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

Supporting information for

Pyrene-Based Blue Emitters with Aggregation-Induced Emission Features for High-Performance Organic Light-Emitting Diodes

Xing Feng,[‡ab] Zeng Xu[‡c] Zhen Hu,[a] Chunxuan Qi,[c] Dongxiang Luo,[a] Xingyu Zhao,[d] Zhongfei Mu,[a] Carl Redshaw,[e] Jacky W. Y. Lam,[b] Dongge Ma,*[c] Ben Zhong Tang*[bc]

[a] School of Materials and Energy, Guangdong University of Technology, Guangzhou 510006, P.R. China.

[b] Department of Chemistry, Hong Kong Branch of Chinese National Engineering Research Center for Tissue Restoration and Reconstruction Division of Life Science Institute for Advanced Study and Division of Biomedicine Engineering The Hong Kong University of Science and Technology Clear Water Bay, Kowloon, Hong Kong, P. R. China. E-mail: tangbenz@ust.hk

[c] NSFC Center for Luminescence from Molecular Aggregates, SCUT-HKUST Joint Research Laboratory, State Key Laboratory of Luminescent Materials and Devices, South China University of Technology, Guangzhou 510640, P.R. China. E-mail: msdgma@scut.edu.cn, tangbenz@ust.hk

[d] China Science and Technology Exchange Center, Beijing 100045, P. R. China.

[e] Department of Chemistry & Biochemistry, University of Hull, Cottingham Road, Hull, Yorkshire HU6 7RX, UK..

NMR spectrum

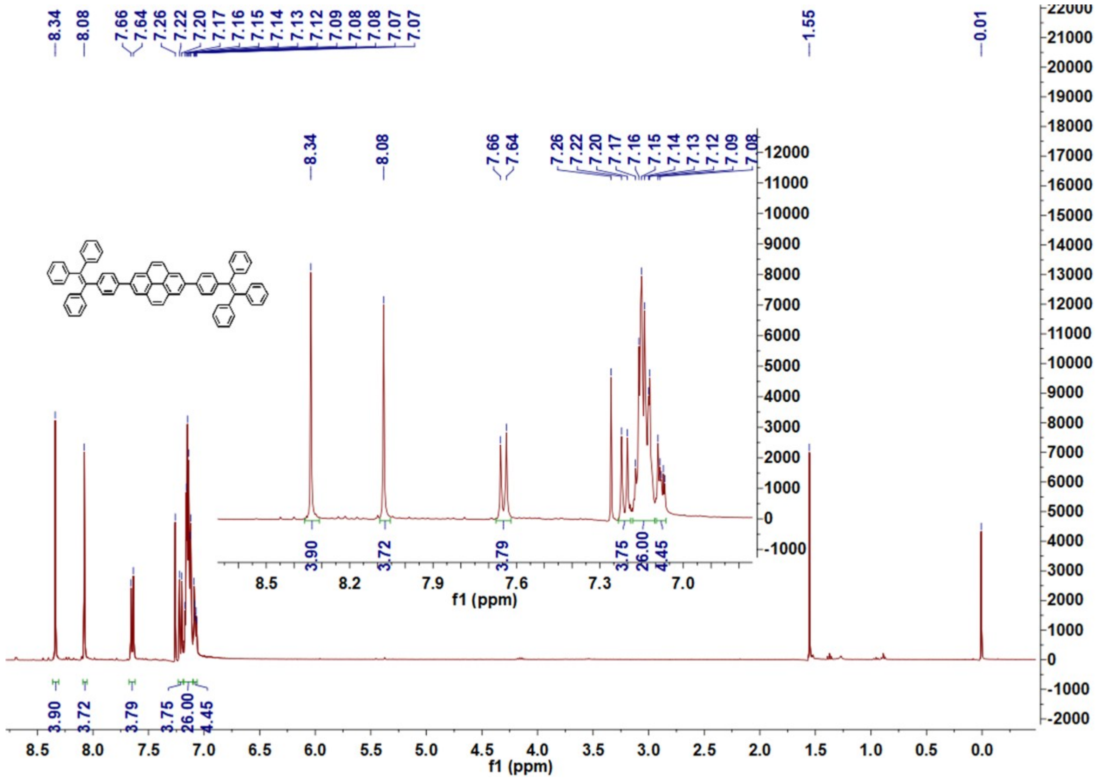

Figure S1. [1]H NMR spectrum of **Py-TPE** (400 MHz, $CDCl_3$, 293 K).

