Electronic Supplementary Information (ESI)

Cross-dipole stacking molecule of an anthracene derivative: integrating optical and electrical properties

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Experimental section:

Materials and Instrumentations

All reagents were used as received from commercial resources unless otherwise specified.

^{1}H and ^{13}C NMR spectra were recorded using a Bruker ADVANCE 400 NMR Spectrometer. ^{1}H NMR spectra were referenced to $CDCl_3$ (7.26 ppm) and ^{13}C NMR spectra were referenced to $CDCl_3$ solvent (77.36 ppm). UV-vis absorption spectra were measured with Hitachi (model U-3010) UV-Vis spectrophotometer in a 1-cm quartz cell. Photoluminescence (PL) spectra were recorded on a Perkin-Elmer LS 55 spectrofluorometer. Absolute quantum yield measurement (LabSphere®, FluoroMax-4, HORIBA JobinYvon, PLQY software package) was used for powder sample. In this experimental setup, it is possible to measure the Photoluminescence Quantum Yields (PLQY) *via* using the integrating sphere in combination with a commercial fluorometer. Emission spectra including the scattering region of excitation light were measured for both blank and test samples, and these spectra were corrected with instrumental factors to calculate the quantum yield. Florescence quantum efficiency of TES-DPA solution was measured with fluorescence in as reference. Time-resolved peak fluorescence of TES-DPA in THF and solid state were determined by F906 (Edinburgh instrument).

High-quality single crystals of TES-DPA were grown from a chlorobenzene at room temperature. X-ray diffraction intensity data were collected at 113 K on a Rigaku Saturn724 CCD diffract meter with graphite monochromated Mo K\α radiation. And the structure and refinement were carried out using the Crystal Clear (Rigaku Inc., 2008).

OFET characteristics were recorded by a Keithley 4200 SCS and Micromanipulator 6150 probe station in a clean and shielded box. EL spectra were recorded by PR 655 spectrometer and the J-V test was taken by Keithley 2400.

