTP-TPI

CE 2.10 cd/A, EQE 5.02%, λ_{EL} 424 nm, CIE (0.16,0.05)



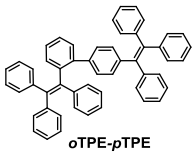
DPT-TPI

CE 3.13 cd/A, EQE 5.25%, λ_{EL} 432 nm, CIE (0.16,0.07)



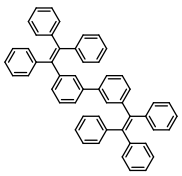
***m*TPE-*p*TPE**

CE 2.8 cd A^{-1}, EQE 1.9%, λ_{EL} 459 nm; CIE (0.16, 0.16)



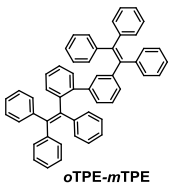
***o*TPE-*p*TPE**

CE 2.2 cd A^{-1}, EQE 1.7%, λ_{EL} 454 nm, CIE (0.16, 0.14)



***m*TPE-*m*TPE**

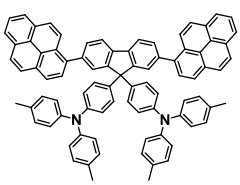
CE 2.1 cd A^{-1},EQE 1.9%, λ_{EL} 452 nm, CIE (0.15, 0.11)



***o*TPE-*m*TPE**

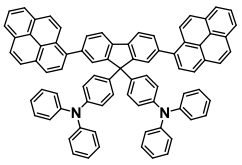
CE 1.8 cd A^{-1}, EQE 1.4%, λ_{EL} 435 nm, CIE (0.16, 0.14)

Chart S1. Some good blue materials with twisted conformations to restrict the π-π stackings.[1]



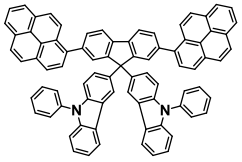
DTDPF

CE 1.31 cd/A, EQE 1.83%, λ_{max} 456 nm, CIE (0.15, 0.16)



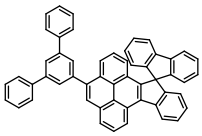
BPTF

CE 2.06 cd/A, EQE 0.56%, λ_{max} 438 nm, CIE (0.15, 0.13)



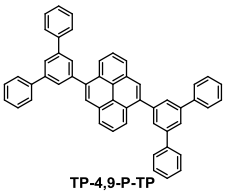
DCDPF

CE 4.4 cd/A, λ_{max} 458 nm, CIE (0.15, 0.15)



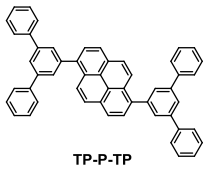
TP-PFF

CE 3.24 cd/A, λ_{max} 457 nm, CIE (0.15, 0.13)



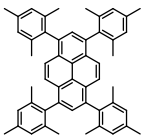
TP-4,9-P-TP

CE 2.11 cd/A, λ_{max} 455 nm, CIE (0.16, 0.14)



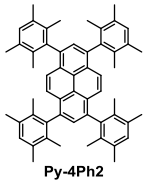
TP-P-TP

CE 2.51 cd/A, EQE 3.16%, λ_{max} 454 nm, CIE (0.16, 0.14)



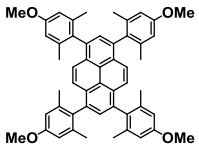
Py-4Ph1

CE 2.2 cd/A, EQE 2.6%, λ_{max} 450 nm, CIE (0.15, 0.10)



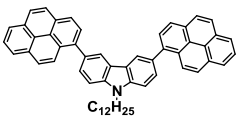
Py-4Ph2

CE 0.9 cd/A, EQE 1.01%, λ_{max} 448 nm, CIE (0.14, 0.08)



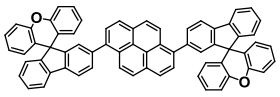
Py-4Ph3

CE 2.7 cd/A, EQE 3.26%, λ_{max} 448 nm, CIE (0.14, 0.09)



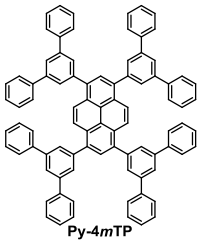
CP2

CE 3.33 cd/A, λ_{max} 436 nm, CIE (0.16, 0.14)



