

## Supporting Information (SI)

### Creation of Efficient Blue AIE Luminogens for High-Performance

#### Nondoped Blue OLEDs and Hybrid White OLEDs

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## 1. General Information

All chemicals and reagents were purchased from commercial sources and used as received without further purification.  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were measured on a Bruker AV 500 spectrometer in appropriated deuterated solution at room temperature. High resolution mass spectra (HRMS) were recorded on a GCT premier CAB048 mass spectrometer operating in MALDI-TOF mode. TGA analysis was carried out on a TA TGA Q5000 and DSC analysis was performed on a DSC Q1000 under dry nitrogen at a heating rate of  $10\text{ }^\circ\text{C min}^{-1}$ . UV-vis absorption spectra were measured on a Shimadzu UV-2600 spectrophotometer. Photoluminescence spectra were recorded on a Horiba Fluoromax-4 spectrofluorometer. Fluorescence quantum yields were measured using a Hamamatsu absolute PL quantum yield spectrometer C11347 Quantaaurus\_QY. Fluorescence lifetimes were determined with a Hamamatsu C11367-11 Quantaaurus-Tau time-resolved spectrometer. The frontier orbitals of the molecules based on the ground state geometries are calculated at B3LYP/6-31G (d) by Gaussian 09 program. Cyclic voltammetry was measured on a CHI 610E A14297. The anisotropy of the neat film was carried out on VB-400 VASE Ellipsometer.

## 2. Experimental Section

### 2.1 Synthesis and characterization

**9-(4-(2,6-Di-*tert*-butyl-10-(4-(1,2,2-triphenylvinyl)phenyl)anthracen-9-yl)phenyl)-9H-carbazole (TPE-TAC):** **1** (1.15 g, 1.6 mmol), **2** (460 mg, 1.6 mmol),  $\text{Pd}(\text{PPh}_3)_4$  (184 mg, 0.16 mmol),  $\text{Na}_2\text{CO}_3$  (678 mg, 6.4 mmol), THF (60 mL) and deionized water (15 mL) were added into a 250 mL two-necked round bottom flask and heated to reflux for 8 h under nitrogen. After cooled down to room temperature, the mixture was poured into water and extracted with dichloromethane for several times. The combined organic layers were dried over anhydrous magnesium sulfate. After filtration, the

solvent was removed by a rotary evaporation. The crude product was purified by column chromatography on silica-gel using dichloromethane/petroleum as eluent to afford TPE-TAC as white solid in 71% yield (980 mg). <sup>1</sup>H NMR (500 MHz, CD<sub>2</sub>Cl<sub>2</sub>), δ (TMS, ppm): 8.23 (s, 1H), 8.21 (s, 1H), 7.84–7.81 (m, 3H), 7.72–7.69 (m, 3H), 7.65–7.63 (m, 4H), 7.55–7.49 (m, 4H) 7.37–7.30 (m, 4H), 7.25–7.13 (m, 17H), 1.34 (s, 9H), 1.32 (s, 9H). <sup>13</sup>C NMR (125 MHz, CD<sub>2</sub>Cl<sub>2</sub>), δ (TMS, ppm): 147.90, 147.69, 144.59, 144.56, 141.96, 141.67, 137.86, 137.42, 135.93, 133.57, 132.05, 132.03, 131.97, 131.34, 130.29, 129.22, 128.50, 128.42, 128.40, 127.65, 127.28, 127.22, 127.20, 126.73, 125.38, 125.22, 124.06, 121.93, 121.49, 120.99, 120.68, 110.54, 35.59, 35.56, 31.32, 31.14. HRMS (C<sub>66</sub>H<sub>55</sub>N): *m/z* 861.4332 (M<sup>+</sup>, calcd 861.4335).