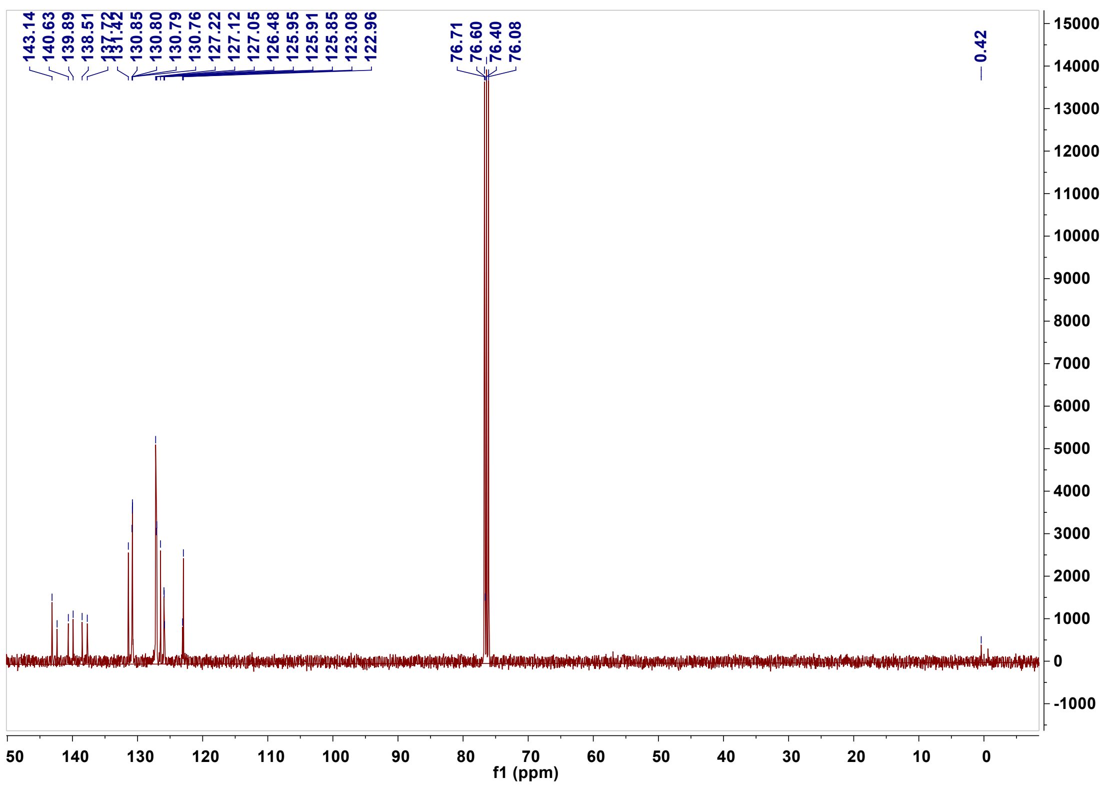

Figure S2.[13]C NMR spectrum of **Py-TPE** (100 MHz, $CDCl_3$, 293 K).

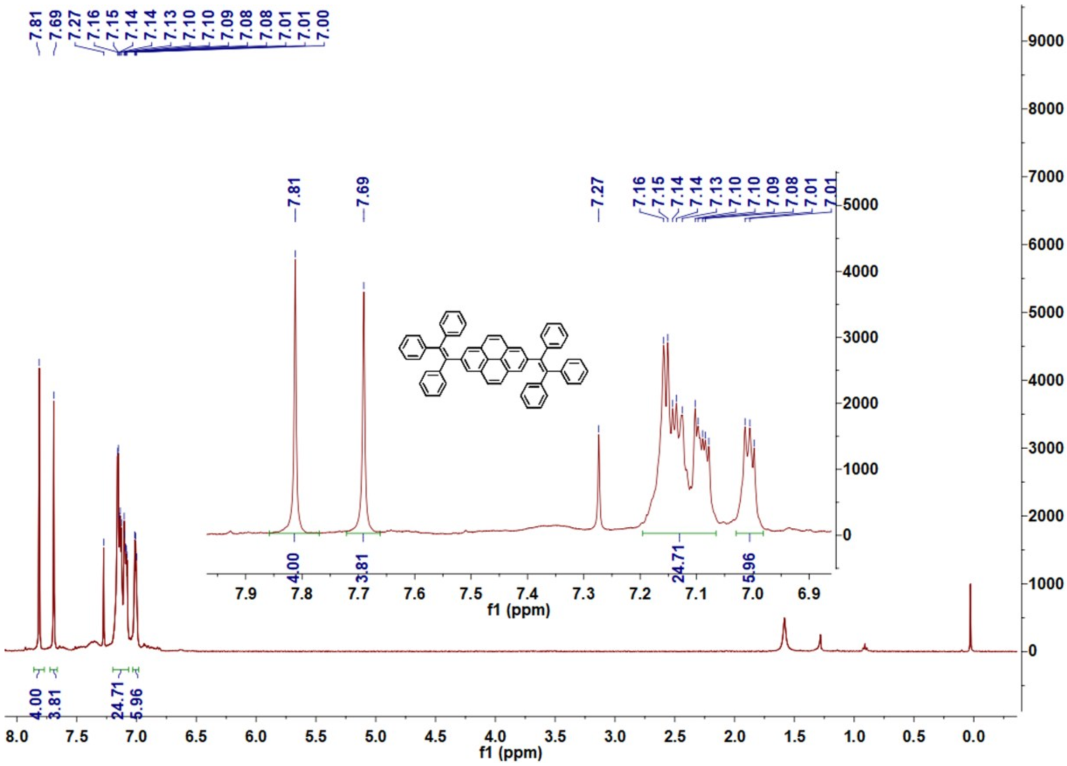

Figure S3. ^{1}H NMR spectrum of **Py-TriPE** (400 MHz, $CDCl_3$, 293 K).