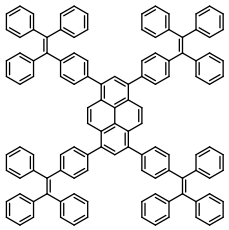
DSFXPy

CE 5.6 cd/A, EQE 3.6%, λ_{max} 448 nm, CIE (0.16, 0.16)



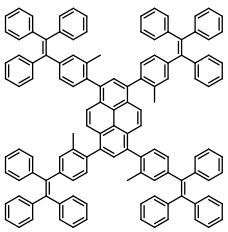
Py-4*m*TP

CE 3.26 cd/A, CIE (0.15,0.11)



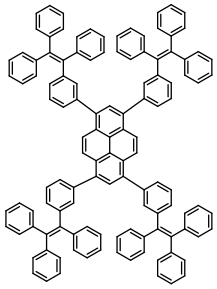
TTPEPy

EQE 4.95%; CE 12.3 cd A^{-1}; λ_{max} 488 nm



Py-4MethylTPE

EQE 2.5%; CE 5.14 cd A^{-1}; λ_{max} 472 nm; CIE (0.19, 0.27)



Py-4*m*TPE

EQE 2.5%; CE 4.02 cd A^{-1}; λ_{max} 436 nm; CIE (0.18, 0.16)

Chart S2. Some good blue materials based on pyrene derivatives with restricted π-π stacking.[2]

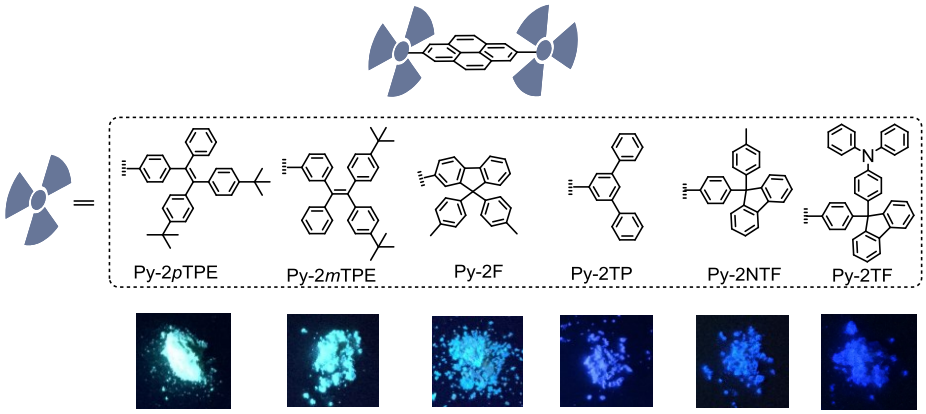


Figure S1. The chemical structures of Py-2*p*TPE, Py-2*m*TPE, Py-2F, Py-2TP, Py-2NTF, Py-2TF and their corresponding solid photographs.

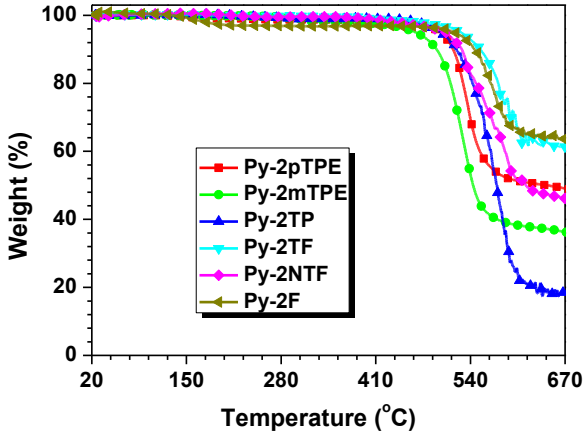
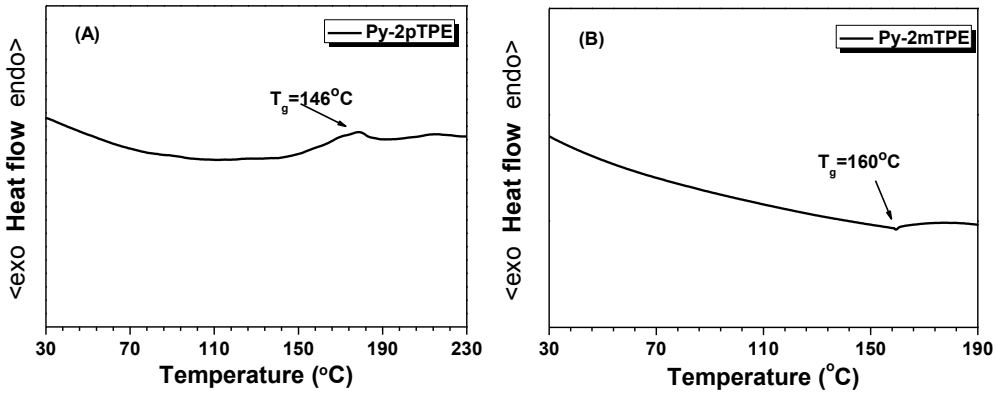


