Supporting Information

Novel Blue Fluorescent Emitters structured by Linking Triphenylamine and Anthracene Derivatives for Organic Light-Emitting Devices with EQE exceeding 5%

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Experimental section

Materials and methods

All the reagents and solvents used for the syntheses and measurements were purchased from commercial suppliers and were used without further purification unless otherwise noted. ^{1}H NMR and ^{13}C NMR spectra were measured with a Switzerland Bruker DR × 600. UV-vis absorption spectra were measured using Lambda Bio 40. The Photoluminescence (PL) spectra were recorded using HORIBA FluoroMax-4 spectrophotometer. The absolute quantum yields were determined through an absolute method employing an integrating sphere. Thermogravimetric analysis (TGA) curves were undertaken using a Netzsch TG 209F3 under a dry nitrogen atmosphere heating from room temperature up to 800 °C at a rate of 10 °C/min. Differential scanning calorimetry (DSC) was performed on a DSC Q2000 at a heating rate of 10 °C/min from 40 to 300 °C, then cooling down to room temperature rapidly, and heating up to 300 °C at a heating rate of 10 °C/min again; the melting temperature (T_m) was obtained from the first heating scan and the glass transition temperature (T_g) was determined from the second heating scan. Cyclic voltammetry (CV) was carried out in a solution of tetrabutylammonium perchlorate (0.1 M) in acetonitrile at a scan rate of 100 mV/s at room temperature using a conventional three electrode cell, which consisted of the working electrode platinum plate, the counter electrode platinum wire, and the reference electrode calomel electrode.

DFT calculation

Theoretical calculations were performed using the Gaussian 03 package. Geometry optimization was performed by density functional theory (DFT) in B3LYP/6-31G(d) basis sets.

OLED fabrication and characterization

The OLEDs with area of 3 × 3 cm^2 were fabricated by vacuum deposition onto the indium tin oxide (ITO) glass substrates. The substrates were cleaned, in the following order, with deionized water, acetone, and ethanol. The electroluminescence (EL) spectra and CIE coordinates were measured by a PR-655 spectrophotometer. The current density-voltage-luminance (*J-V-L*) characteristics of the OLEDs were recorded using Keithley 2400 Source Meter and ST-900M Spot Brightness Meter.

Synthesis of **TPA-AN-NA** and **TPA-AN-TFP**

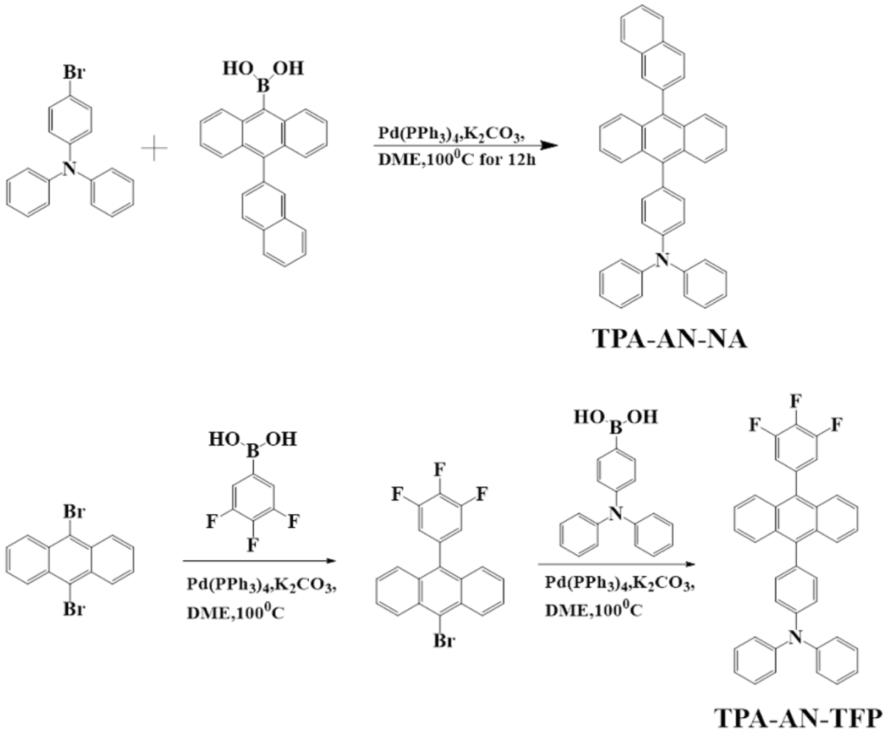
Synthesis of 4-(10-(naphthalen-2-yl)anthracen-9-yl)-N,N-diphenylaniline (**TPA-AN-NA**)

