

Supporting Information

Ambipolar 3,3'-dimethyl-9,9'-bianthracene derivative as blue host material for high-performance OLEDs

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S1. Synthesis and characterization

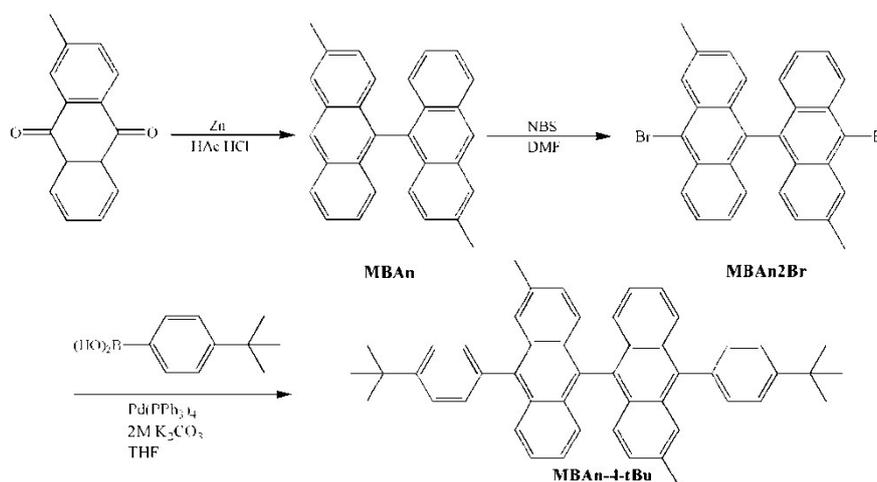
MBAn-(4)-tBu was synthesized by palladium(0)-catalyzed Suzuki cross-coupling reaction between [4-(*tert*-butyl)phenyl]boronic acid and brominated 3,3'-dimethyl-[9,9']bianthracene (MBAn2Br), as shown in the Scheme S1. After purification by column chromatography and recrystallization, the newly synthesized MBAn-(4)-tBu was purified further by train sublimation at a reduced pressure below 10^{-3} Pa and fully characterized with ^1H NMR.

S1.1 Synthesis of 9,9'-bi(2,2'-bimethyl)anthracene (MBAn)

2-methyl anthraquinone (13.32 g, 60 mmol), Zn (22.5 g, 346 mmol) and acetic acid (300 mL) were mixed in a flask under nitrogen. All reagents and solvents were used as purchased from commercial sources without further purification. When the reaction mixture was heated to 90 °C and slowly add concentrated hydrochloric acid (70 mL) at this temperature. After the reaction came to an end for 10-15 h, (inspected by thin layer chromatography), the product was filtrated and then purified by toluene. MBAn was obtained as a pale yellow powder. Yield: 91.6%. ^1H NMR (CDCl_3 , 400 MHz): δ 2.30-2.54 (s, 6H), 6.88-7.07 (m, 8H), 7.30-7.39 (m, 2H), 7.80-8.08 (m, 4H), 8.47-8.58 (m, 2H). Anal. Calcd (%) for $\text{C}_{30}\text{H}_{22}$: C, 94.20%; H, 5.80%. Found: C, 94.36%; H, 5.64%.

S1.2 Synthesis of 10,10'-dibromo-9,9'-bi(2,2'-bimethyl)anthracene (MBAn2Br).

BAn (2.0 g, 5.2 mmol) and DMF (10 mL) were mixed in a flask. *N*-bromosuccinimide (NBS) (2.8 g, 15.6 mmol) and DMF (67 mL) were mixed in a constant pressure funnel. When the reaction mixture was cooled at 5°C, NBS solution was slowly added to the reaction mixture. After the reaction mixture was stirred for 10 h at room temperature, the product was filtrated and then purified by toluene. MBAn2Br was obtained as a pale yellow powder. Yield: 80%. ¹H NMR (CDCl₃, 400 MHz): δ 2.46-2.69 (s, 6H), 6.96-7.65 (m, 10H), 8.44-8.50 (m, 2H), 8.67-8.73 (m, 2H). Anal. Calcd (%) for C₃₀H₂₀Br₂: C, 66.69%; H, 3.73%. Found: C, 66.42%; H, 3.66%.



Scheme S1 Synthetic procedures for MBAn-(4)-tBu.

S2. Theoretical calculations

In order to gain insights into the geometrical configuration of the compound, density function theory (DFT) calculations were carried out using the Gaussian 09 program at the B3LYP/6-31G* level. The optimized molecular geometries of these molecules are shown in Fig. S1.

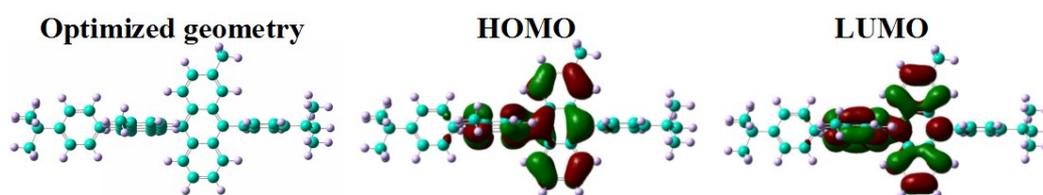


Fig. S1 The optimized geometry and frontier molecular orbital surfaces of MBAn-(4)-tBu.