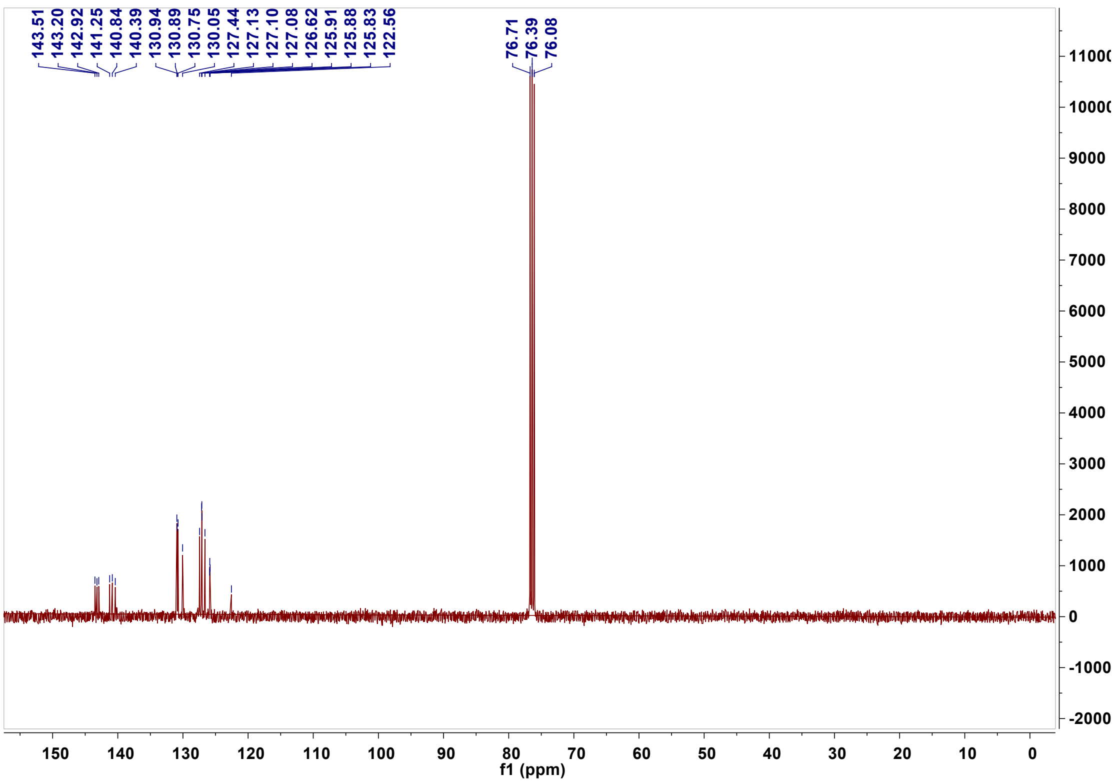

Figure S4. ^{13}C NMR spectrum of **Py-TriPE**(100 MHz, $CDCl_3$, 293 K).

Mass spectra

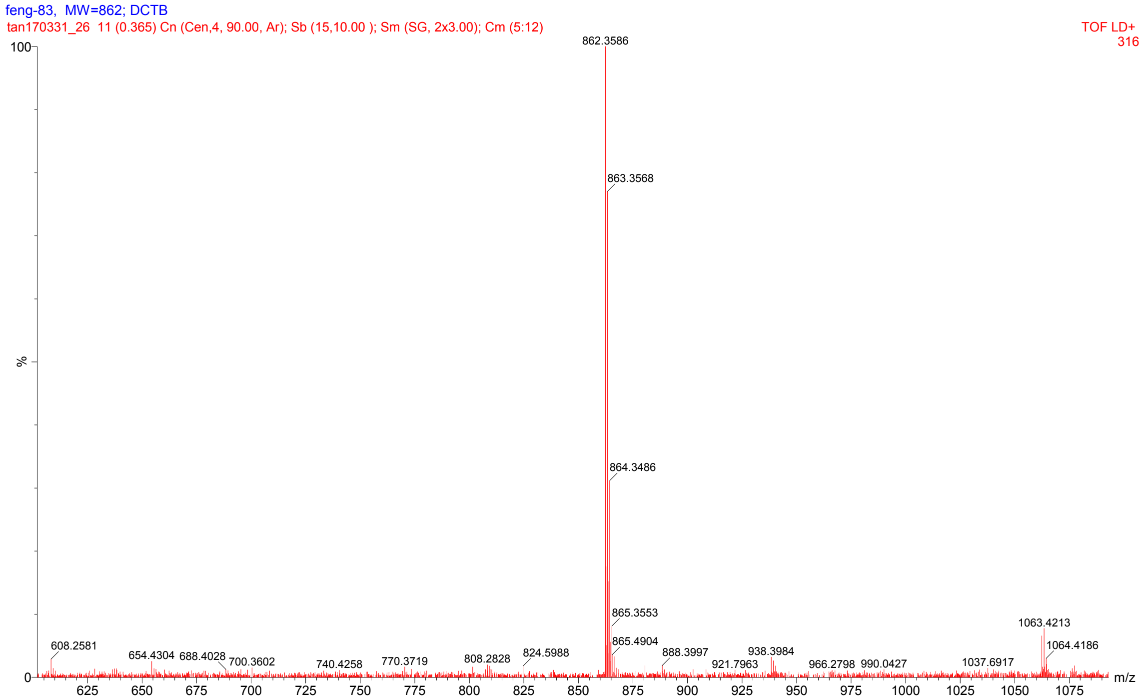

Figure S5. HRMS spectrum of **Py-TPE**.

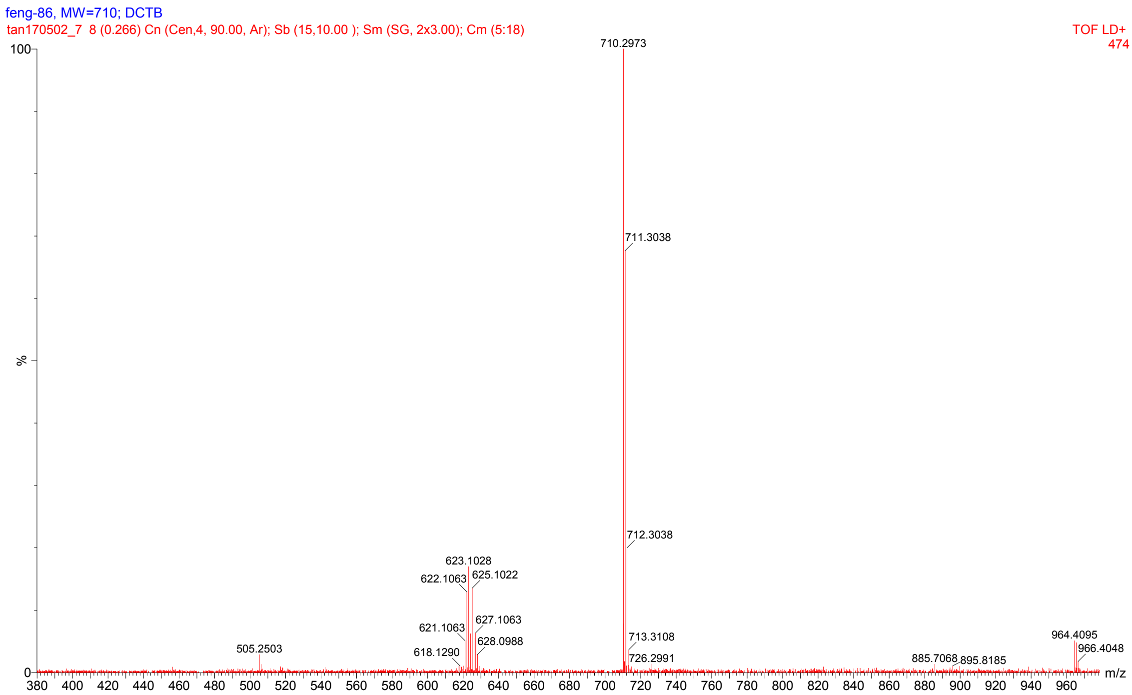

Figure S6. HRMS spectrum of **Py-TriPE**.

