The Color Tunable OLEDs with an Anthracene Derivative Doped Single-Emitting Component Layer Controlled by Doping Ratio and Driving Voltage

Ming-Yu Teng, Qiu-Lei Xu, Hong-Yan Li, Lin Wu, You-Xuan Zheng*, Chen Lin*, Leyong Wang

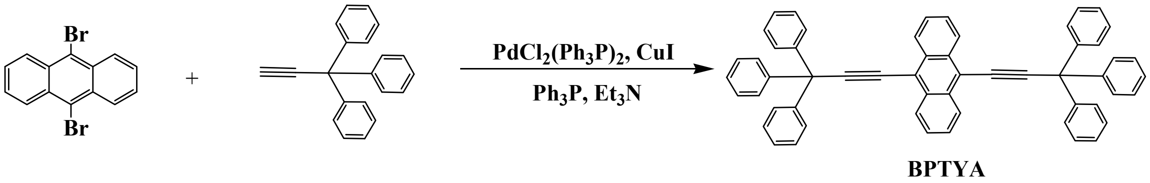
State Key Laboratory of Coordination Chemistry, Nanjing National Laboratory of Microstructures, School of Chemistry and Chemical Engineering, Nanjing, P.R. China, 210093, yxzheng@nju.edu.cn , linchen@nju.edu.cn.

Supporting Information

1. General information

TLC: TLC Plates 60 F 254, visualized by UV light (254 nm). Column chromatography (CC): silica gel (300 400 mesh). Solvents used for CC were untreated prior to use, while reagents were used as purchased. NMR Spectra: BRUKER NMR spectrometer (^{1}H: 300 MHz, ^{13}C: 77 MHz); δ values in ppm relative to Me4Si as internal standard for ^{1}H-NMR; for ^{13}C-NMR: CDCl$_3$ (δ 77.0) and Me$_4$Si as internal standard. IR Spectra: BRUKER Vector 22, using KBr as pellets. Melting points: X-4 microscope melting point apparatus. The electroluminescence spectra were measured with a Hitachi F-4600. UV Spectra: Lambda 35 UV/Vis spectrometer. On the basis of the uncorrected PL and EL spectra, the Commission Internationale de l'clairage (CIE) coordinates were calculated using a test program of the Spectra scan PR650 spectrophotometer. The temperature was uncorrected before use. Elemental analysis: VARIO EL III instrument.

2. Preparation of BTPYA



Scheme S1 The synthetic routes to **BTPYA**[S1].

A three-neck 50 mL round-bottom flask was charged with substituted dibromoanthracene (0.101 g, 0.30 mmol), CuI (0.005 g, 0.025 mmol), PPh_3 (0.020 g, 0.075 mmol) and $(PPh_3)_2PdCl_2$ (0.036 g, 0.050 mmol) dissolved in 10 mL of Et_3N and warmed to 85ºC. Prop-2-yne-1,1,1-triyltribenzene (0.182g, 0.66 mmol) dissolving in 5 mL of Et_3N was added at once via syringe. The reaction flask was heated at 85 °C in an oil bath for 24 h to give a yellow precipitation. The solid was filtered and washed several times with Et_3N and petroleum, dissolved in $CHCl_3$ and filtered once more to remove residual CuI, the solvent was removed under reduced pressure to give pure product.

Yellow solid; m.p. 281-283ºC; R_f =0.65 (petroleum ether/ethyl acetate = 10:1); product 0.18g (yield 85.7%),

^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.54 (dd, 4H, *J*=6.6 Hz, 3.3 Hz; anthracenyl 1,4,5,8-H), 7.51 (d, 16H, *J*=9.0 Hz, 3.3 Hz; anthracenyl 2,3,6,7-H, phenyl H), 7.40 – 7.25 (m, 18H; phenyl H).