Figure S2. TGA thermograms of Py-2*p*TPE, Py-2*m*TPE, Py-2TP, Py-2TF, Py-2NTF and Py-2F recorded under N_2 at a heating rate of 10 °C/min



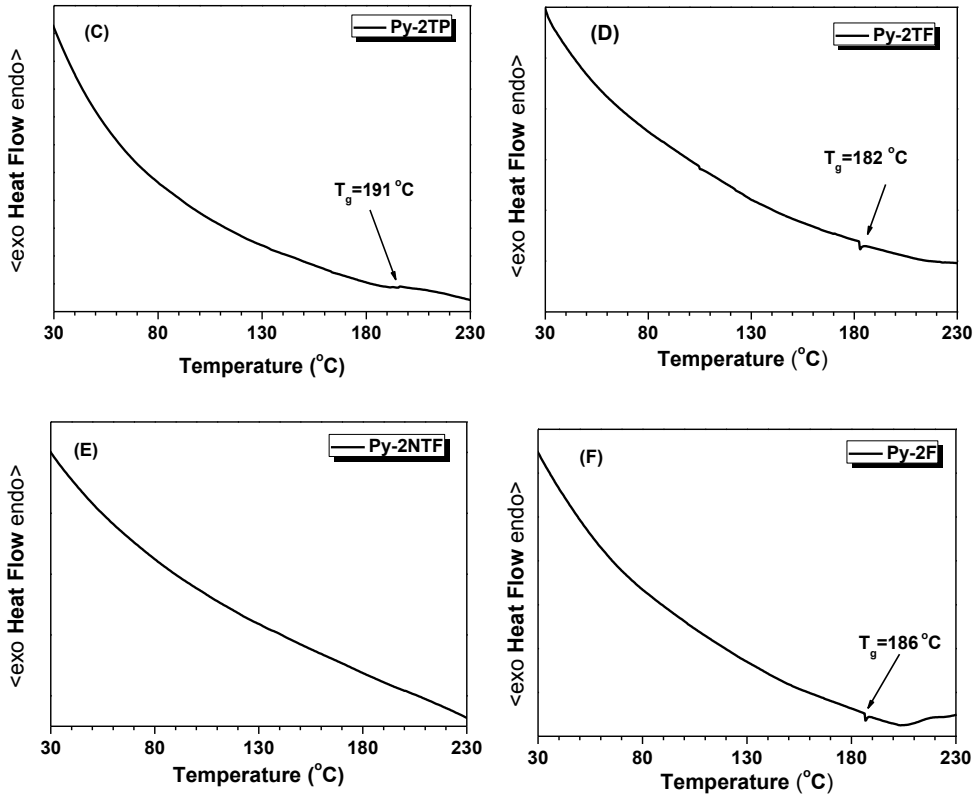


Figure S3. DSC thermograms of Py-2*p*TPE (A), Py-2*m*TPE (B), Py-2TP (C), Py-2TF (D), Py-2NTF (E) and Py-2F (F) recorded under N_2 at a heating rate of 10 °C/min.

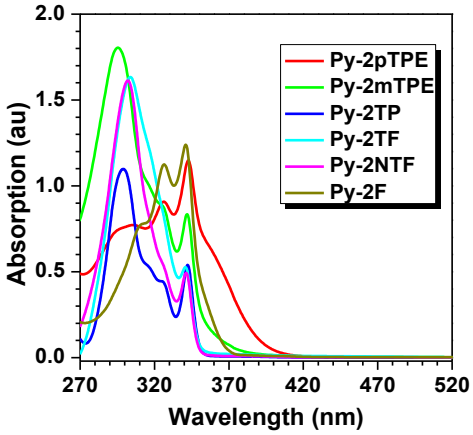


Figure S4. UV-vis spectra in THF solution. Concentration (μM): 12.0, 14.7, 14.0, 12.1, 15.8 and 11.9 for Py-2*p*TPE, Py-2*m*TPE, Py-2TP, Py-2TF, Py-2NTF and Py-2F, respectively.