Photophysical Properties

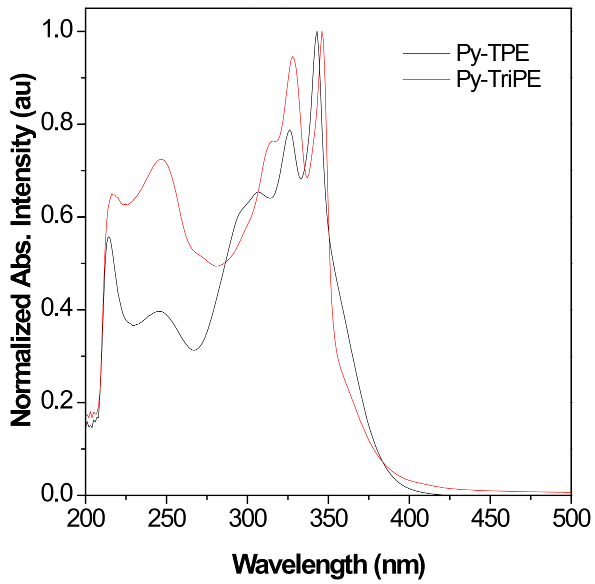

Figure S7 Normalized UV-vis absorption spectra of **Py-TPE** and **Py-TriPE** recorded in THF solutions at ~10^{-5} M at 25 °C.

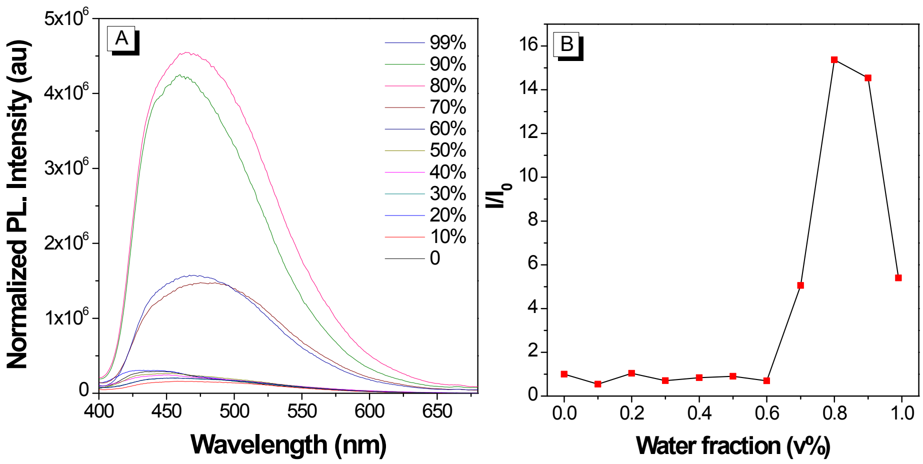

Figure S8. (A) PL spectra of **Py-TriPE** in THF/water mixture with different water fractions (f_w). (B) Plot of I/I_0 *versus* the composition of THF/water mixture of **Py-TriPE**, where I_0 is the PL intensity in pure THF solution at 465 nm.

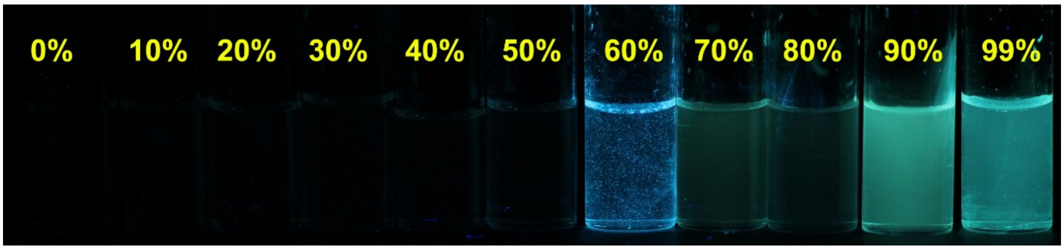

Figure S9. Fluorescent photographs of **Py-TPE**in THF/water mixtures from f_w = 0, to 99% taken under UV illumination (λ_{ex} = 365 nm).

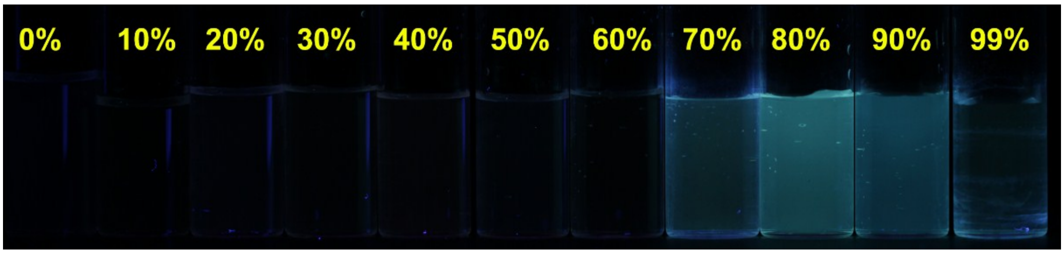

Figure S10. Fluorescent photographs of **Py-TriPE**in THF/water mixtures from f_w = 0, to 99% taken under UV illumination (λ_{ex} = 365 nm).