^{13}C-NMR (*δ,* ppm): 145.4, 132.7, 129.5, 128.4, 127.4, 127.2, 126.8, 118.6, 108.5, 82.7, 57.4;

IR (cm^{-1}): ν_{max}(KBr/cm^{-1}), 3454, 1595, 1489, 1444, 1387, 1155, 770, 756, 738, 696, 638.

Anal. Calc. for $C_{56}H_{38}$: C, 94.61; H, 5.39. Found: C, 94.51; H, 5.21.

3. Crystallographic information for BTPYA

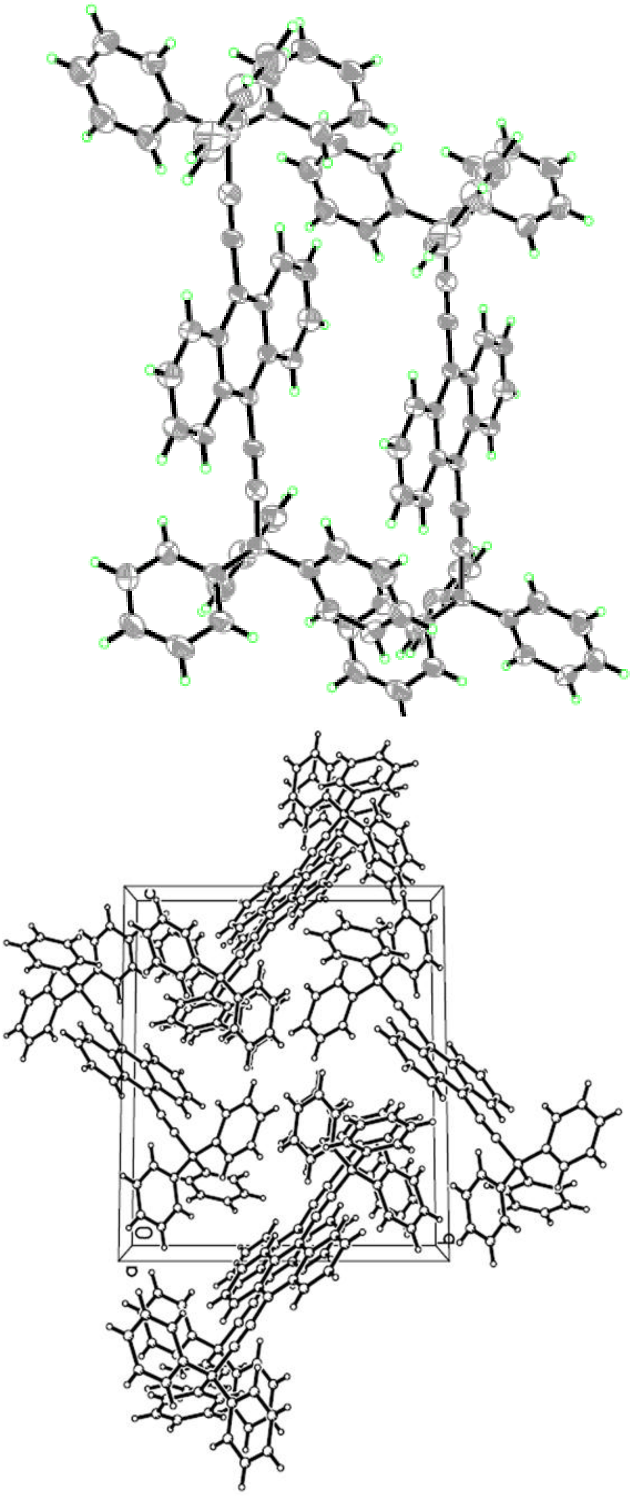


Fig. S1. The X-ray crystallography of **TPBYA** (packing view).

Table S1. Crystallographic data for **BTPYA**.