A mixture of 4-bromo-N,N-diphenylaniline (0.973 g, 3 mmol), 9,9-diphenyl-9,10-(10-(naphthalen-2-yl)anthracen-9-yl)boronic acid (1.15 g, 3.3 mmol), $Pd(PPh_3)_4$ (0.173 g, 0.15 mmol) and K_2CO_3 (2.0 M aqueous solution, 10.0 mL) were dissolved in 30 mL of 1,2-dimethoxyethane, and then heated to reflux for 12 h. After cooling to room temperature, the solution was extracted with dichloromethane. The organic material was dried by anhydrous $MgSO_4$ and concentrated. Then crude product was purified by silica gel chromatography. The desired product was obtained as yellow powder (1 g, yield: 63%). ^1H NMR (600 MHz, DMSO, δ): 8.19 (d, *J* = 8.7 Hz, 1H), 8.12 (d, *J* = 7.8 Hz, 1H), 8.05-8.01 (m, 2H), 7.77 (dd, *J* = 5.4, 4.3 Hz, 2H), 7.67-7.59 (m, 5H), 7.48 (td, *J* = 8.8, 6.4, 1.3 Hz, 2H), 7.43-7.38 (m, 8H), 7.25-7.22

(m, 6H), 7.13 (td, J = 7.4, 1.1 Hz, 2H). ^{13}C NMR (151 MHz, CDCl$_3$, δ): 146.01, 145.38, 135.32, 134.88, 131.62, 130.89, 130.32, 128.36, 127.76, 127.56, 126.26, 126.08, 125.24, 124.57, 124.36, 123.20, 122.88, 121.40.

Synthesis of N, N-diphenyl-4-(10-(3,4,5-trifluorophenyl)anthracen-9-yl)aniline (**TPA-AN-TFP**)

9-bromo-10-(3,4,5-trifluorophenyl)anthracene (**1**) and N,N-diphenyl-4-(10-(3,4,5-trifluorophenyl) anthracen-9-yl)anilin (**TPA-AN-TFP**) were prepared with a similar procedure as that of **TPA-AN-NA**. The desired product was obtained as yellow-green powder (0.6 g, yield: 60%). ^{1}H NMR (600 MHz, CDCl$_3$, δ): 7.88-7.84 (m, 2H), 7.64-7.59 (m, 2H), 7.42-7.39 (m, 4H), 7.34 (t, J = 7.9 Hz, 4H), 7.30-7.25 (m, 8H), 7.10 (dt, J = 18.2, 7.1 Hz, 4H). ^{13}C NMR (151 MHz, CDCl$_3$, δ):150.68, 150.31, 141.23, 136.01, 134.93, 132.94, 132.59, 132.33, 130.28, 128.78, 128.06, 127.71, 126.14, 125.87, 118.58.



Scheme S1. The molecular structures of **TPA-AN-NA** and **TPA-AN-TFP**.