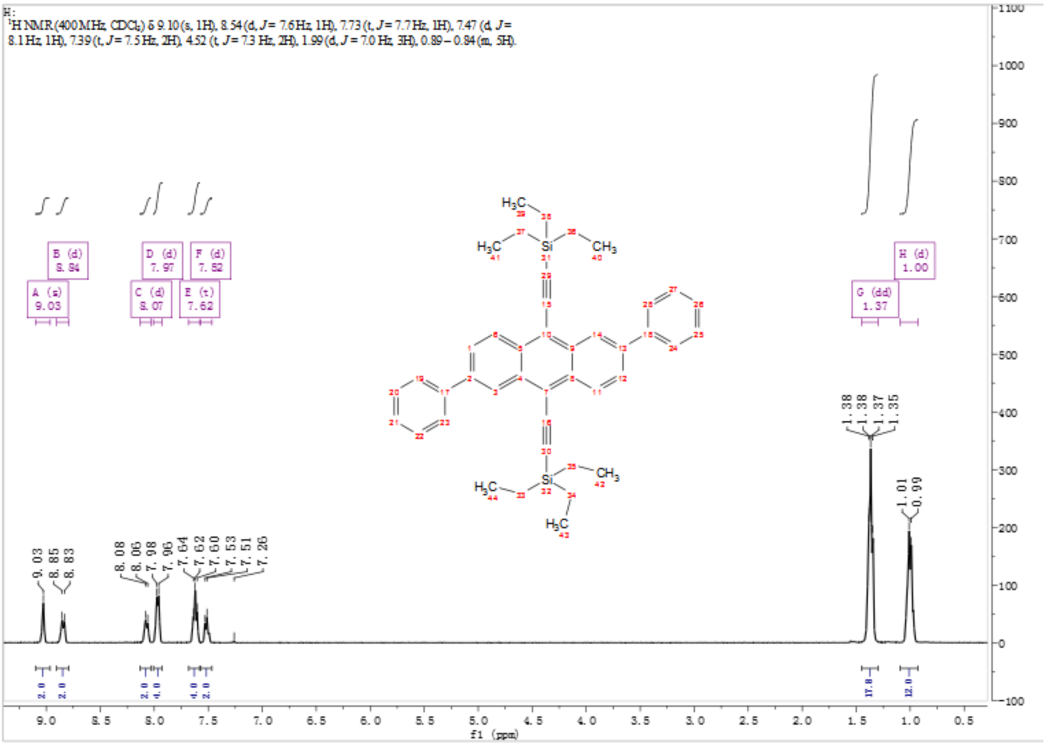
Synthesis

2,6-dibromoanthracene-9,10-dione, 2. A solution of compound 1 (2,6-diaminoanthracene-9,10-dione) 10 g (41.4 mmol) in anhydrous acetonitrile (200 mL) was added $CuBr_2$ 20.8 g (93.2 mmol), then t-BuONO 9.6 g (93.2 mmol) was added to the above suspension, the whole system was allowed to warm up 63°C for 3 h. After cooling down to room temperature, the reaction was quenched by adding 20% HCl (100 mL). Then water (200 mL) was added and the brown crude product was obtained by filtration washed with water and air dried. Dioxane (800 mL) was used to dissolve the crude product at refluxing and then active charcoal was added, after filtration, the filtrate was allowed to cool down to room temperature give **2** as light yellow crystals 9.85 g (65%). ^{1}H NMR (400 MHz, CDCl3, δ): 8.64 (s, 2H), 8.18 (d, *J* = 8.0 Hz, 2H), 7.98 (d, *J* = 8.1 Hz, 2H).MS (EI) m/z: 366 (M+).

2,6-diphenylanthracene-9,10-dione, 3. Compound 3 was synthesized by Suzuki coupling reaction. To a 250 mL flask, 1.1 g (3mmol) compound **2**, 0.8 g (6.6mmol) phenylboronic acid and $Pd(PPh_3)_4$ 190 mg (0.15mmol) was added under argon. Then 24 mL ethanol, 120 mL toluene and 24mL 2M K_2CO_3 aqueous solution was added. The whole system was heated to 90 °C and kept overnight. The mixture was separated, and the water layer was extracted with CH_2Cl_2 (50 mL × 3), the combined organic layer was dried over anhydrous Na_2SO_4. Solvent was removed under vacuum. Further purification by column chromatography on silica gel using petroleum ether: CH_2Cl_2 (3 : 1) as eluent afforded the product as a yellow solid (0.92 g, 85% yield). ^{1}H NMR (400 MHz, $CDCl_3$, δ): 8.58 (d, *J* = 1.7 Hz, 1H), 8.42 (d, *J* = 8.1 Hz, 1H), 8.04 (dd, *J* = 8.1, 1.8 Hz, 1H), 7.76 (d, *J* = 7.5 Hz, 2H), 7.53 (t, *J* = 7.4 Hz, 2H), 7.47 (t, *J* = 7.3 Hz, 1H). MS (EI) m/z: 360 (M+).

((2,6-diphenylanthracene-9,10-diyl)bis(ethyne-2,1-diyl))bis(trialkylsilane) 4. To a 250 mL round-bottom flask containing 100 mL anhydrous THF, triethyl(ethynyl)silane 4.03 g (27.88 mmol) was added and the stirring system was placed in an ice-water bath, then 7.8 mL (6.25 mmol 2M) *n*-BuLi was added slowly and this mixture was stirred for 1 h at 0 °C. Then compound 3 1.8 g (5 mmol) was added quickly, and the mixture was stirred overnight. Stannous chloride dihydrate 2.83 g (12.5 mmol) and 12.5 mL 10% HCl was added to the mixture which was stirred for another 7 h. Then the whole system was extracted with hexanes (60 mL × 3) and the combined organic layer was washed with saturated brine solution, dried over anhydrous Na_2SO_4 and concentrated. The final TES-DPA was to be obtained after silica chromatography (eluent: petroleum ether) with a yield of 46% (1.4 g). ^{1}H NMR (400 MHz, $CDCl_3$, δ): 9.10 (s, 2H), 8.54 (d, *J* = 7.6 Hz, 2H), 7.73 (t, *J* = 7.7 Hz, 2H), 7.47 (d, *J* = 8.1 Hz, 4H), 7.39 (t, *J* = 7.5 Hz, 4H), 4.52 (t, *J*=

7.3 Hz, 2H), 1.99 (d, J = 7.0 Hz, 18H), 0.89 – 0.84 (m, 12H).^{13}C NMR (101 MHz, CDCl3, δ): 140.91, 139.32, 132.96, 132.20, 129.26, 128.23, 128.05, 127.65, 127.13 (s), 125.25, 118.95, 106.38, 103.08,8.21, 5.03.MS (EI) m/z: 606 (M$^+$).Anal.calcd for $C_{42}H_{46}Si_2$(%):C: 83.11, H: 7.64. Found: C: 83.72, H: 7.88.