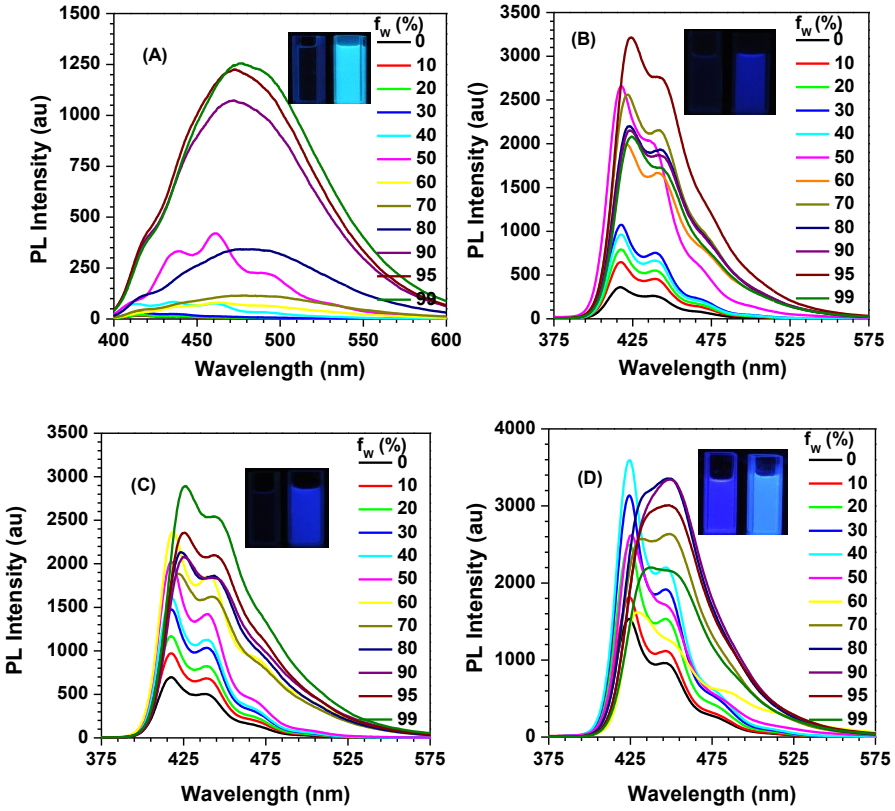


Figure S5. PL spectra in THF/H_2O mixtures with different water fractions: (A) Py-2*m*TPE, concentration (μM): 14.7 ; excitation wavelength 310 nm; (B) Py-2TF, concentration (μM): 12.1; excitation wavelength 300 nm; (C) Py-2NTF, concentration (μM): 15.8; excitation wavelength 310 nm; (D) Py-2F, concentration (μM): 11.9 ; excitation wavelength 310 nm. Inset: photos of Py-2*m*TPE, Py-2TP, Py-2NTF and Py-2F in THF/H_2O mixtures (f_w = 0 and 99%) taken under the illumination of a 365 nm UV lamp.