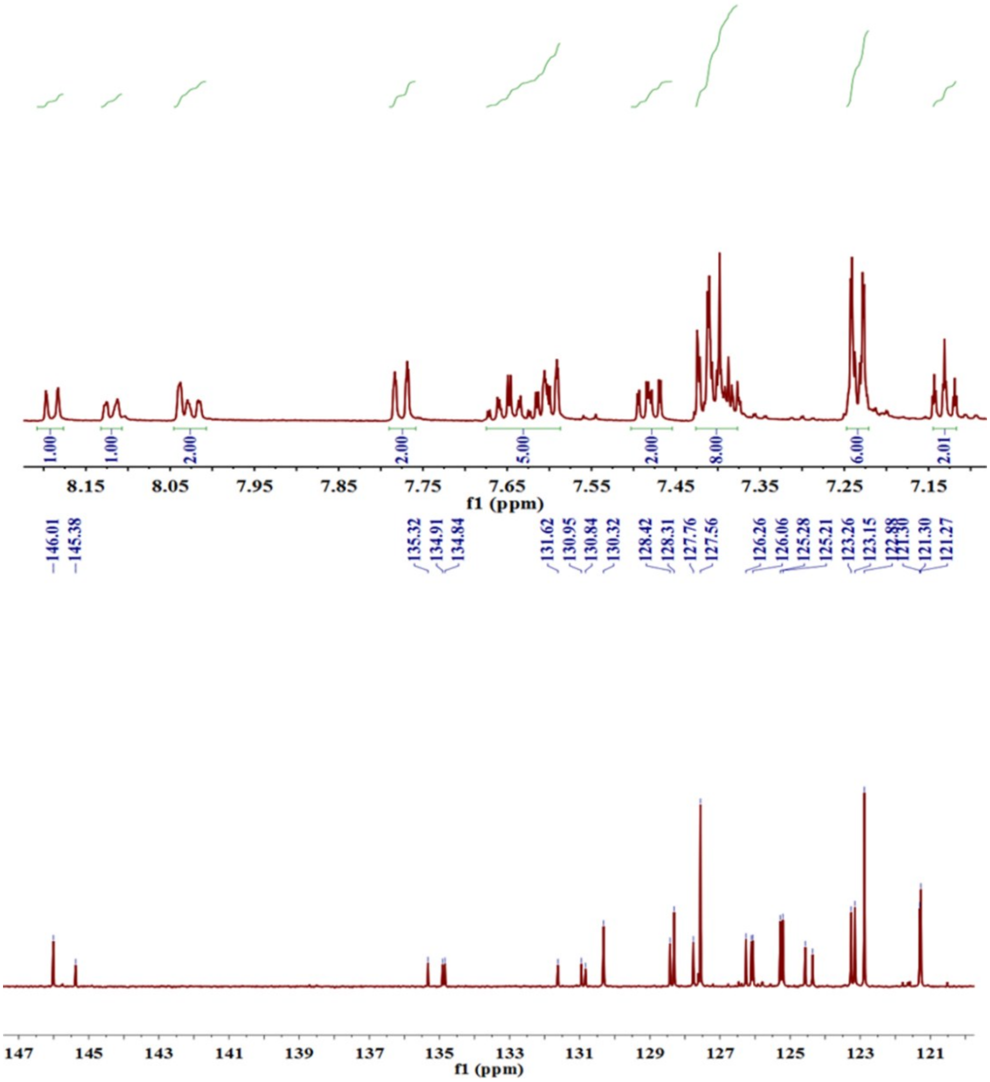


Figure S1. ^{1}H NMR and ^{13}C NMR spectra of **TPA-AN-NA** in DMSO and $CDCl_3$ respectively.