**9-(4-(2,6-Di-*tert*-butyl-10-(4-(1,2,2-triphenylvinyl)phenyl)anthracen-9-yl)1,3-di(9H-carbazol-9-yl)benzene (TPE-TADC):** This compound was synthesized by a similar method to that for TPE-TAC, in which **1** (1.05 g, 1.5 mmol), **3** (678 mg, 1.5 mmol), Pd(PPh<sub>3</sub>)<sub>4</sub> (173 mg, 0.15 mmol) and Na<sub>2</sub>CO<sub>3</sub> (636 mg, 6.0 mmol) were used. TPE-TADC was obtained as white solid in 56% yield (860 mg). <sup>1</sup>H NMR (500 MHz, CD<sub>2</sub>Cl<sub>2</sub>), δ (TMS, ppm): 8.16–8.14 (m, 4H), 8.05–8.04 (m, 1H), 7.95–7.92 (m, 1H), 7.85–7.82 (m, 3H), 7.72–7.70 (m, 4H), 7.65–7.60 (m, 3H), 7.53–7.50 (m, 1H), 7.46–7.43 (m, 4H), 7.31–7.27 (m, 6H), 7.22–7.10 (m, 17H), 1.39 (s, 9H), 1.31 (s, 9H). <sup>13</sup>C NMR (125 MHz, CD<sub>2</sub>Cl<sub>2</sub>), δ (TMS, ppm): 148.48, 147.83, 144.55, 144.52, 143.98, 143.83, 141.98, 141.55, 141.30, 140.05, 137.79, 137.62, 134.46, 132.03, 132.01, 131.95, 131.27, 129.18, 128.48, 128.40, 128.38, 127.27, 127.18, 126.87, 124.27, 122.03, 120.98, 110.46, 35.68, 35.60, 31.29. HRMS (C<sub>78</sub>H<sub>62</sub>N<sub>2</sub>): *m/z* 1026.4913 (M<sup>+</sup>, calcd 1026.4937).

## 2.2 Devices fabrication and measurement

The devices fabrication and measurement were carried out according to the reported methods.<sup>1</sup> Devices

with active areas of  $4 \times 4 \text{ mm}^2$  were grown on patterned ITO glass substrates with a sheet resistance of  $10 \Omega \text{ sq}^{-1}$ . Before OLED fabrication, the ITO glass substrates were cleaned with detergent and deionized water, dried in an oven at  $120^\circ\text{C}$  for 1 hour, then treated with UV-ozone for 15 minutes, and finally loaded into a deposition chamber with a basic pressure of  $1 \times 10^{-4} \text{ Pa}$ . The organic layers were fabricated by evaporating organic layers at a rate of  $1\text{--}2 \text{ \AA s}^{-1}$ . A layer of LiF with 1 nm thickness was deposited at a rate of  $0.1 \text{ \AA s}^{-1}$ , and finally Al was deposited at a rate of approximately  $5.0 \text{ \AA s}^{-1}$  as the cathode. The current–voltage–brightness characteristics and EL spectra were measured with a Keithley 2400 source meter and a Konica Minolta chromameter CS-200, and EL spectra were measured with a Flame-S-VIS-NIR (Serial Number: FLMS03334). All measurements were done at room temperature under ambient conditions.

### 2.3 Carrier transport calculation

The SCLC characteristics can be described by the following Mott-Gurney equation:

$$J = \frac{9}{8} \epsilon_0 \epsilon_r \mu \frac{E^2}{L} \quad (1)$$

where  $\epsilon_0$  is the free-space permittivity ( $8.85 \times 10^{-14} \text{ C V}^{-1} \text{ cm}^{-1}$ ),  $\epsilon_r$  is the relative dielectric constant (assumed to be 3.0 for organic semiconductors),  $E$  is the electric field of  $V/L$  and  $L$  is the thickness of emitter (80 nm). In general, the carrier mobility ( $\mu$ ) can be expressed via the Poole-Frenkel formula:

$$\mu = \mu_0 \exp(\gamma \sqrt{E}) \quad (2)$$

where  $\gamma$  is the Poole-Frenkel factor and  $\mu_0$  is the zero-field mobility. According to equations (1) and (2), the current density ( $J$ ) of SCLC region can be further expressed as:

$$J = \frac{9}{8} \epsilon_0 \epsilon_r \frac{V^2}{L^3} \mu_0 \exp(0.891 \gamma \sqrt{\frac{V}{L}}) \quad (3)$$