	BTPYA
Formula	$C_{56}H_{38}$
Formula weight	710.9
Temperature	293(2) K
λ (Å)	0.71073
Crystal system	Monoclinic
Space group	P2(1)/n
a (Å)	8.5972(17)
b (Å)	14.442(3)
c (Å)	16.327(3)
α (º)	90.00
β (º)	102.573(3)
γ (º)	90.00
V (Å^3)	1.202
Z	4
ρ_{calcd} (g/cm^3)	1.202
μ (Mo K α) (mm^{-1})	0.067
F(0 0 0)	770
Range of transmission factors (º)	1.90 - 28.30
Reflections collected	4757
Unique	1687
Goodness-of-fit (GOF) on F^2	0.746
R_1[a], wR_2[b] (I >2r(*I*))	0.0491, 0.1082
R_1[a], wR_2[b] (all data)	0.1379, 0.1287
CCDC No.	833615

Table S2. Selected bond lengths (Å) and angles (º) for **BTPYA**.

$C_{56}H_{38}$					
C(23)-C(24)	1.134 (2)	C(24)-C(28)	1.469 (2)	C(25)-C(28)	1.402 (3)
C(20)-C(21)	1.415 (3)	C(20)-C(22)	1.354 (3)	C(22)-C(25)	1.418 (2)
C(26)-C(27)	1.424 (3)	C(27)-C(28)	1.401 (2)	C(23)-C(29)	1.516 (3)
C(23)-C(24)-C(28)	172.4 (2)	C(24)-C(23)-C(29)	176.5 (2)	C(21)-C(20)-C(22)	120.4 (2)
C(20)-C(22)-C(25)	121.7 (2)	C(22)-C(25)-C(27a)	118.0 (2)	C(28)-C(25)-C(27a)	119.5 (2)
C(25a)-C(27)-C(28)	119.7 (2)	C(25a)-C(27)-C(26)	118.0 (2)	C(21a)-C(26)-C(27)	122.3 (2)

4. Preparation of OLEDs

All OLEDs with the emission area of 0.1 cm^2 were fabricated on the pre-patterned ITO-coated glass substrate having an ITO sheet resistance of 15 Ω/sq. Substrates were cleaned by ultrasonic baths in organic solvents and de-ionized water followed by ozone treatment for 20 min. The hole-transporting material of NPB film was first deposited on the ITO glass substrates. The **BTPYA** (x wt%) and **TPBi** host were co-evaporated from two separate sources to form emitting layer. And then, **TPBi**, LiF (1 nm), and Al (100 - 200 nm) were evaporated. All chemicals used for EL devices were sublimed in vacuum prior to use. The vacuum was less than 1×10^{-5} Pa during all materials deposition. The current density-voltage-luminance (J-V-L) characteristics and current efficiency versus J curves of the devices were measured with a computer controlled KEITHLEY 2400 source meter with a calibrated silicon diode in air without device encapsulation.