S3. Physical properties of MBAn-(4)-tBu

A summary of the precise photophysical data of the compound is given in Table S1.

Table S1 Physical properties of MBAn-(4)-tBu

Compound	$\lambda_{\text{Abs max}}(\text{nm})$	λ_{PL}	E_{ox}^c	Φ_{F}^d	HOMO/LUMO _{exp} ^e	HOMO/LUMO _{cal}	$T_{\text{g}}/T_{\text{m}}/T_{\text{d}}^f$
	soln ^a /film ^b	max(nm)	(V)		(E_{g}) (eV)	($\Delta E_{\text{HOMO-LUMO}}$)	(°C)
		soln ^a /film ^b				(eV)	
MBAn-(4)-tBu	344,363,384,404	460/461	0.52	7.1	-5.3/-2.4(2.9)	-5.0/-1.5(3.5)	-/402/407
	/343,364,384,406						

^a Measured in CH₂Cl₂. ^b Measured in solid thin film on quartz plates. ^c Measured in CH₃CN. ^d Absolute photoluminescence quantum yield determined in solid. ^e Values from DFT calculation. ^f T_{g} : glass-transition temperature; T_{m} : melting point; T_{d} : decomposition temperature.

S4. EL properties of MBAn-(4)-tBu as deep-blue dopants

We chose MBAn-(4)-tBu as the dopant for device fabrication. In this device, the well known ambipolar conductive 4,4'-bis(*N*-carbazolyl)biphenyl (CBP) was used as host material. As shown in Fig. S2, the device D was fabricated with the following configuration: ITO/HAT-CN (5 nm)/TAPC (40 nm)/CBP: MBAn-(4)-tBu (20 nm)/TPBi (40 nm)/Liq (1 nm)/Al (120 nm). The dopant was co-evaporated with CBP to give the optimal doping concentration of 5 wt% in the EML. Fig. S3 and Fig. S4 exhibited the J - V - L - η characteristics of the MBAn-(4)-tBu-doped CBP device. The

key device performance parameters and EL emission characteristics were summarized in Table S2. Device D successfully realized deep-blue emissions with CIE coordinates of (0.15, 0.07), which not only meet the NTSC standard, but also approach to the criterion of European Broadcasting Union standard of (0.15, 0.06). The MBAn-(4)-tBu-doped CBP device exhibits good performance with a low turn-on voltage of 3.2 V, luminance of 3874 cd m⁻², which has been greatly improved when compared with the non-doped devices. Notably, these efficiencies show little roll-off at high brightness, although the EQE of device B (3.00%) is lower than device A (3.94%) in the deep-blue visible region with a CIE chromaticity coordinates (0.16, 0.07).

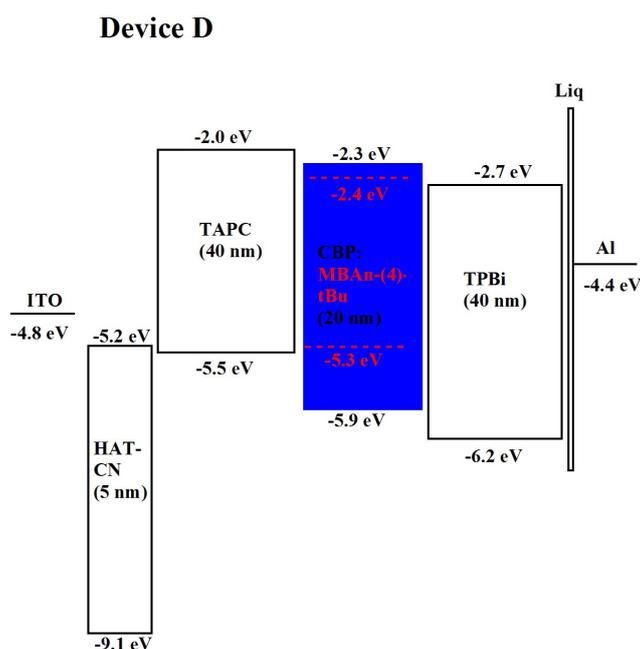


Fig. S2 Structure of device D and the energy levels of the material.