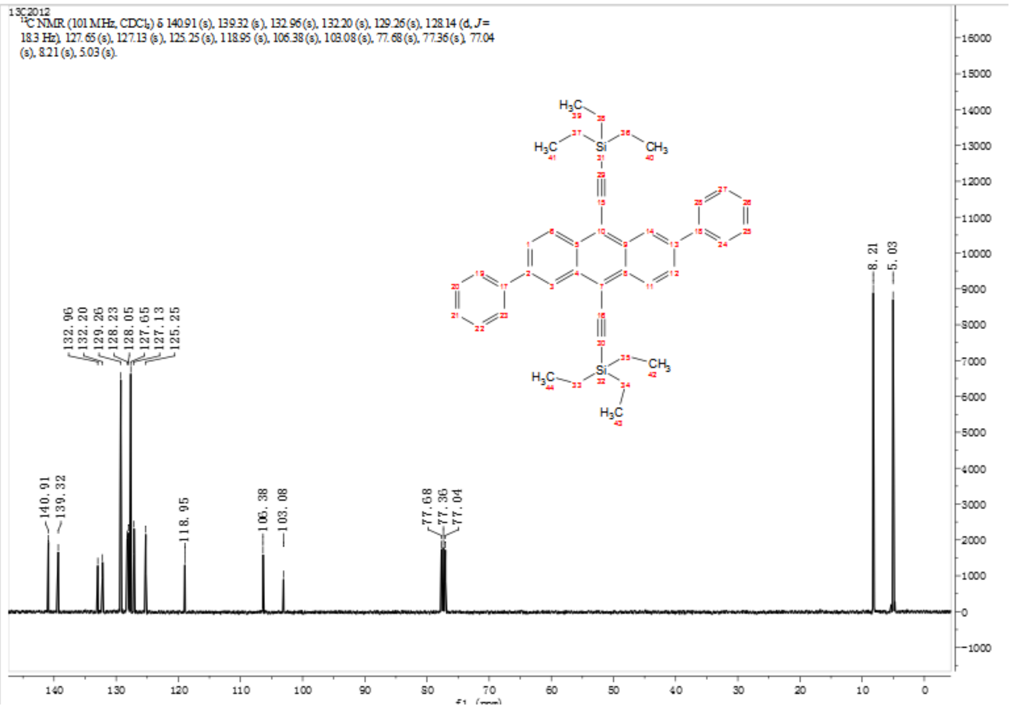


Figure S1 ^{1}HNMR and ^{13}C NMR of TES-DPA.

Table S1. Crystal Data and Structure Refinement for*TES-DPA*(CCDC998335)

Empirical formula	C42 H46 Si2
Formula weight	606.97
Temperature	113.0 K
Wavelength	0.71075 Å
Crystal system	Monoclinic
Space group	P2(1)/c
Unit cell dimensions	a = 26.848(2) Å □α = 90°
	b = 34.169(2) Å □β = 90. 500（5）°
	c = 7.6508(6) Å □γ = 90°.
Volume	7018.3(9) Å^3
Z	8
Density (calculated)	1.149mg/m^3
Absorption coefficient	0.129mm^{-1}
F(000)	2608
Crystal size	0.24×0.12 × 0.10 mm^3
Theta range for data collection	1.40° to 27.90°
Index ranges	-31 ≤h≤ 31, -40 ≤k≤ 40, -8≤l≤ 9
Reflections collected	73565
Independent reflections	12348 [R(int) = 0.0600]
Completeness to theta = 25.00°	100 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9872 and 0.9697
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	12348 / 46 / 844
Goodness-of-fit on F2	1.377
Final R indices [I>2sigma(I)]	R1 = 0.0762, wR2 = 0.1643
R indices (all data)	R1 = 0.0899, wR2 = 0.1720
Largest diff. peak and hole	0.544 and -0.680 e.Å^{-3}