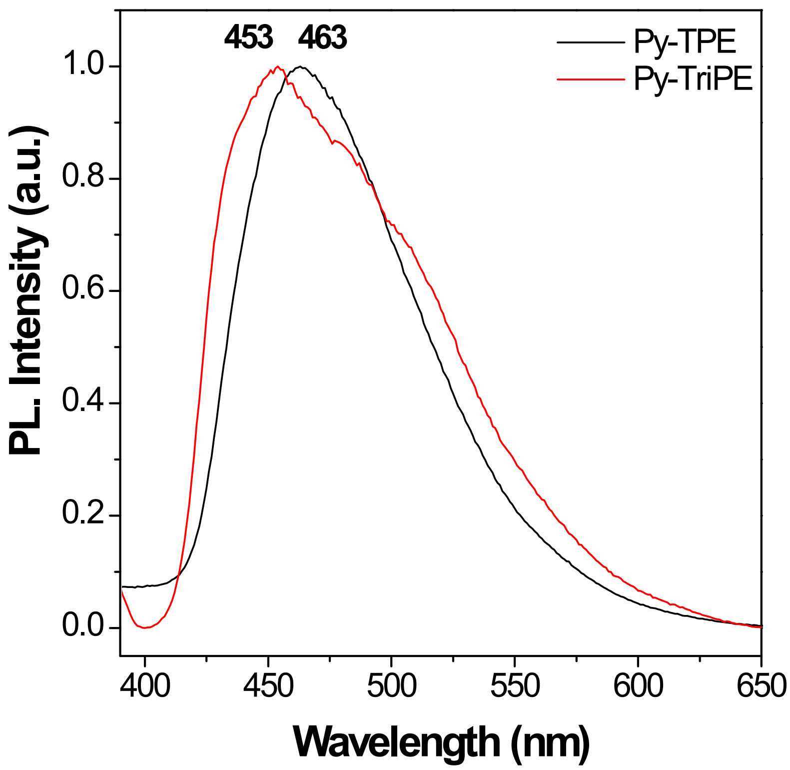

Figure S11.PL spectra of **Py-TPE** and **Py-TriPE**inthe solid state.

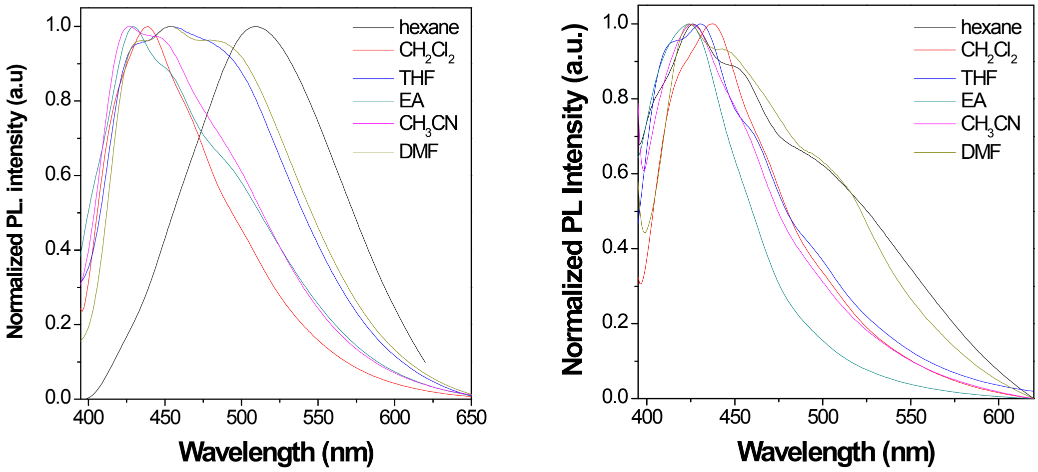

Figure S12. Fluorescence spectra of **Py-TPE**and**Py-TriPE** recorded in six different solvents (hexane, dichloromethane, tetrahydrofuran, ethyl acetate, acetonitrile and N,N-dimethylformamide) at ~10–5 M and 25 °C.

Table S1. Emission spectrum data for Py-TPE and Py-TriPE in various solvents (10μM) at room temp.[a]

Compd.	hexane	CH_2Cl_2	THF	EA	CH_3CN	DMF
Py-TPE	510 (346)	439 (368)	454 (341)	429 (364)	427 (364)	454 (346)
Py-TriPE	426, 451 (369)	438 (369)	431 (366)	424 (369)	425 (369)	425 (369)

[a] All measurements were performed under degassed conditions.The excitation wavelength data (λ_{ex}) is listed in parenthesis.

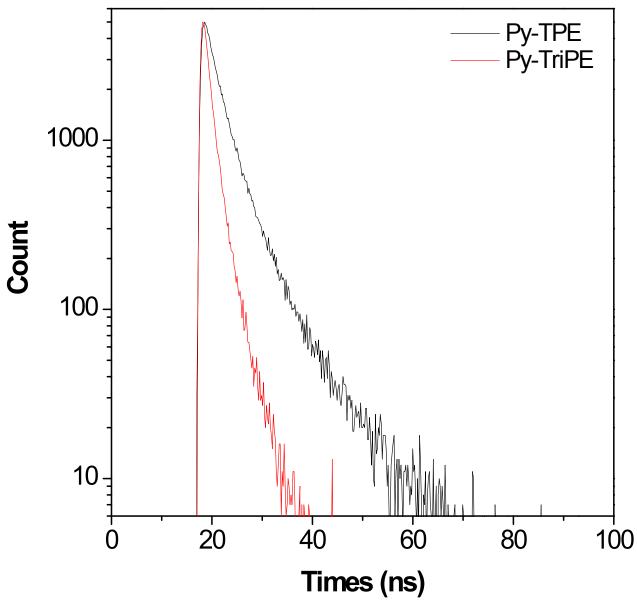

Figure S13. Fluorescence decays of **Py-TPE** and **Py-TriPE**in the solid state.