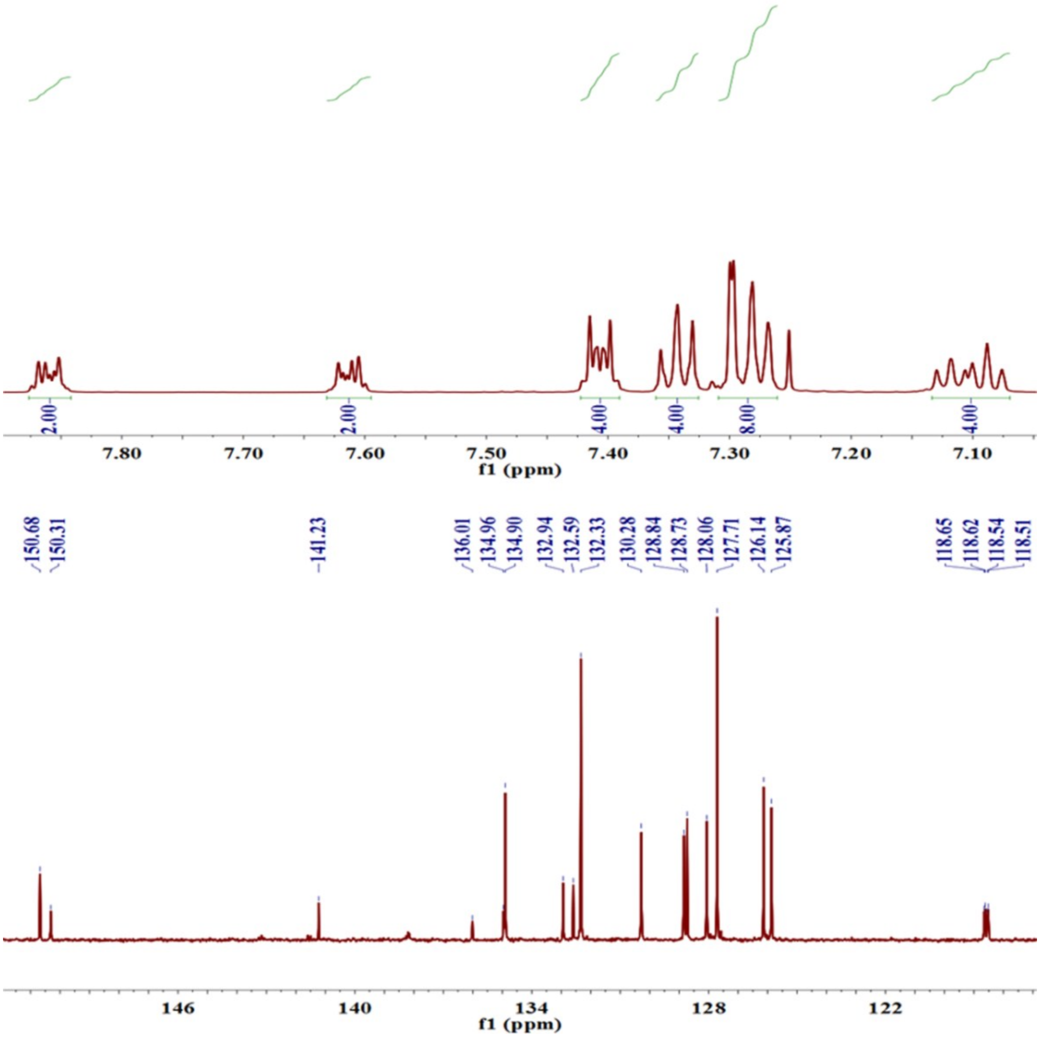


Figure S2. ^{1}H NMR and ^{13}C NMR spectra of **TPA-AN-TFP** in $CDCl_3$.

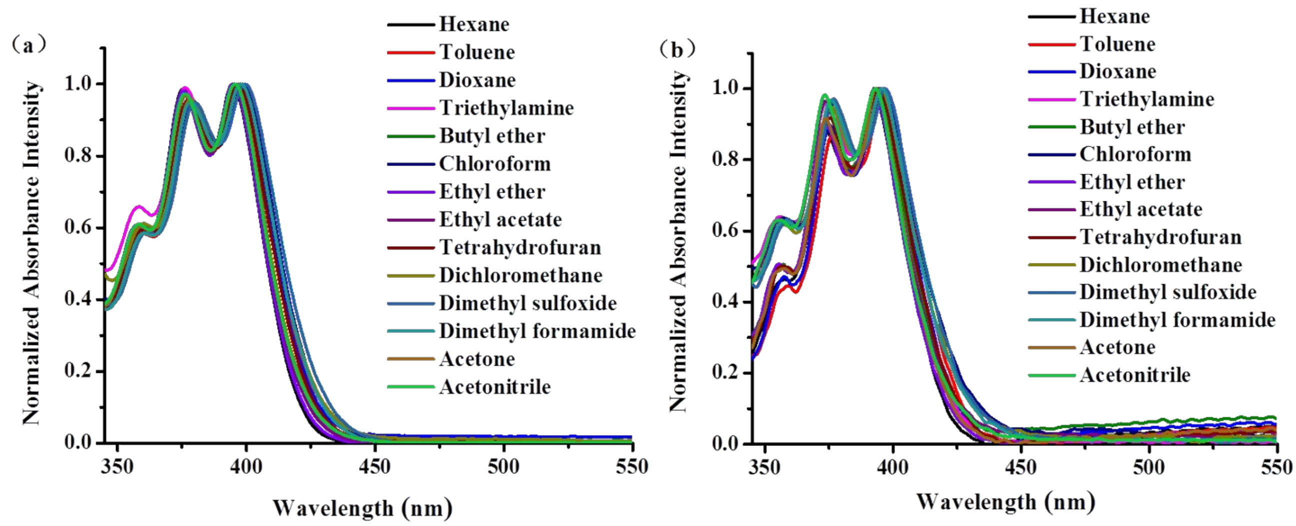


Figure S3. The UV-vis absorption spectra of **TPA-AN-NA** (a) and **TPA-AN-TFP** (b) in different solvents.