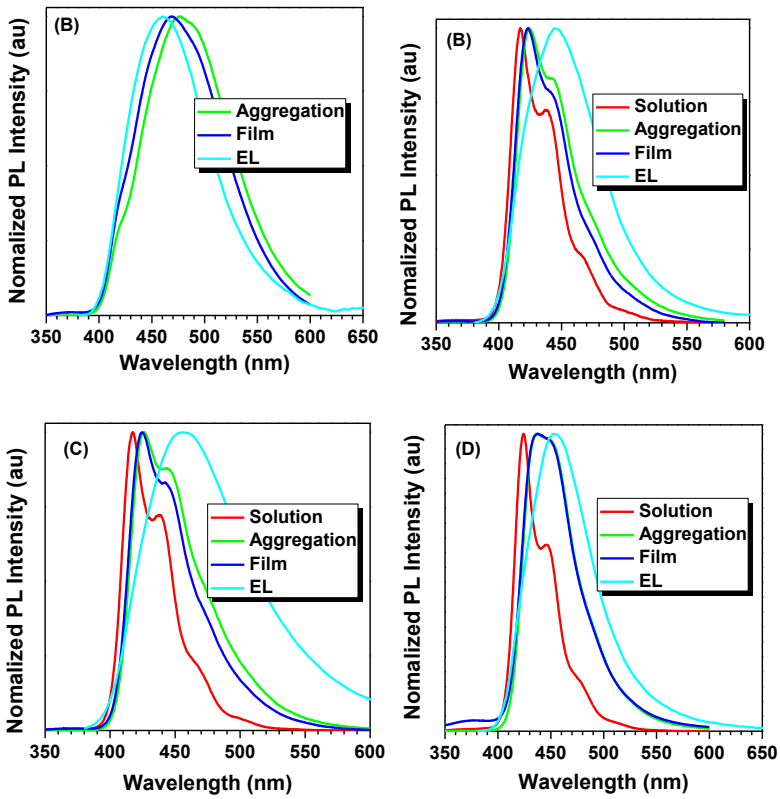


Figure S6. The solution, aggregation, film and EL spectra for (A) Py-2*m*TPE, (B) Py-2TF, (C) Py-2NTF and (D) Py-2F.

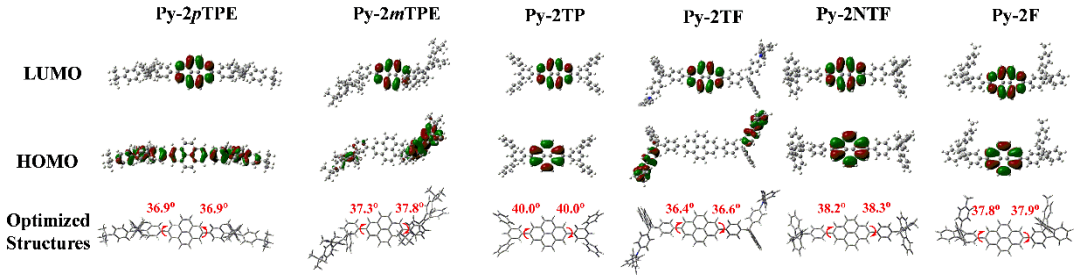


Figure S7. Calculated molecular orbital amplitude plots of LUMO, HOMO levels and optimized molecular structures for Py-2*p*TPE, Py-2*m*TPE, Py-2TP, Py-2TF, Py-2NTF and Py-2F.

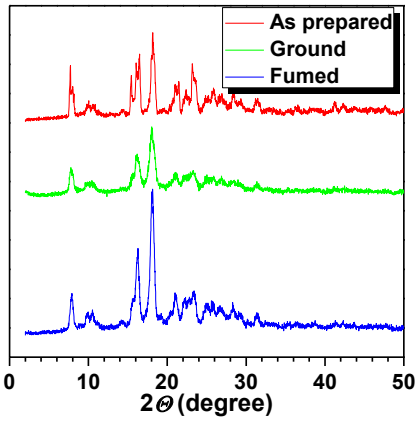


Figure S8 The XRD patterns of the as-prepared, ground and fumed TPE-*p*Br solids

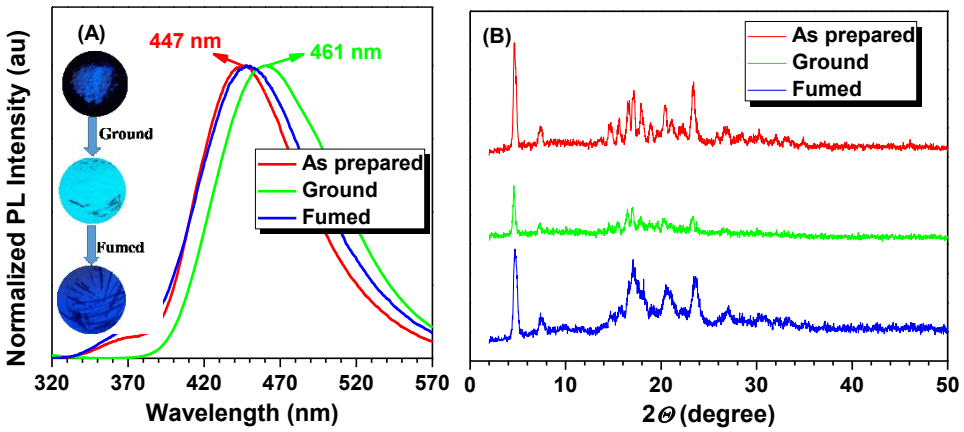


Figure S9. (A) Their emission spectra of the as-prepared, ground and fumed TPE-*m*Br solids, Insert: Their photographs taken under UV illumination (365 nm); (B) their XRD patterns.