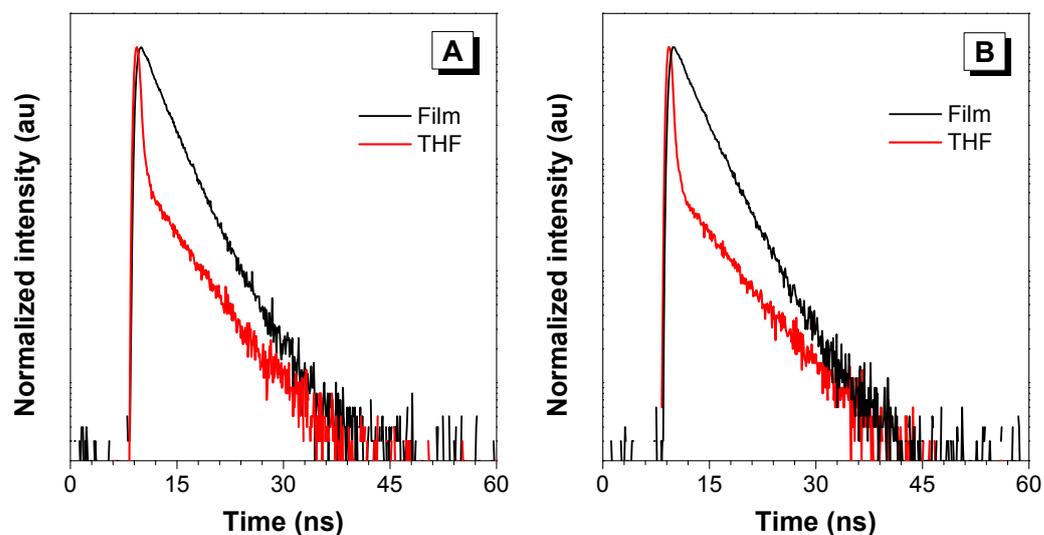
By fitting the  $J$ - $V$  curves in SCLC region to equation 3, the  $\mu_0$  and  $\gamma$  values are obtained as  $2.09 \times 10^{-9}$

and 0.008581 (TPE-TAC, EOD),  $1.00 \times 10^{-8}$  and 0.00743 (TPE-TAC, HOD),  $2.73886 \times 10^{-10}$  and 0.01158 (TPE-TADC, EOD),  $7.44752 \times 10^{-8}$  and 0.00481 (TPE-TADC, HOD), respectively, then generating the field-dependent electron mobility according to equation 2.

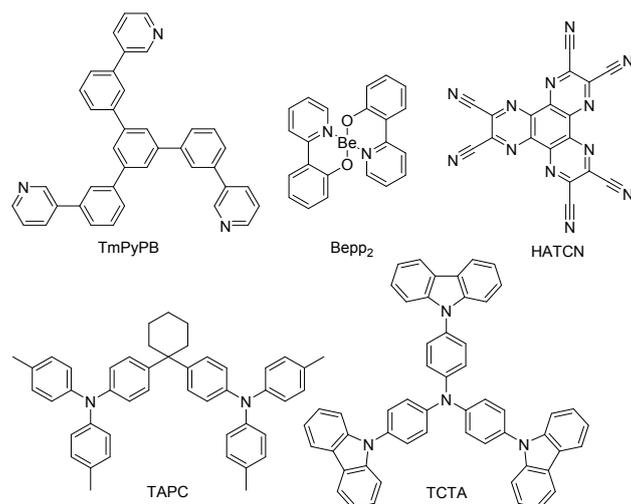
### 3. Reference

(1) Chen, B.; Liu, B.; Zeng, J.; Nie, H.; Xiong, Y.; Zou, H.; Ning, H.; Wang, Z.; Zhao, Z.; Tang, B. Z. Efficient Bipolar Blue AIEgens for High-Performance Nondoped Blue OLEDs and Hybrid White OLEDs. *Adv. Funct. Mater.* **2018**, 28, 1803369.