Electrochemical Analysis

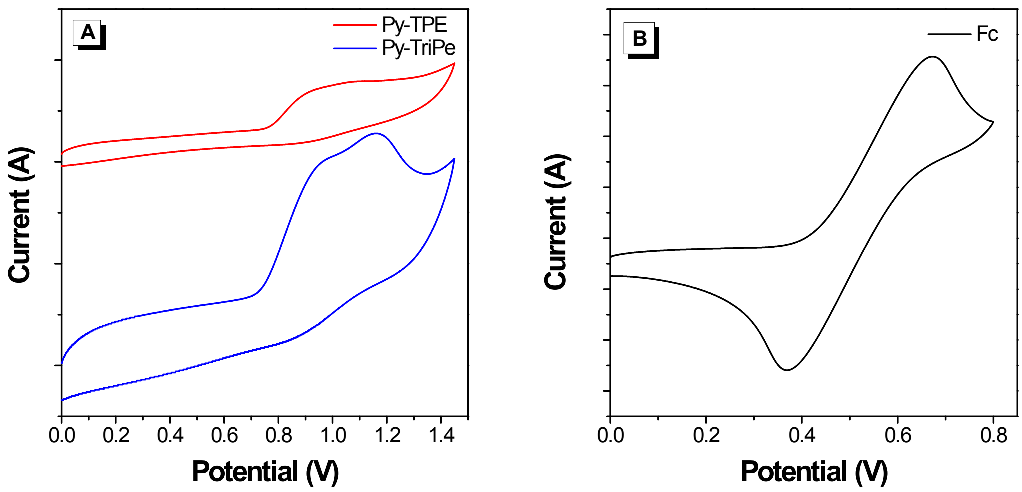

Figure 14. CV of (A) **Py-TPE** and **Py-TriPE**and (B) ferrocenerecorded from a CH_2Cl_2 solution on a platinum plate electrode at a scan rate of 100 mV•s^{-1}.

Table S2. Electrochemical properties of**Py-TPE** and **Py-TriPE**

Compound	λ_{edge} (nm)	$E_{ox}^{1/2}$ eV	$E_{ox,onset}$ eV	$E_{ox, onset}$ (Fc) (eV)	HOMO eV	LUMO eV	E_g eV
Py-TPE	384	0.83	0.77	0.43	5.14	-1.91	3.23
Py-TriPE	390	0.82	0.75	0.43	5.12	-1.94	3.18

$E_{ox}^{1/2}$ is half-wave potentials of the oxidative waves, $E_{ox,onset}$ is the onset potentials of the first oxidative wave, with potentials *versus* Fc/Fc$^+$ couple. HOMO and LUMO energy levels were calculated according to equations: HOMO = -(4.8 + $E_{ox,onset}$ - $E_{ox,onest}$(Fc)) and LUMO =HOMO+E_g.E_g: estimated from UV-vis absorption spectra in in dichloromethane at room temperature.

OLED Device fabrication and characterization

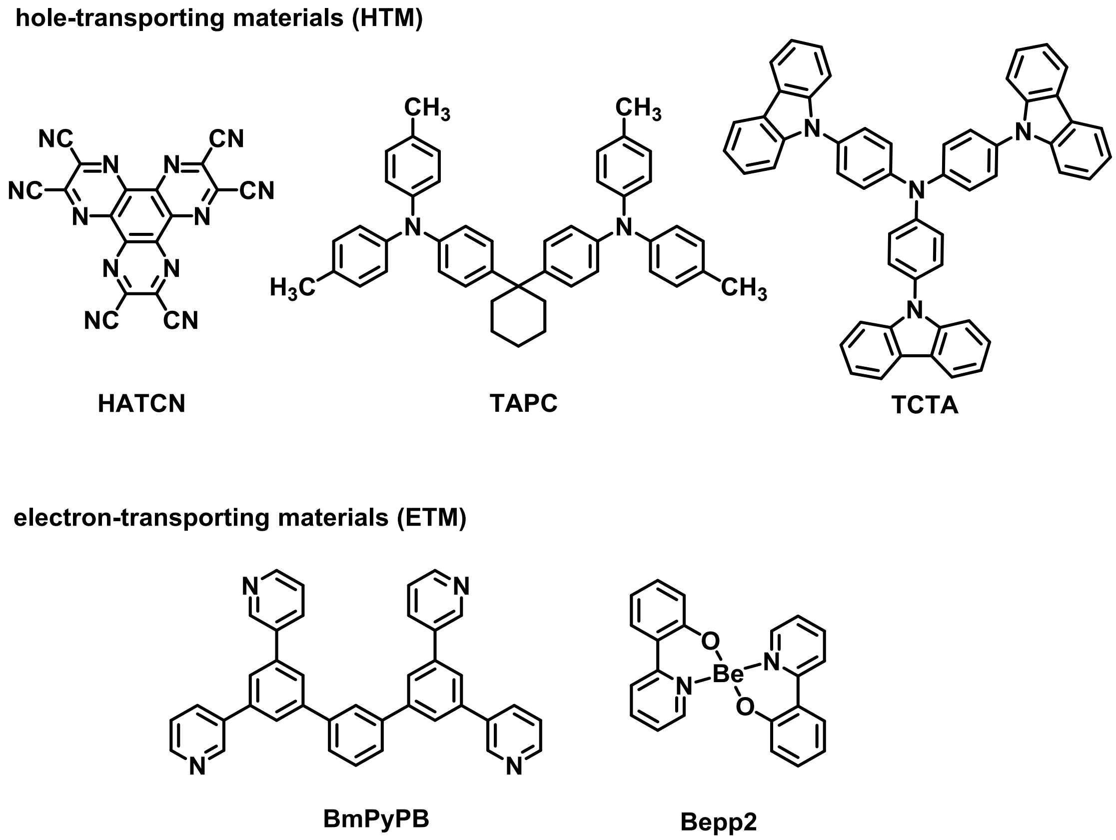

Figure S15. The molecular structures of **HTM** and **ETM**.

