Electronic Supplementary Information

Aromatic-imide-based TADF enantiomers for efficient circularly

polarized electroluminescence

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1. General information

All reagents were purchased from commercial sources and used without further purification. ¹H and ¹³C NMR spectra were recorded on AVIII 500 MHz NMR spectrometers in CDCl₃ solutions. High-resolution mass spectra were measured on a Thermo Fisher® Exactive high resolution LC-MS spectrometer. Single crystal data was collected on a Bruker Smart APEXII CCD diffractometer using graphite monochromated Cu Ka radiation. The calculation was carried out with the Gaussian 09 software package.^[S1] Geometry optimizations were conducted under the B3LYP/6-31g(d) level of theory. The ground state geometries of **OBN-AICz** are optimized by density functional theory (DFT) using the B3LYP functional. The thermogravimetric analysis (TGA) was performed on a Q600 SDT thermal analyzer at a heating rate of 10 °C min⁻¹ in nitrogen. And differential scanning calorimetric (DSC) were performed on a Q2000 at a heating rate of 10 °C min⁻¹ in nitrogen. Cyclic voltammetry was performed using a CHI600A analyzer with a scan rate of 100 mV/s at room temperature to investigate the oxidation potentials. A conventional three electrode cell was used as electrolytic cell with a glassy carbon working electrode, an Ag/Ag⁺ (0.01 M AgNO₃) as the reference electrode, and Pt wire as the counter electrode. The oxidation potential was measured in CH₂Cl₂ with 0.1 M of tetra-*n*-butylammonium hexafluorophosphate (n-Bu₄NPF₆) as a supporting electrolyte. Ferrocene used as internal standard for calibrating the reference electrode.

UV-Vis spectra were recorded on PerkinElmer[®] UV/Vis/NIR spectrometer (Lambda 950). The photoluminescence spectra, transient PL decay characteristics and absolute photoluminescence quantum yields (PLQYs) were measured on an Edinburgh Instruments FLS 1000 spectrometer. The circular dichroism (CD) spectra were recorded on a JASCO J810 spectropolarimeter. The circularly polarized photoluminescence (CPL) measurements were performed utilizing a commercialized instrument JASCO CPL-300 spectrophotometer.

The OLED devices were fabricated by vacuum deposition onto pre-coated ITO glass substrates at a low pressure (1×10^{-5} mbar) for organic and metal deposition successively.

Indium tin oxide (ITO) coated glass with a sheet resistance of 10 Ω per square was used as the anode substrate. Before the fabrication of devices, the ITO glass substrates were cleaned with Decon 90, rinsed in ultrapure water and ethanol, dried in an oven at 120 °C, and finally treated with O₂ plasma for 2 minutes to enhance the surface work function of ITO anode. The electroluminescence and current-voltage-luminance characteristics of the devices were measured with a computer-controlled Spectrascan PR 670 spectrophotometer and Keithley 2400 SourceMeter after device packaging. Circularly polarized electroluminescence (CPEL) spectra were recorded on an instrument JASCO CPL-300 spectrophotometer.

2. X-ray crystal structure analysis



Fig. S1 Crystal packing of S-OBN-AICz (CCDC: 2107122).

Identification code	2107122			
Empirical formula	$C_{116}H_{82}N_6O_8$			
Formula weight	1687.87			
Temperature/K	169.99(10)			
Crystal system	monoclinic			
Space group	P21			
a/Å	12.3309(2)			
b/Å	20.9732(4)			
c/Å	18.7365(4)			
α/°	90			
β/°	91.942(2)			
$\gamma^{/\circ}$	90			
Volume/Å ³	4842.82(16)			
Z	2			
$\rho_{calc}g/cm^3$	1.157			
μ/mm^{-1}	0.576			
F(000)	1768			
Crystal size/mm ³	0.5 imes 0.3 imes 0.2			
Radiation	Cu Ka ($\lambda = 1.54184$)			
2Θ range for data collection/°	4.718 to 151.512			
Index ranges	$-15 \leq h \leq 15, -26 \leq k \leq 25,$			
	$0 \leq 1 \leq 23$			
Reflections collected	19174			
Independent reflections	19174 [R _{sigma} = 0.0369]			
Data/restraints/parameters	19174/558/1300			
Goodness-of-fit on F ²	2.232			
Final R indexes [I>= 2σ (I)]	$R_1 = 0.1020, wR_2 = 0.2862$			
Final R indexes [all data]	$R_1 = 0.1087, wR_2 = 0.2907$			
Largest diff. peak/hole / e Å ⁻³	0.67/-0.49			
Flack parameter	0.21(6)			

 Table S1 Crystal data and structure refinement for S-OBN-AICz.

3. Thermal and electrochemical properties



Fig. S2 TGA thermogram of *R*-**OBN-AICz** recorded under nitrogen at a heating rate of 10 $^{\circ}$ C min⁻¹.



Fig. S3 DSC curves of *R*-OBN-AICz recorded under nitrogen at a heating rate of 10 $^{\circ}$ C min⁻¹.



Fig. S4 Cyclic voltammograms of *R*-OBN-AICz measured in dichloromethane.

4. Photophysical properties



Fig. S5 UV-Vis absorption spectra of *R*-OBN-AICz in different solvents.



Fig. S6 PL spectra of *R*-OBN-AICz in different solvents.