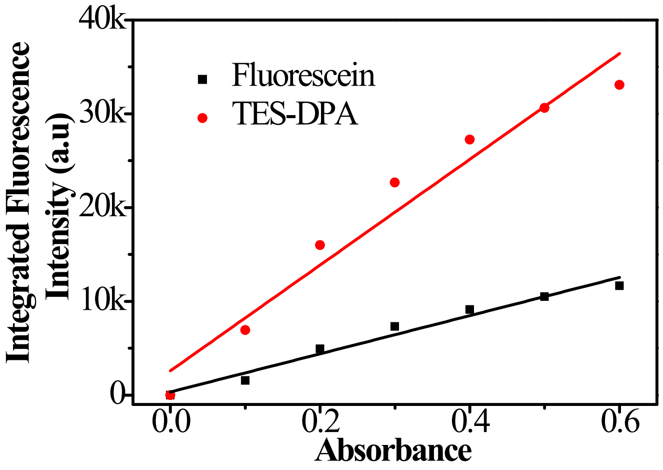


Figure S2. Fluorescence quantum efficiency of TES-DPA solution. The efficiency of TES-DPA solution was measured in comparison with fluorescence. Acetone was used as solvent for the two compounds and the excited wavelength was fixed at 430 nm, Φ_F of 79% was reported for fluorescence, and a 2.7 times stronger fluorescence was obtained for TES-DPA under the same condition, thus the ΦF of TES-DPA was estimated as 100%.

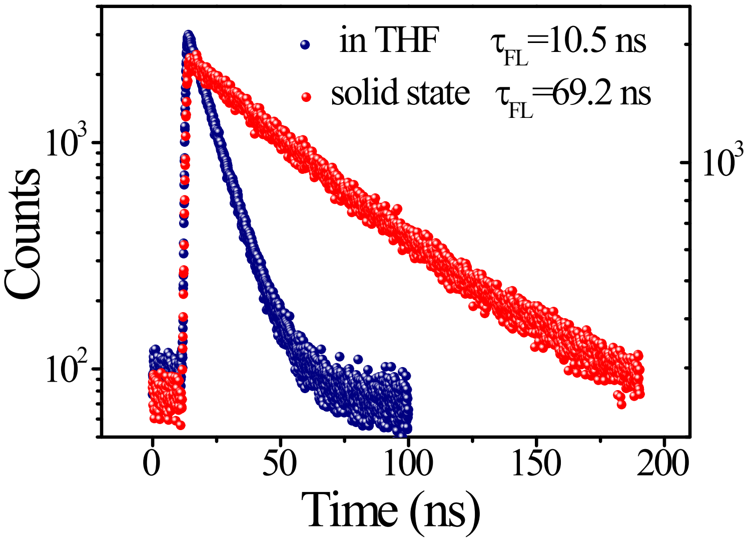


Figure S3 Time-resolved peak florescence of TES-DPA in THF and in crystalline solid state recorded on F906 (Edinburgh instrument)

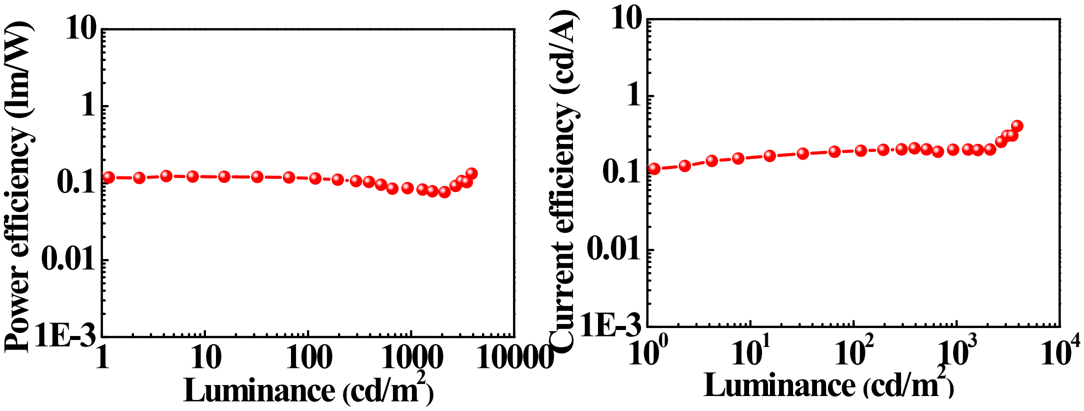


Figure S4 Power efficiency and current efficiency of the OLED devices based on TES-DPA, the relatively poor efficiencies might be derived from the high hole-transport property of TES-DPA and easy crystallization of the material, which can be improved by further optimization of the fabrication process, correlated study was under way.