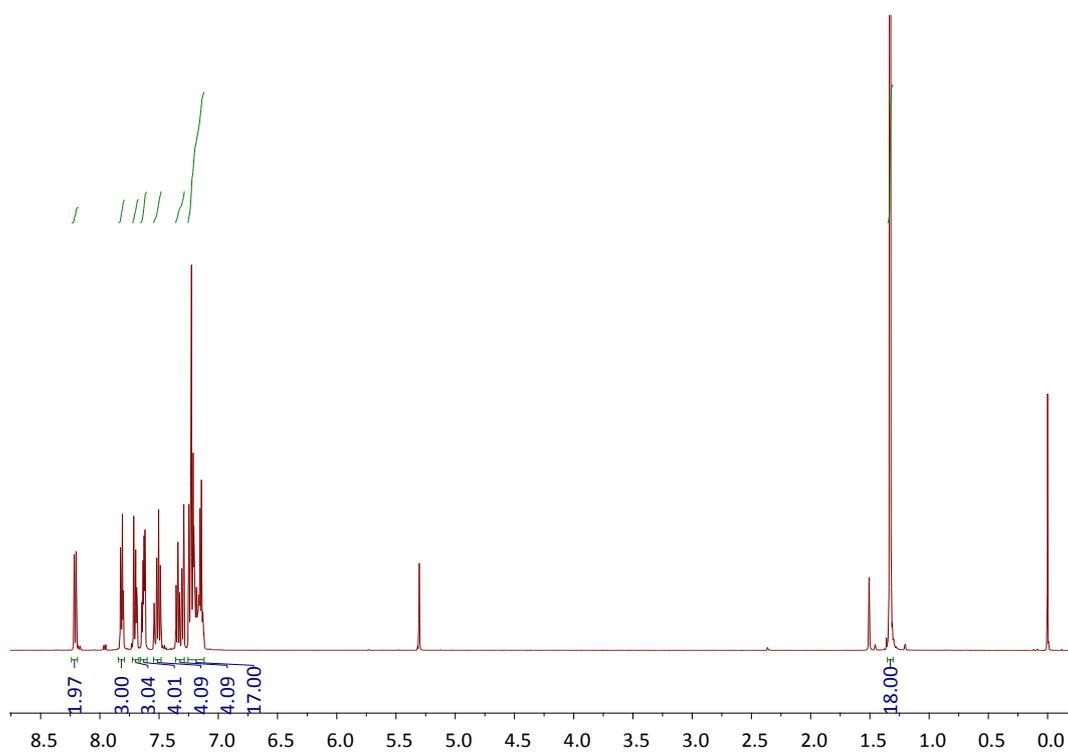
### 4. Additional Spectra



**Figure S1.** Fluorescence decay profiles of TPE-TAC (A) and TPE-TADC (B) in THF and films.



**Figure S2.** Chemical structures of TmPyPB, Bepp<sub>2</sub>, HATCN, TAPC and TCTA.



**Figure S3.** <sup>1</sup>H NMR spectrum of TPE-TAC in CD<sub>2</sub>Cl<sub>2</sub>.

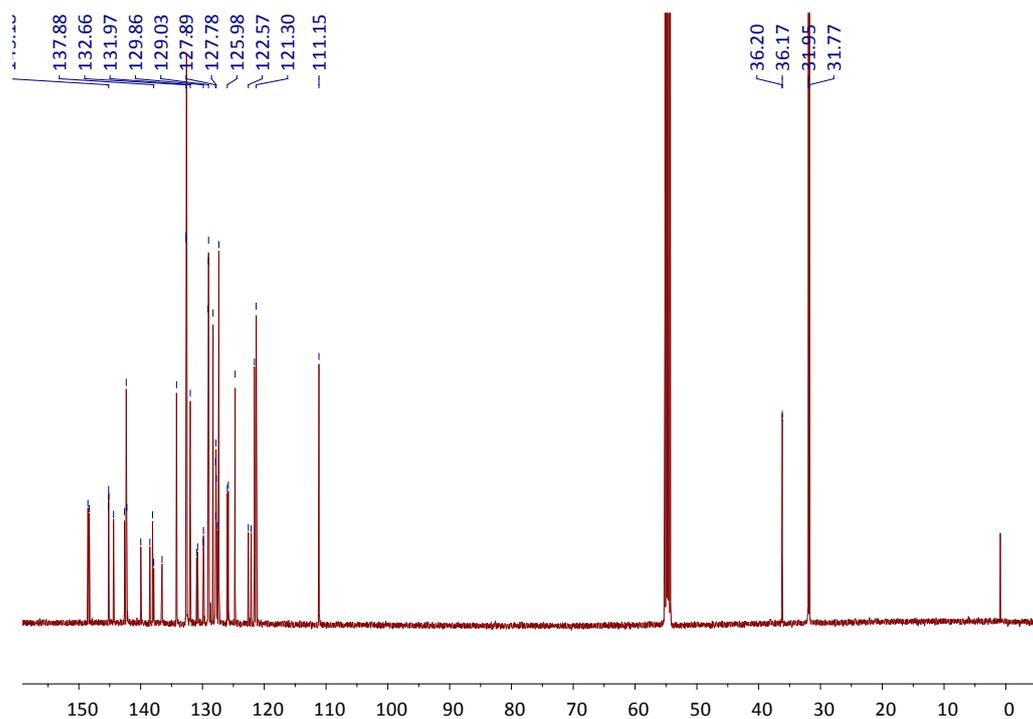


Figure S4.  $^{13}\text{C}$  NMR spectrum of TPE-TAC in  $\text{CD}_2\text{Cl}_2$ .