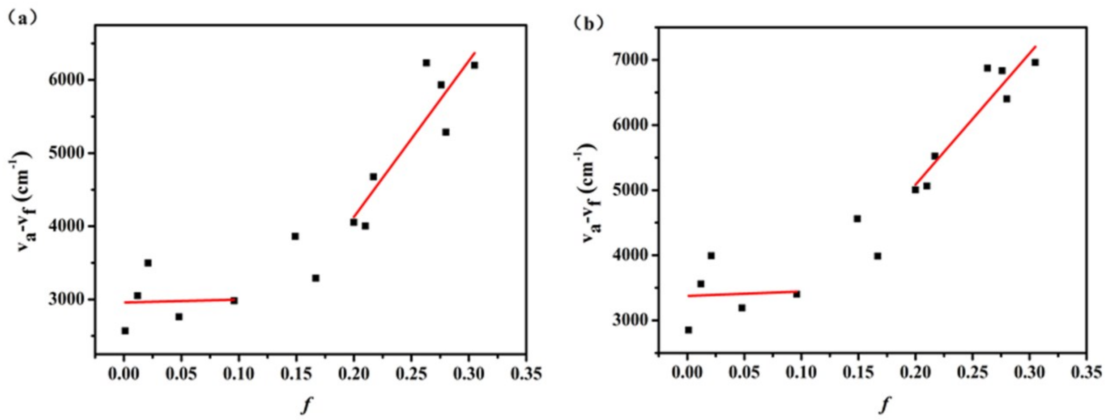


Figure S4. Fitted correlation of the Stokes Shift as a function of solvent polarity for **TPA-AN-NA** (a) and **TPA-AN-TFP** (b).

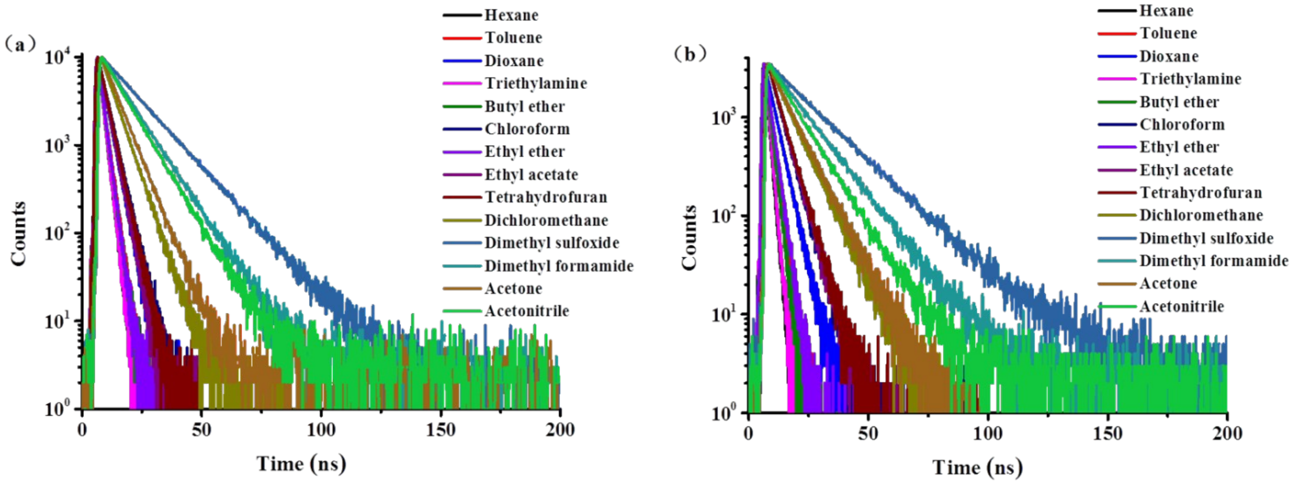


Figure S5. The transient decay spectra of **TPA-AN-NA** (a) and **TPA-AN-TFP** (b) in different solutions.