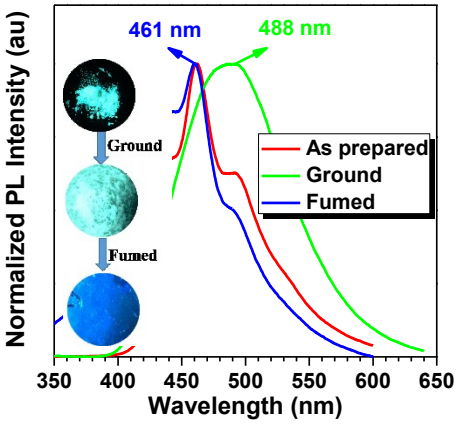


Figure S10. Their emission spectra of the as-prepared, ground and fumed Py-2*m*TPE solids. Insert: Their photographs taken under UV illumination (365 nm).

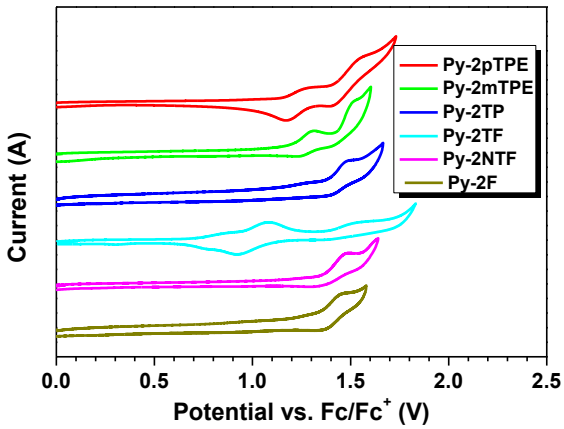


Figure S11. Cyclic Voltammograms of Py-2*p*TPE, Py-2*m*TPE, Py-2TP, Py-2TF, Py-2NTF and Py-2F in CH_2Cl_2.

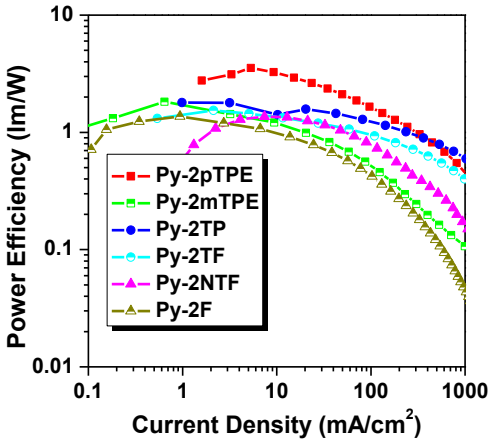


Figure S12. Changes in power efficiency with the current density. Device configuration: ITO/PEDOT:PSS/NPB (40 nm)/Py-2*p*TPE, Py-2*m*TPE, Py-2TP, Py-2TF, Py-2NTF and Py-2F (10-20 nm)/TPBI (35 nm) /Ca:Ag.

Table S1. The selected EL data for Py-2TP.

V(V)	L(cd m^{-2})	η_C(cd A^{-1})	η_C roll off (%)	η_{EQE}(%)	η_{EQE} roll off (%)
5.2	93	2.94	0	3.46	0
6.1	1210	2.83	3.7	3.34	3.5
7.1	5407	2.30	21.8	2.70	22.0
7.8	10435	1.95	33.7	2.30	33.5
8.7	18287	1.38	53.1	1.63	52.9

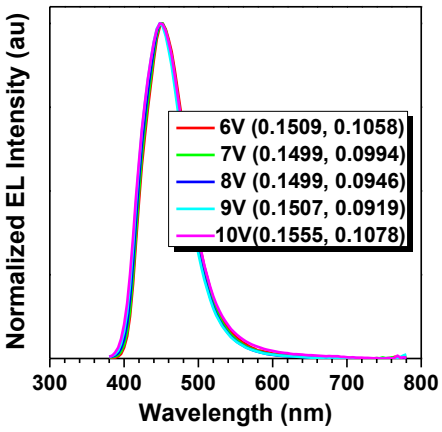


Figure S13. Normalized EL spectra of Py-2TP recorded at various driving voltage.