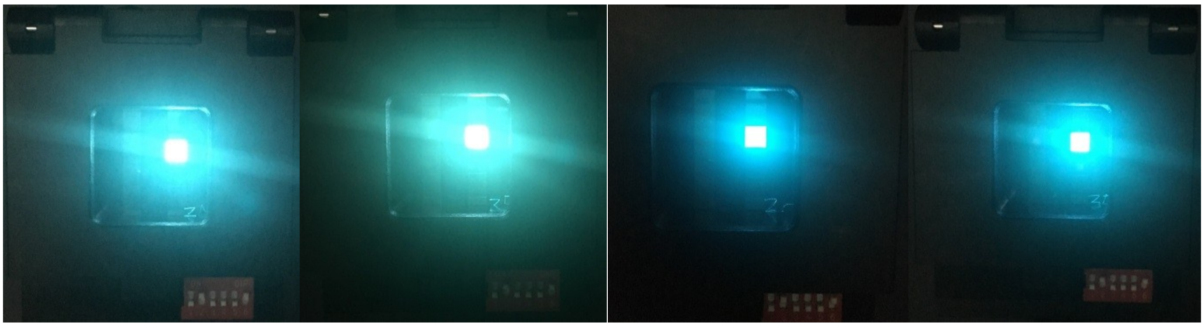

Figure S16. Photos of the OLED devices, using **Py-TPE** as host material in EL devices**1-2** and**Py-TriPE** as host material in EL devices **3-4**.

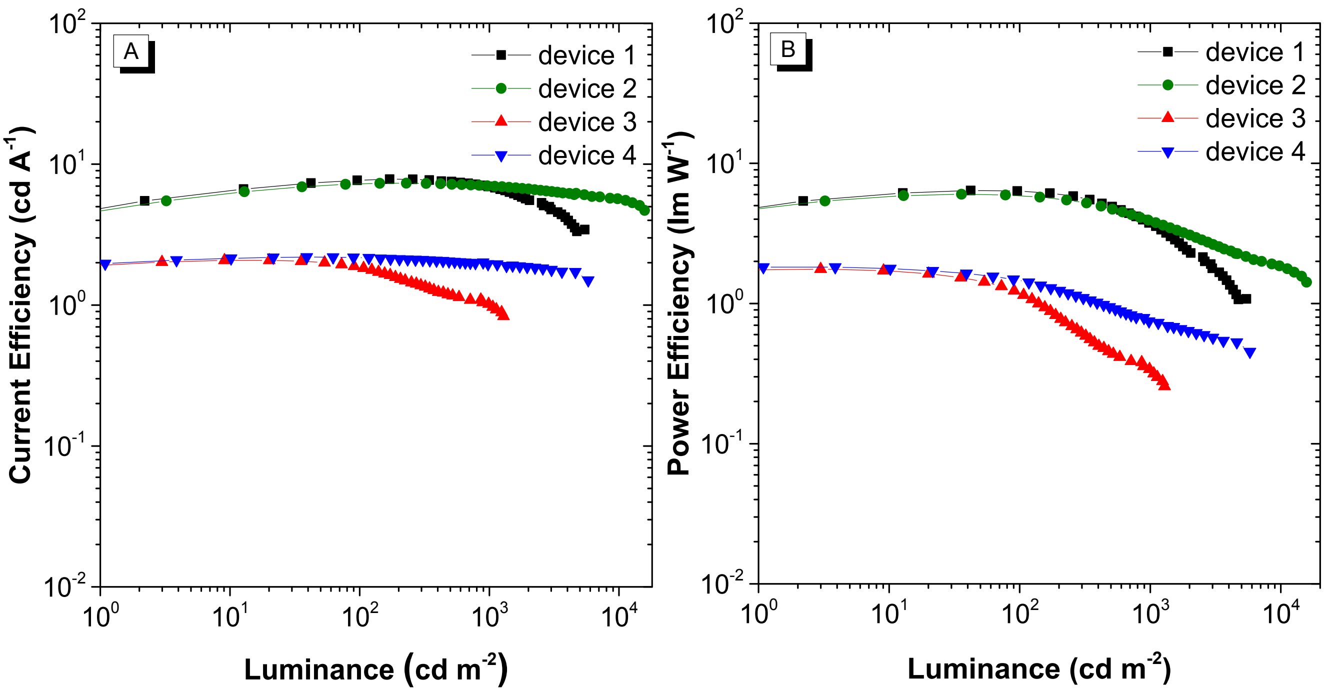

Figure S17. (A) Luminance–Current efficiencycurves and (B) Luminance–power efficiencycurves for non-doped OLED devices, using **Py-TPE** as host material in EL devices**1-2** and**Py-TriPE** as host material in EL devices **3-4**.