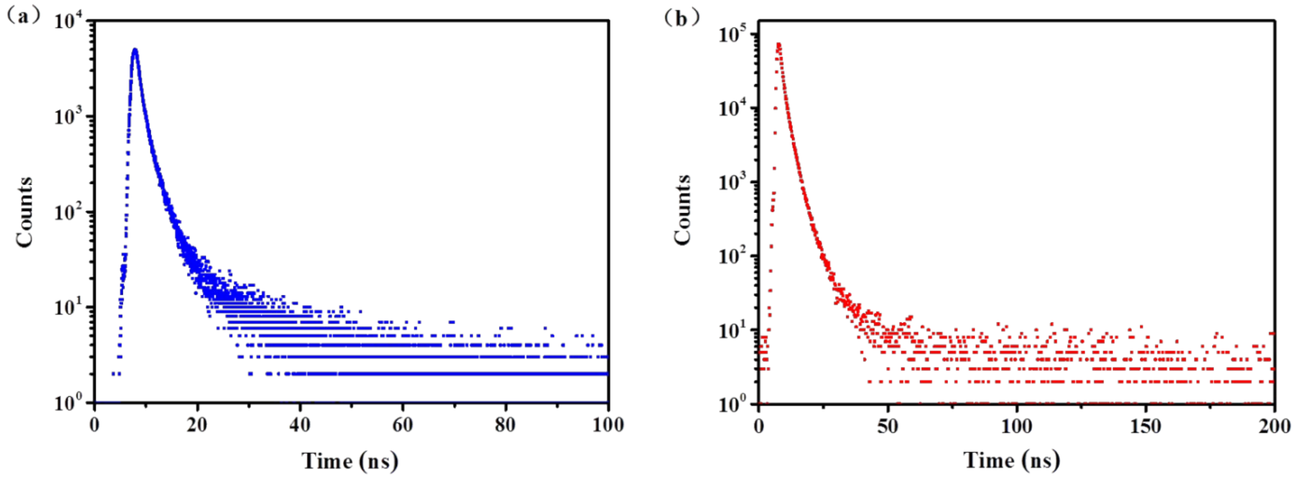


Figure S6. Transient decay spectra of **TPA-AN-NA** (a) and **TPA-AN-TFP** (b) in thin films.

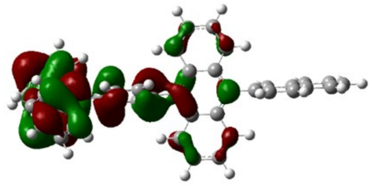
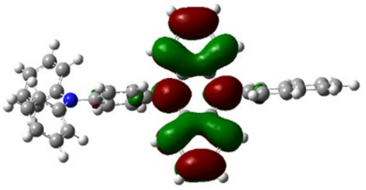
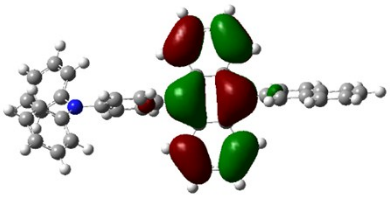
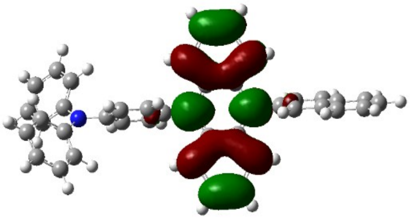
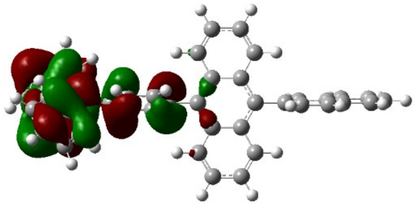
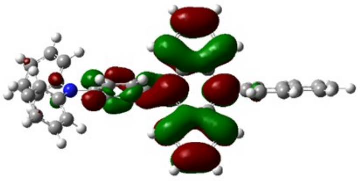
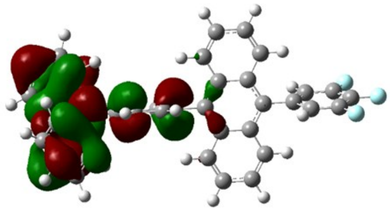
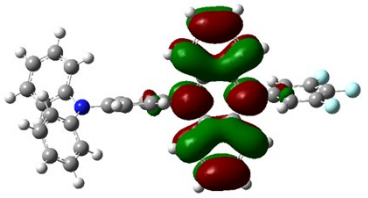
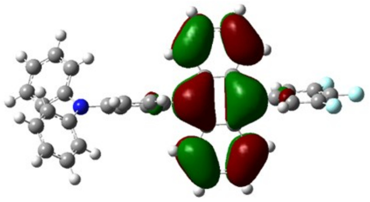
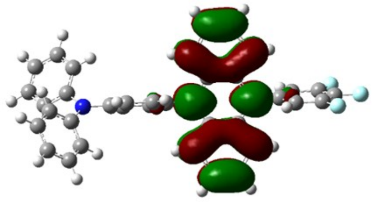
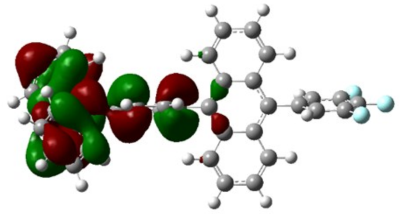
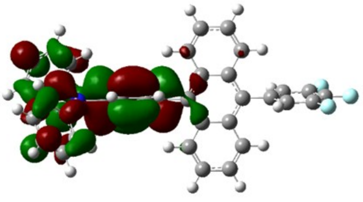
Molecule	State	Hole（HONTO）	Particle(LUNTO)
CHN	S_1		
	T_1		
	T_3		
CHNF	S_1		
	T_1		
	T_3		