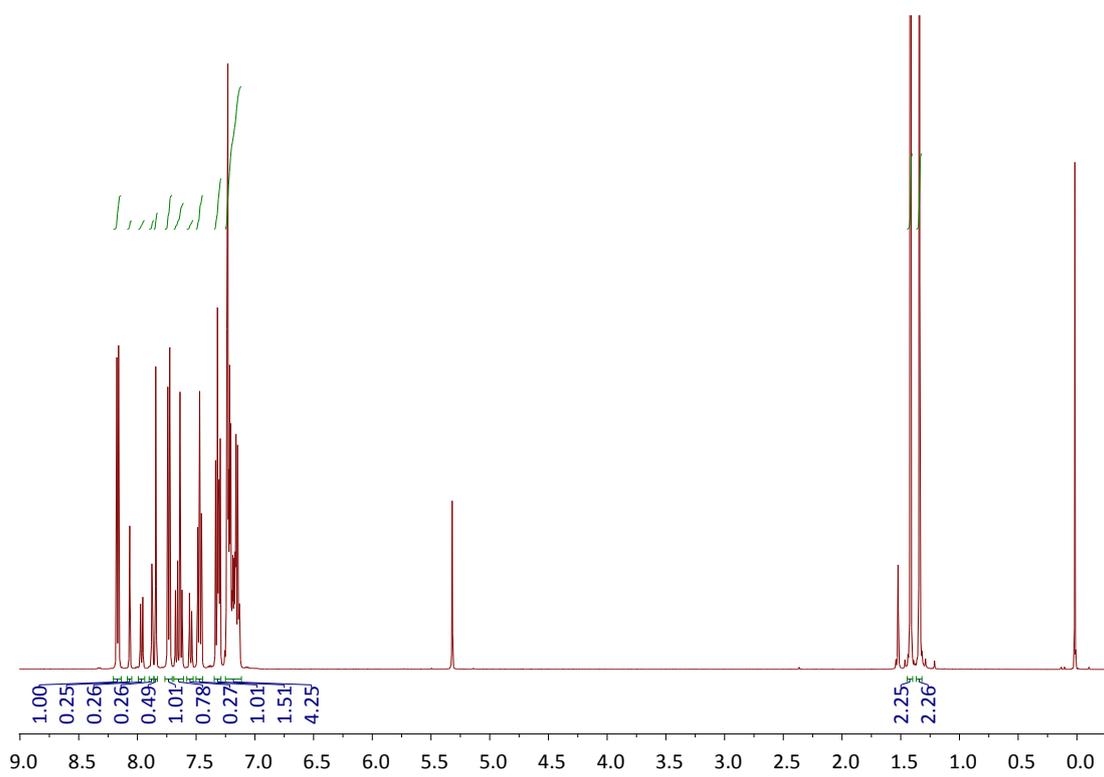
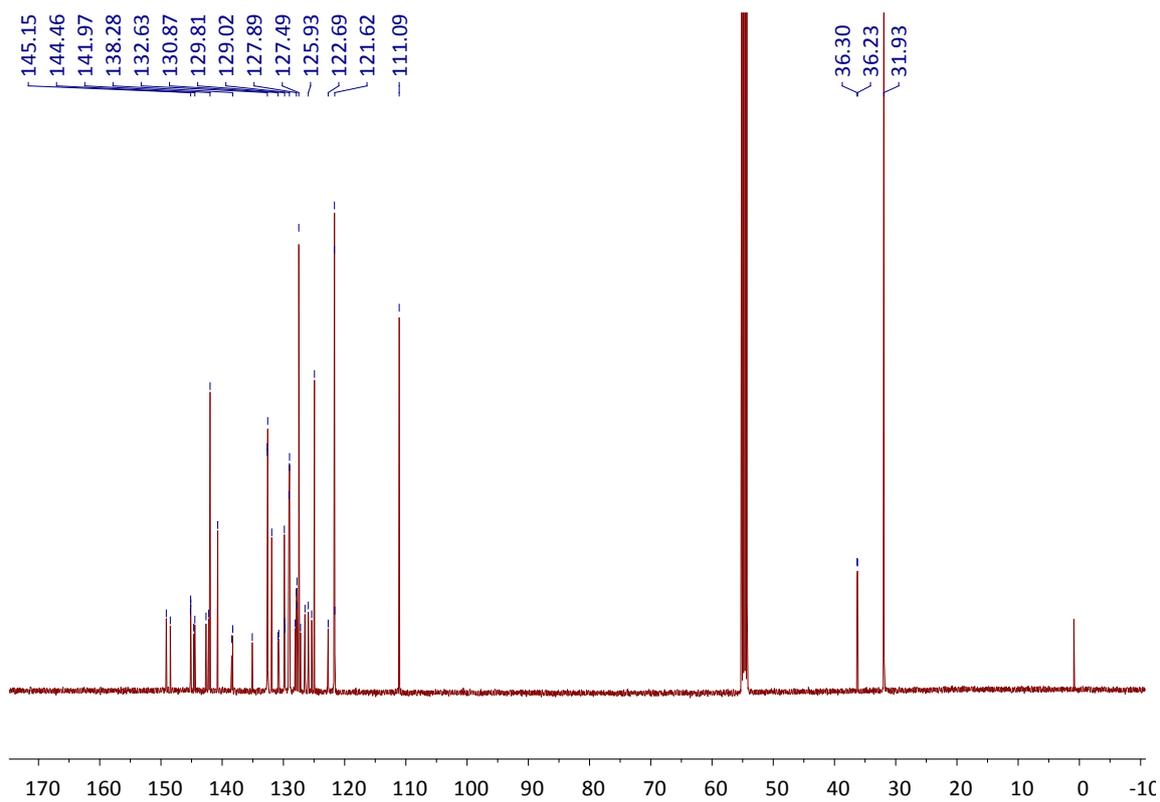


Figure S5.  $^1\text{H}$  NMR spectrum of TPE-TADC in  $\text{CD}_2\text{Cl}_2$ .



**Figure S6.**  $^{13}\text{C}$  NMR spectrum of TPE-TADC in  $\text{CD}_2\text{Cl}_2$ .