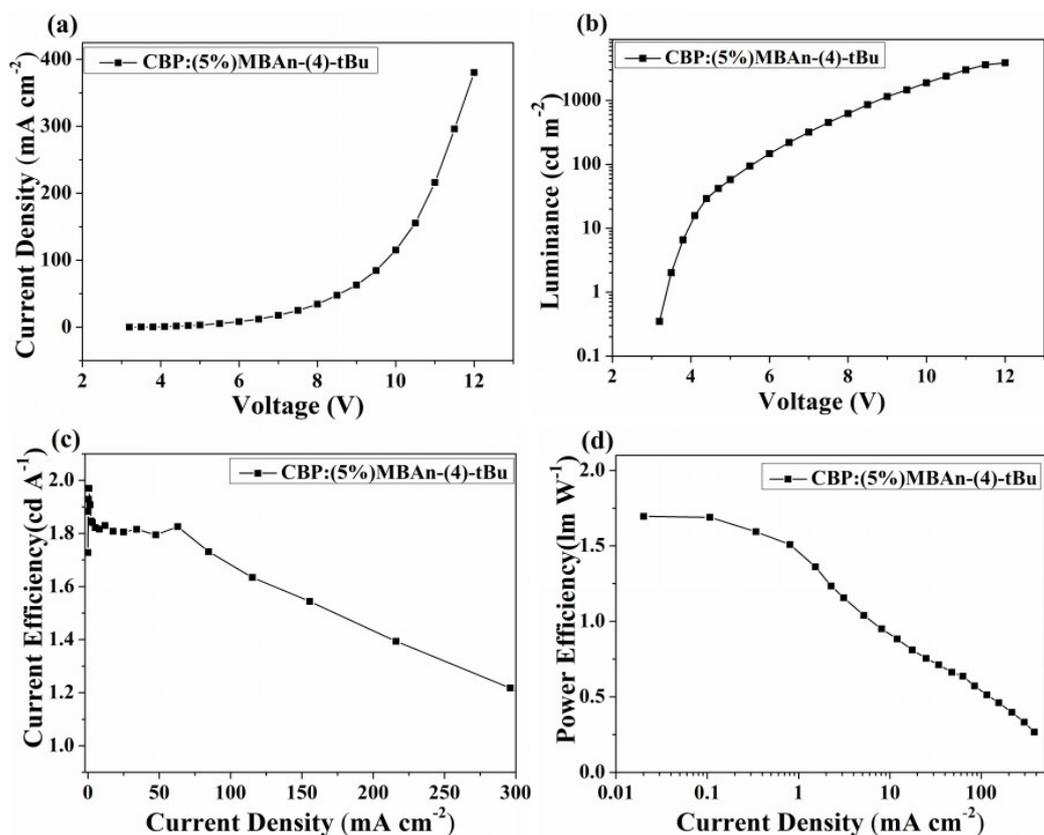


Fig. S3 (a) Current density-voltage curve, (b) Brightness-voltage curve, (c) Current efficiency-current density curve, and (d) Power efficiency-current density curve for MBAn-(4)-tBu-doped CBP device.

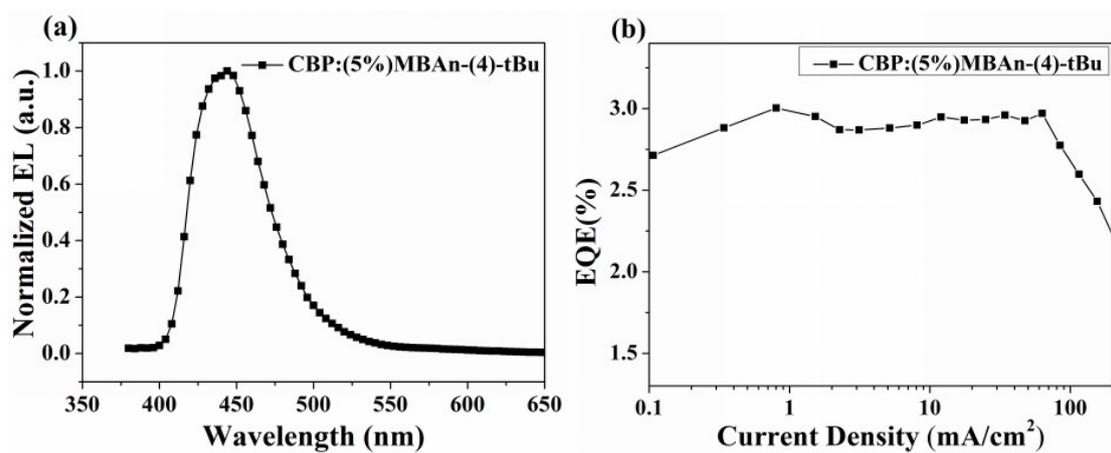


Fig. S4 (a) Normalized EL spectra of MBAn-(4)-tBu device, (b) External quantum efficiency-current density curves for MBAn-(4)-tBu-doped CBP device.

Table S2 EL performance of the MBAn-(4)-tBu-doped CBP device

EML	V_{on}^a	λ_{EL}^b	L_{max}^c	η_c^d	η_p^d	η_{ext}^d	FWHW	CIE (x, y) ^b
	(V)	(nm)	(cd m ⁻²)	(cd A ⁻¹)	(lm W ⁻¹)	(%)	^b (nm)	
CBP: MBAn-(4)-tBu	3.3	444	3874	1.96	1.69	3.00	55	(0.15, 0.07)

^a Turn-on voltage at 1 cd m⁻². ^b Values collected at 8 V. ^c Maximum luminance. ^d Values collected at a peak efficiency.