Fig. S7 Natural transition orbitals of **TPA-AN-NA** and **TPA-AN-TFP**

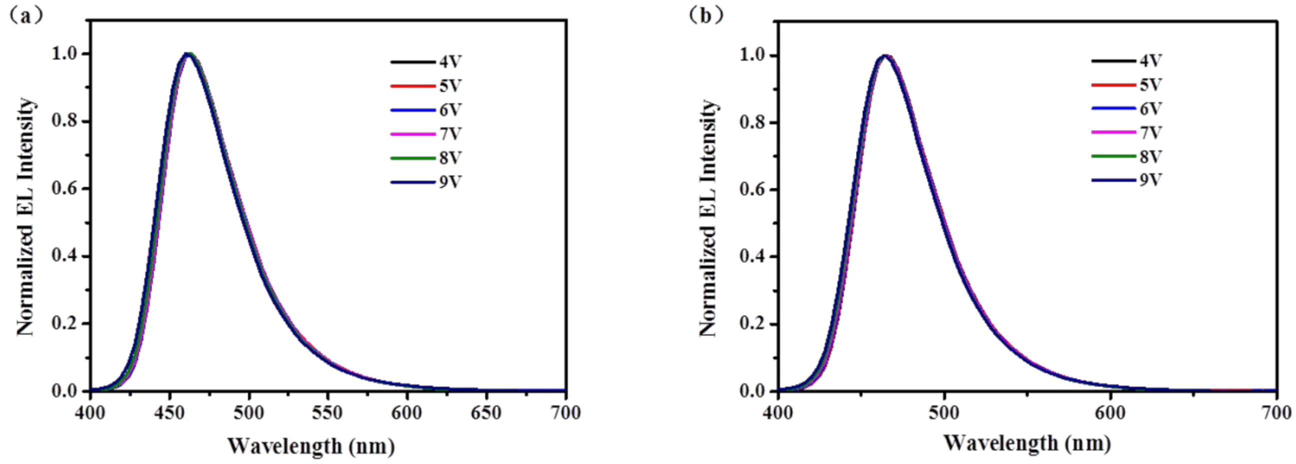


Figure S8. EL spectra of non-doped (a) and doped (b) devices based on **TPA-AN-NA** at different voltages.

