Incorporating tercarbazole donor in spiro-type host material for efficient RGB phosphorescent organic light-emitting diodes

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1. Chemicals and instruments

All chemicals and reagents were used as received from commercial resources without further purification. Tetrahydrofuran (THF), 1,4-dioxane and N,N-dimethylformamide (DMF) used in synthetic routes were purified by PURE SOLV (Innovative Technology) purification system. ¹H NMR and ¹³C NMR spectra were measured on a Bruker 400 spectrometer at room temperature. Mass spectra and time of Flight MS-MALDI (MALDI-TOF) were performed on a Thermo ISQ mass spectrometer using a direct exposure probe and Bruker Autoflex II/Compass 1.0, respectively. UV-vis absorption spectra were recorded on a Perkin Elmer Lambda 750 spectrophotometer. Photoluminescence (PL) spectra and phosphorescent spectra were performed on Hitachi F-4600 fluorescence spectrophotometer. Differential scanning calorimetry (DSC) was performed on a TA DSC 2010 unit at a heating rate of 10 °C/min under nitrogen. The glass transition temperature (T_g) was determined from the second heating scan. Thermogravimetric analysis (TGA) was performed on TA SDT 2960 instrument at a heating rate of 10 °C/min under nitrogen, the temperature at 5% weight loss was used as the decomposition temperature (T_d).

The electrochemical measurement was made using a CHI600 voltammetric analyzer. A conventional three-electrode configuration consisting of a platinum working electrode, a Pt-wire counter electrode, and an Ag/AgCl reference electrode were used. The solvent in the measurement was CH_2Cl_2 , and the supporting electrolyte was 0.1 M [Bu₄N]PF₆. Ferrocene was added as a calibrant after each set of measurements, and all potentials reported were quoted with reference to the ferrocene-ferrocenium (Fc/Fc⁺) couple at a scan rate of 100 mV/s. Theoretical calculations based on density functional theory (DFT) approach at the B3LYP/6-31G (d) level were performed with the use of the Gaussian 09 program.

2. OLED fabrication and measurements

OLED devices were fabricated on ITO glass substrates (15 Ω per square). The emitting area of each device was 0.09 cm². The substrates were cleaned with ethanol, acetone and deionized water, and then dried in an oven before being exposed to UV ozone for 30 minutes. All of the organic materials and metal layers were deposited under a vacuum of ca. 10⁻⁶ Torr. The Electroluminescence spectra and current density-voltage (J-V-L) characteristics of the devices were measured using a constant current source (Keithley 2400 SourceMeter) combined with a photometer (Photo Research SpectraScan PR 655).



Fig. S1 a) PL spectra of the doped films (50 nm) of 15 wt% **FIrpic**: **TCZSO**₂, 12 wt% **Ir(ppy)**₂(**acac**): **TCZSO**₂ and 6 wt% **Ir(MDQ)**₂(**acac**): **TCZSO**₂; b) time-resolved transient PL spectra of the doped films (50 nm) of 15 wt% **FIrpic**: **TCZSO**₂, 12 wt% **Ir(ppy)**₂(**acac**): **TCZSO**₂ and 6 wt% **Ir(MDQ)**₂(**acac**): **TCZSO**₂.



Fig. S2 Current density versus voltage characteristic of the hole- and electron-only devices for TCZSO2.



Fig. S3 Device performance of TCZSO₂ and mCP.



Fig. S4 EQE curve of the TCZSO₂-based devices.

Device	V ^{a)}	CE ^{b)}	PE ^{b)}	EQE ^{b)}	CIE ^{c)}
_	(V)	(cd A ⁻¹)	(lm W ⁻¹)	(%)	
TCZSO ₂	3.6	47.8, 47.7, 45.4	40.3, 34.0, 26.9	22.8, 22.7, 21.6	(0.15, 0.35)
mCP	4.4	40.0, 37.8, 31.5	29.1, 22.4, 14.4	18.7, 17.7, 14.6	(0.16, 0.35)

Table. S1 Electroluminescence characteristics of TCZSO2 and mCP.

^{a)} The driving voltage at 100 cd m⁻²; ^{b)} external quantum efficiency (EQE) and current efficiency (CE) in the order of maximum, at 1000 cd m⁻² and at 5000 cd m⁻²; c) recorded at 10 mA cm⁻².



Fig. S5 Mass (MALDI-TOF) spectrum of TCZSO2.