4. Cyclovoltammetry (CV) diagram of BTPYA

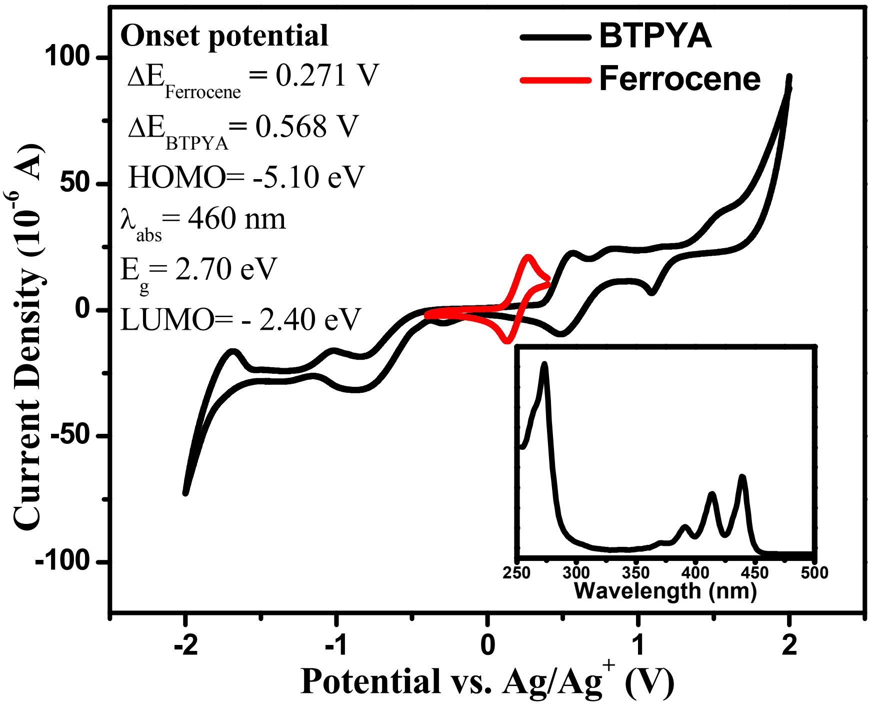


Fig. S2. Cyclovoltammetry (CV) diagram of **BTPYA** in dichloromethane.

The cyclic voltammograms were measured in CH_2Cl_2 solution using ferrocene as the internal standard. During the anodic scan, **BTPYA** shows a reversible oxidation couple as two inflexions with the redox potential in the region of -2.00–2.00 V. On the basis of the potentials of the oxidation and reduction couples, the HOMO/LUMO energy levels of **BTPYA** were estimated as -5.10/-2.40 eV, with regard to the energy level of the ferrocene reference (4.8 eV below the vacuum level). [S2,S3]