Fig. S7 Fluorescence and phosphorescence spectra at 77K in neat film of *R*-OBN-AICz.



Fig. S8 Fluorescence and phosphorescence spectra at 77K in neat film of S-OBN-AICz.

5. Chiroptical properties



Fig. S9 The g_{abs} spectra of *R*-OBN-AICz and *S*-OBN-AICz in toluene.



Fig. S10 The gPL spectra of *R*-OBN-AICz and *S*-OBN-AICz in toluene.



Fig. S11 CPL spectra of *R*-OBN-AICz and *S*-OBN-AICz in doped films.



Fig. S12 The gPL spectra of *R*-OBN-AICz and *S*-OBN-AICz in doped films.

6. Device fabrication and characterization



Fig. S13 Molecular structures of used materials and energy level diagrams of OLEDs.

The OLEDs had the structure: ITO/TAPC (40 nm)/mCBP (10 nm)/mCBP:13 wt% *R*-**OBN-AICz** (20 nm)/ETL (45 nm)/LiF (1 nm)/Al (100 nm). In which, ITO is indium tin oxide, TAPC used as hole-transporting layer, mCBP was acted as electron blocking layer and host, respectively. LiF and Al were utilized as electron-injection layer and the cathode, respectively. Additionally, TmPyPB, TPBi, Bphen and B3PYPB were used as electron-transporting layer, the corresponding devices were **A**, **B**, **C**, and **D**, respectively. The energy diagram and chemical structures of the materials used in device were shown in Fig. S13. The OLED performances were shown in Fig. S14-S18 and summarized in Table S2.



Fig. S14 EQE-luminance characteristics of device A, B, C and D.



Fig. S15 Current density-voltage-luminance (J-V-L) characteristics device A, B, C and D.



Fig. S16 Current efficiency-luminance characteristics of device A, B, C and D.



Fig. S17 Power efficiency-luminance characteristics of device A, B, C and D.



Fig. S18 EL spectra of device A, B, C and D.

Table S2. EL performances of device A, B, C and D.

Device	ETL	V [V]	$\lambda_{_{\rm EL}} [{ m nm}]$	EQE _{max} [%]	CE _{max} [cd A ⁻¹]	PE _{max} [lm W ⁻¹]	<i>L</i> _{max} [cd m ⁻²]
A	TmPyPB	3.8	514	17.5	52.2	43.2	11610
В	TPBi	4.0	514	8.0	23.6	12.3	14470
С	Bphen	3.9	514	8.1	24.0	15.4	13420
D	B3PYPB	3.7	514	16.5	49.7	37.2	13880

Then, we screened the thickness of each layer in the TmPyPB-based devices. Device E: ITO/TAPC (45 nm)/mCBP (10 nm)/mCBP:13 wt% *R*-OBN-AICz (20 nm)/TmPyPB (45 nm)/LiF (1 nm)/Al (100 nm). Device F: ITO/TAPC (40 nm)/mCBP (5 nm)/mCBP:13 wt% *R*-OBN-AICz (20 nm)/TmPyPB (45 nm)/LiF (1 nm)/Al (100 nm). Device G: ITO/TAPC (40 nm)/mCBP (10 nm)/mCBP:13 wt% *R*-OBN-AICz (20 nm)/TmPyPB (50 nm)/LiF (1 nm)/Al (100 nm). Device H: ITO/TAPC (40 nm)/mCBP (10 nm)/mCBP:13 wt% *R*-OBN-AICz (25 nm)/TmPyPB (45 nm)/LiF (1 nm)/Al (100 nm). The OLED performances were shown in Fig. S19-S23 and summarized in Table S3.



Fig. S19 EQE-luminance characteristics of device E, F, G and H.



Fig. S20 Current density-voltage-luminance of device E, F, G and H.



Fig. S21 Current efficiency-luminance characteristics device E, F, G and H.



Fig. S22 Power efficiency-luminance characteristics of device E, F, G and H.



Fig. S23 EL spectra of device E, F, G and H.

Table S3. EL performances of device E, F, G and H.

Device	V [V]	$\lambda_{_{ ext{EL}}}$ [nm]	EQE _{max} [%]	CE _{max} [cd A ⁻¹]	PE _{max} [lm W ⁻¹]	<i>L</i> _{max} [cd m ⁻²]
Ε	3.8	514	16.7	49.4	40.9	14760
F	3.7	512	16.8	49.4	41.9	15440
G	3.8	514	17.8	53.2	43.5	14800
Η	3.9	514	16.7	49.3	39.5	14690



Fig. S24 Current density-voltage-luminance of optimized S-OBN-AICz-based OLEDs.



Fig. S25 EL spectra of optimized S-OBN-AICz-based OLEDs.



Fig. S26 Efficiency-luminance characteristics of optimized *S*-OBN-AICz-based OLEDs.

7. NMR spectra of new compounds



Fig. S27 ¹H NMR spectrum of *R*-OBN-AI2F in CDCl₃ (500 MHz).



Fig. 28¹³C NMR spectrum of *R*-OBN-AI2F in CDCl₃ (126 MHz).





210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 Fig. S30 ¹³C NMR spectrum of *R*-OBN-AICz in CDCl₃ (126 MHz).



210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 Fig. S32 ¹³C NMR spectrum of *S*-OBN-AICz in CDCl₃ (126 MHz).