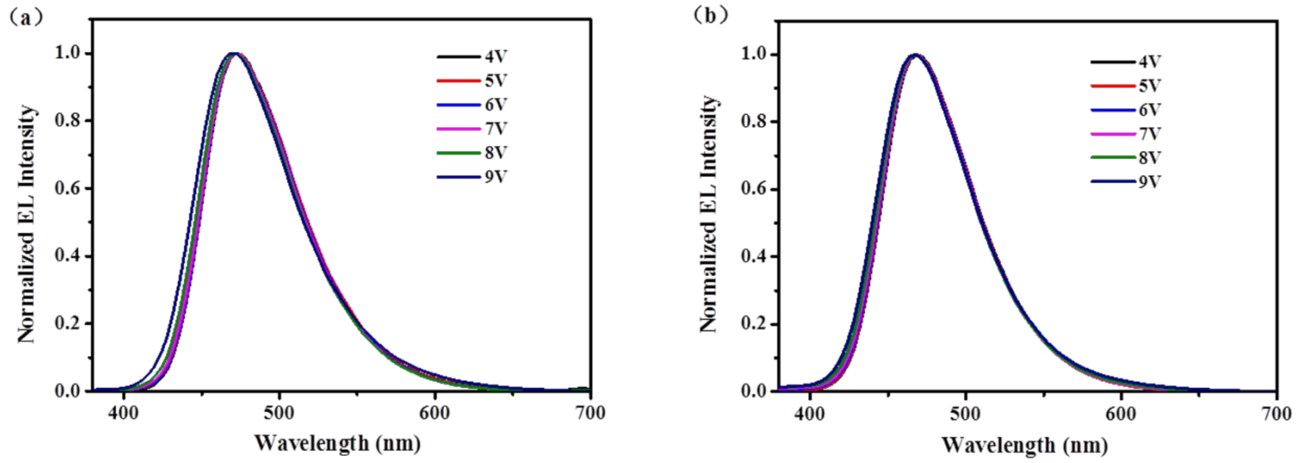


Figure S9. EL spectra of non-doped (a) and doped (b) devices based on **TPA-AN-TFP** at different voltages.

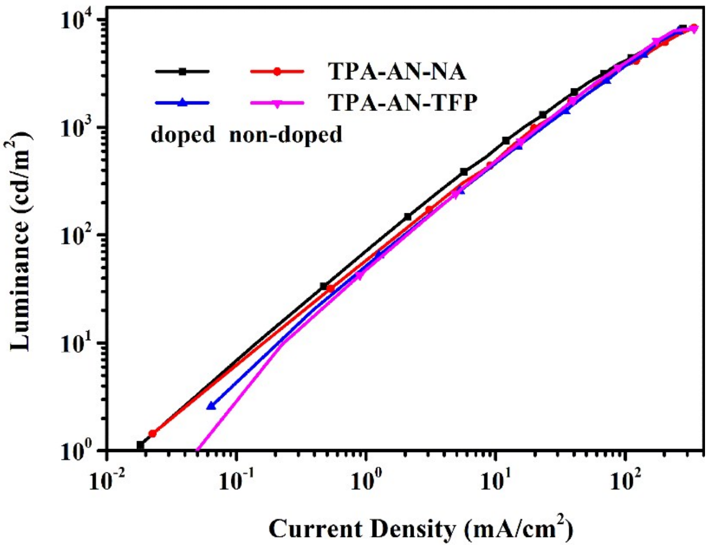


Figure S10. The current density and luminance curves of all devices.

Table S1. The fluorescence lifetime of **TPA-AN-NA** in different solvents and film.

Solvent	τ **[ns]**	**Solvent**	τ **[ns]**	**Solvent**	τ **[ns]**
Hexane Toluene Dioxane Triethylamine Butyl ether	1.44	Chloroform	4.80	Dimethyl sulfoxide	18.6
	2.17	Ethyl ether	2.50	Dimethyl formamide	13.6
	3.88	Ethyl acetate	4.97	Acetone	8.77
	1.62	Tetrahydrofuran	5.20	Acetonitrile	11.0
	2.08	Dichloromethane	8.15	Film	2.12

Table S2. The fluorescence lifetime of and **TPA-AN-TFP** in different solvents and film.

Solvent	τ **[ns]**	**Solvent**	τ **[ns]**	**Solvent**	τ **[ns]**
Hexane	1.75	Chloroform	3.54	Dimethyl sulfoxide	14.6
Toluene	2.15	Ethyl ether	2.06	Dimethyl formamide	10.3
Dioxane	3.08	Ethyl acetate	3.12	Acetone	6.32
Triethylamine	1.76	Tetrahydrofuran	3.42	Acetonitrile	9.38
Butyl ether	2.06	Dichloromethane	5.45	Film	2.31