5. Characteristics of devices

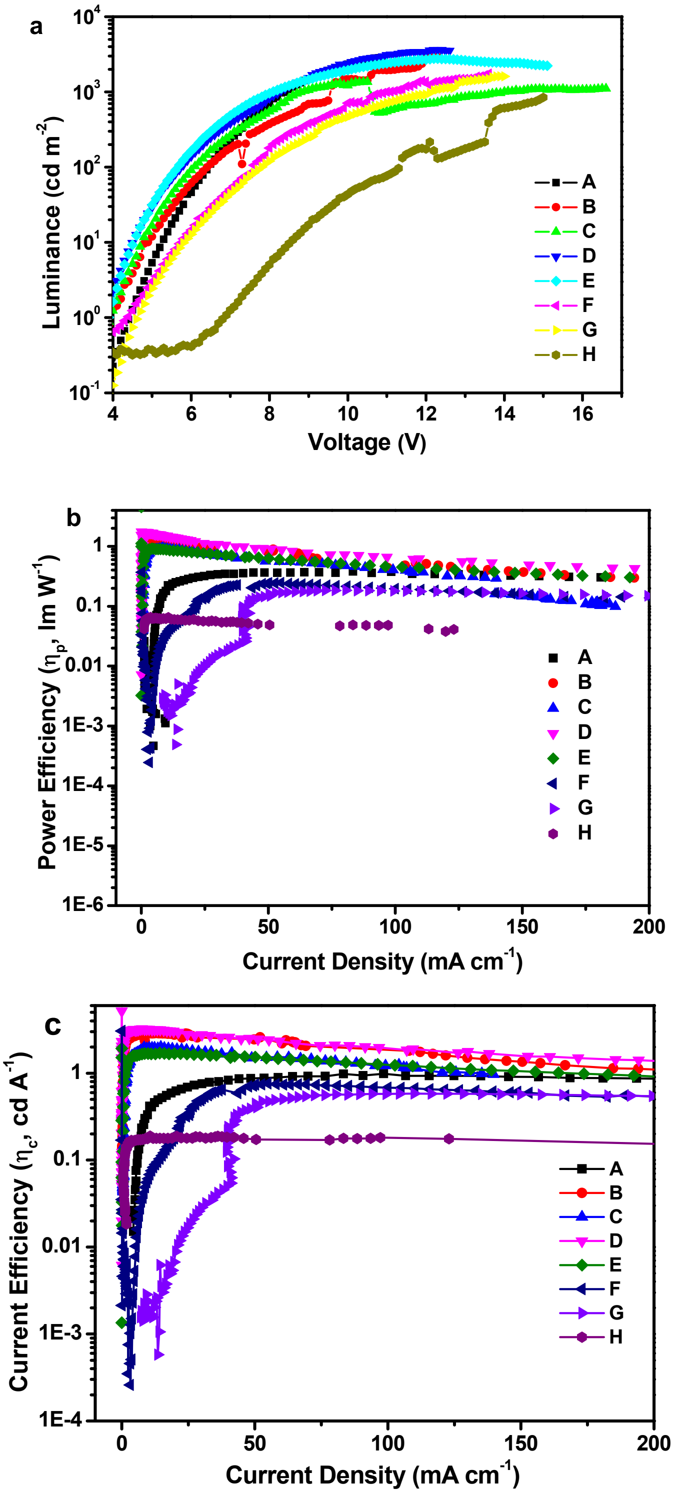


Fig. S3 The brightness versus voltage (V−B, a), power efficiency as a function of current density (η_p-J, b) and current efficiency as a function of current density (η_c-J, c) curves for all the devices.

6. The CIE diagrams of devices A–D at different voltages

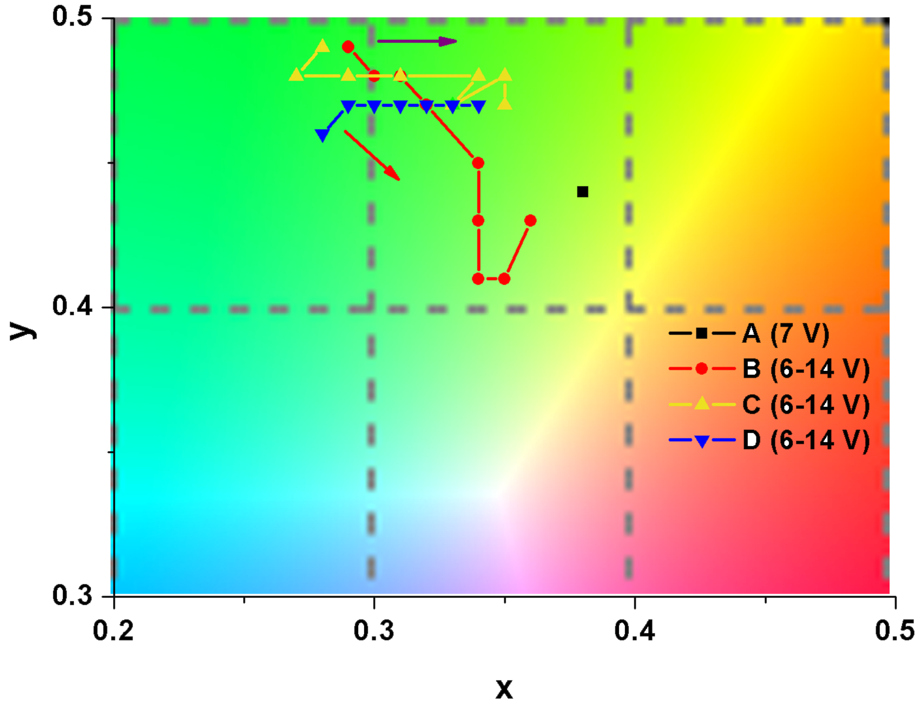


Fig. S4 The CIE x, y chromaticity diagrams of devices A–D at different voltages.

Reference

S1. J. E. Nuñez, A. Natarajan, S. I. Khan, M. Garcia-Garibay, *Org. Lett.* **2007**, *9,* 3559-3561.

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