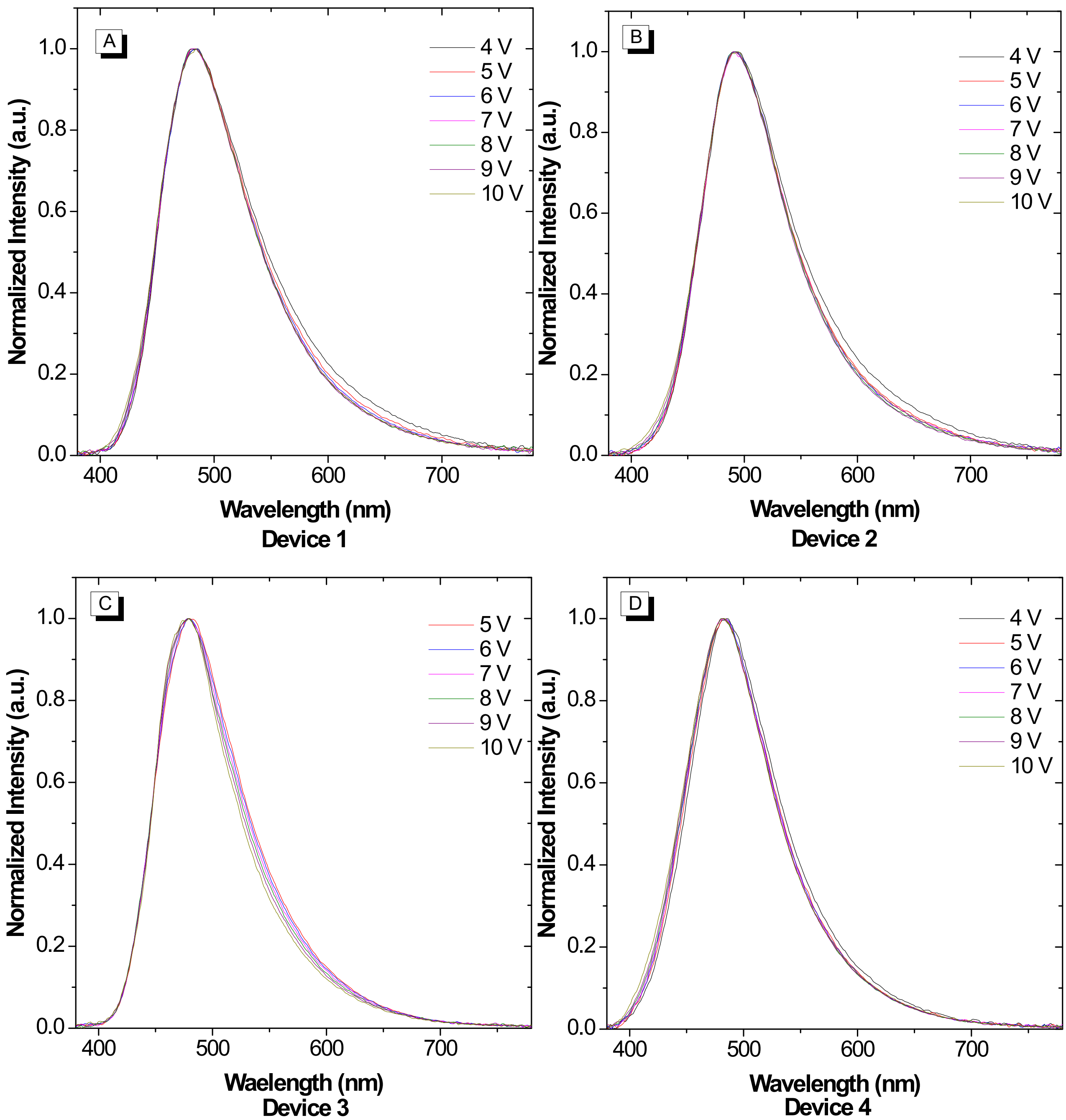

Figure S18.EL spectra of the device using **Py-TPE** and **Py-TriPE** as emittersat various voltages.

Charge Transport Properties

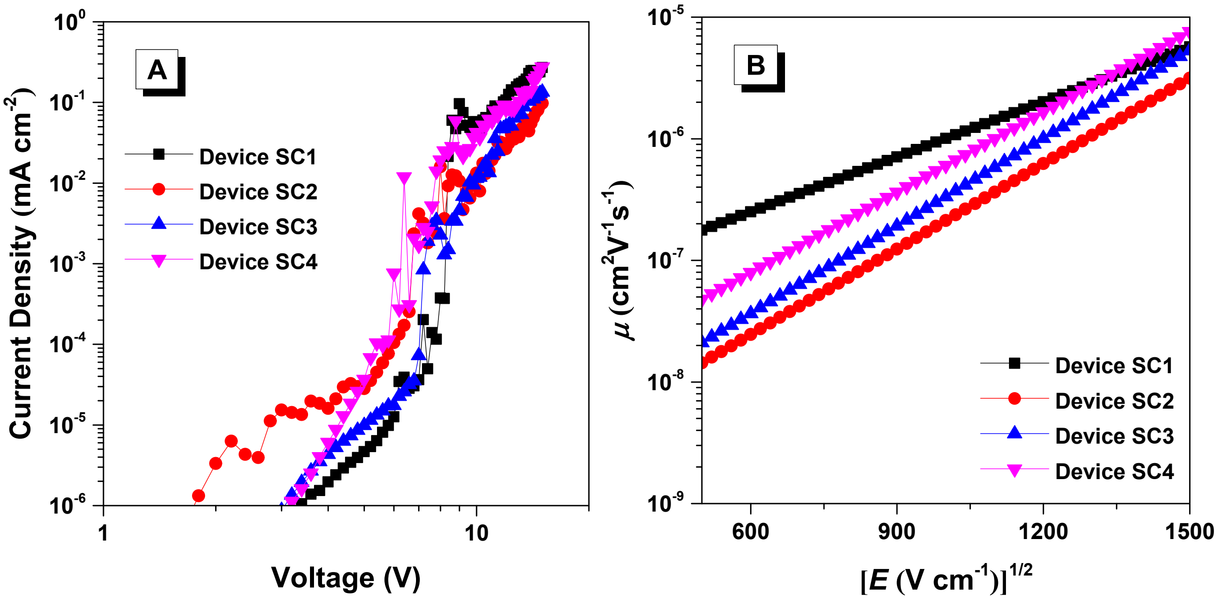

Figure S19.(A) Double logarithmic plots of current density (J) *vs* applied voltage (V) of device SC1-4. Configuration, device SC1: ITO/Py-TPE (80 nm)/TAPC (10 nm)/Al, device SC2: ITO/TmPyPB(10nm)/Py-TPE (80 nm)/LiF (1 nm)/Al, device SC3: ITO/Py-TriPE (80 nm)/TAPC (10 nm)/Al, device SC4: ITO/TmPyPB(10 nm)/Py-TriPE (80 nm)/LiF (1 nm)/Al.(B) Electric field-dependent hole and electron mobilities (μ) of Py-TPE and Py-TriPE.