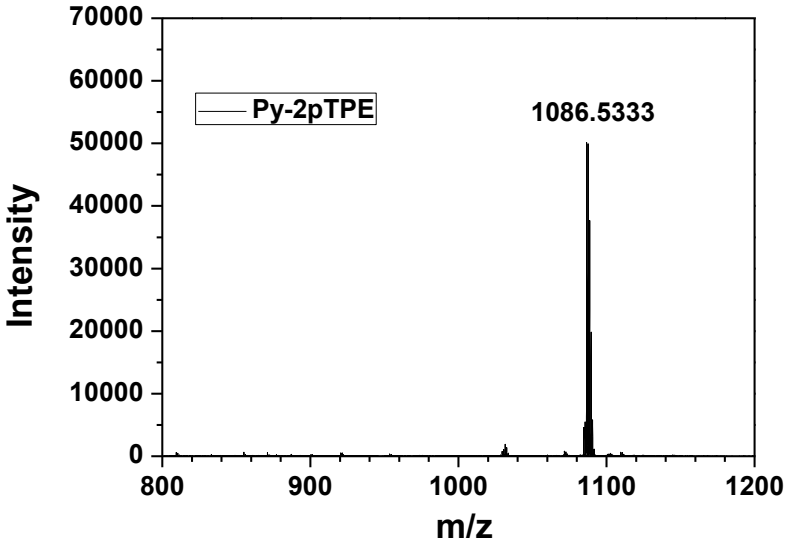


Figure S14. The mass spectrum of Py-2*p*TPE.

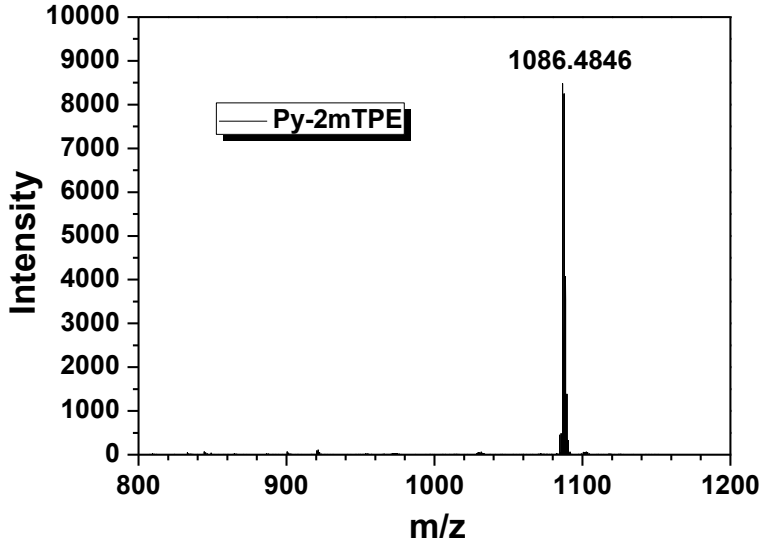


Figure S15. The mass spectrum of Py-2*m*TPE.

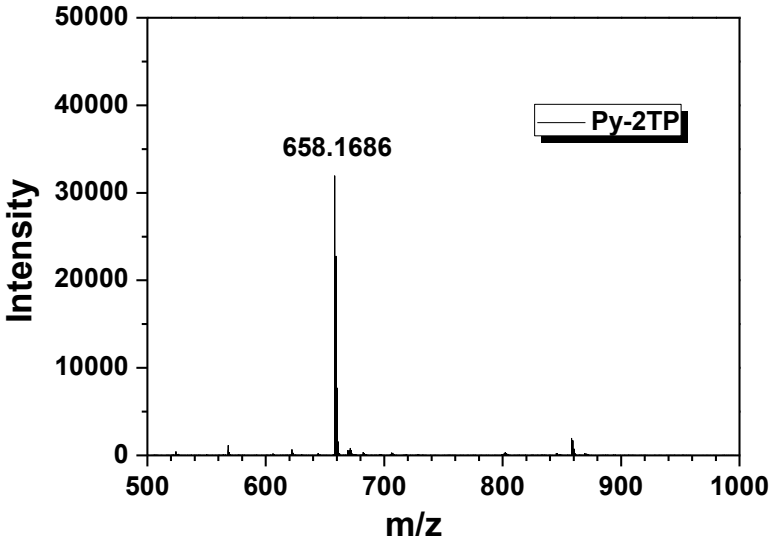


Figure S16. The mass spectrum of Py-2TP.

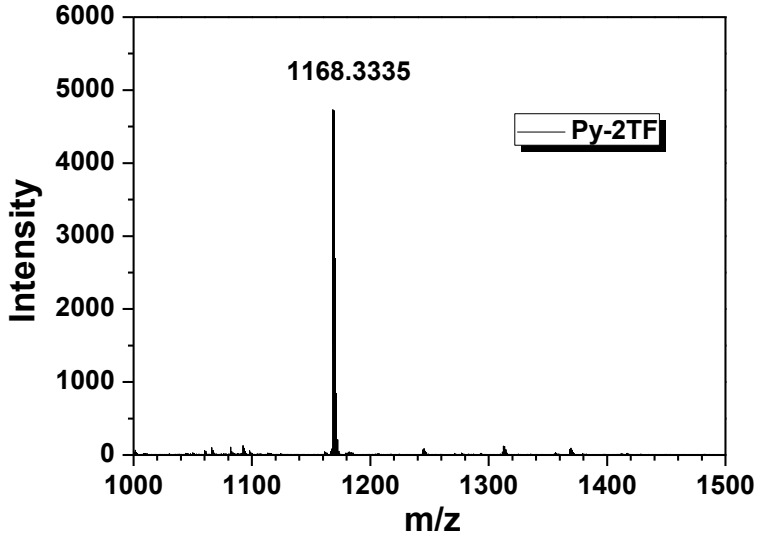


Figure S17. The mass spectrum of Py-2TF.

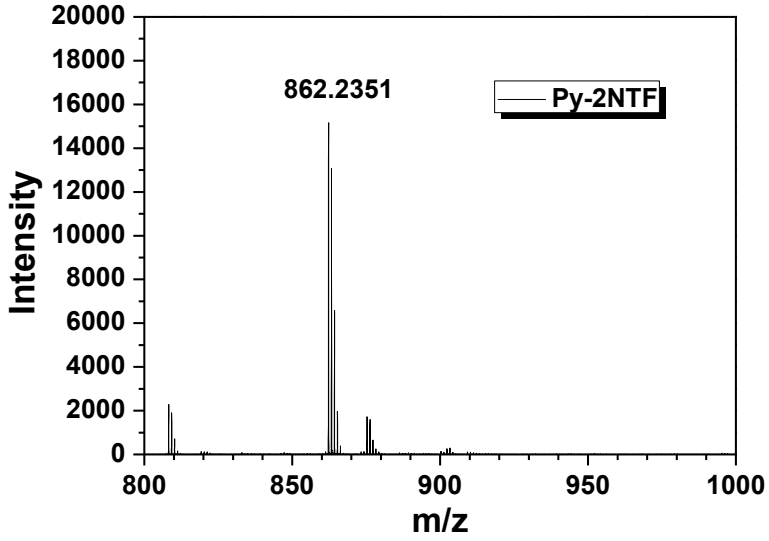


Figure S18. The mass spectrum of Py-2NTF.

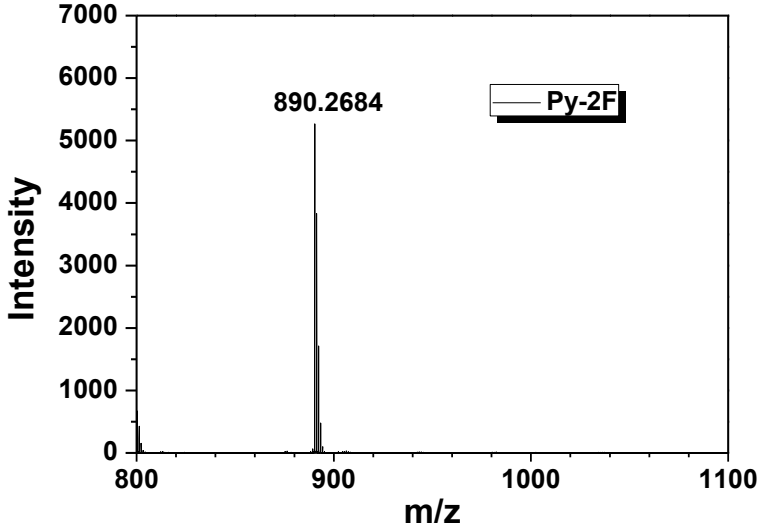


Figure S19. The mass spectrum of Py-2F.

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