

Supporting information for:

A *m*-Terphenyl-modified Sulfone Derivative as a Host Material for High-Efficiency Blue and Green Phosphorescent OLEDs

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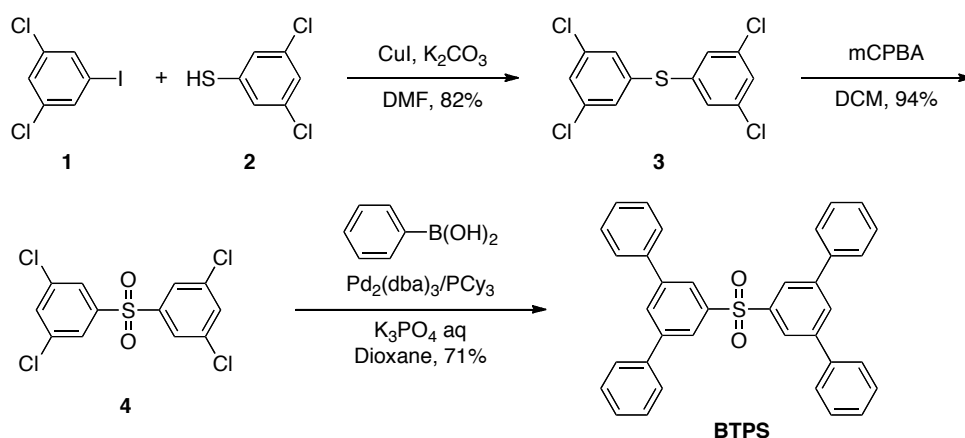
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General Procedures. The optimized structures and single-point energies were calculated by Gaussian09¹ at the RB3LYP 6-31G(d) and 6-311+G(d,p) levels for the ground state. The E_{T1} energy of BTPS was calculated by using TD-DFT method at the RB3LYP 6-31G(d) and 6-31G(d) levels. ¹H NMR spectrum was recorded on JEOL 400 (400 MHz) spectrometer. Mass spectrum was obtained using a JEOL JMS-K9 mass spectrometer. Differential scanning calorimetry (DSC) was performed using a Perkin-Elmer Diamond DSC Pyris instrument under nitrogen atmosphere at a heating rate of 10°C min⁻¹. Thermogravimetric analysis (TGA) was undertaken using a SEIKO EXSTAR 6000 TG/DTA 6200 unit under nitrogen atmosphere at a heating rate of 10°C min⁻¹. UV-Vis spectra were measured using a Shimadzu UV-3150 UV-vis-NIR spectrophotometer. Photoluminescence spectra were measured using a FluroMax-2 (Jobin-Yvon-Spex) luminescence spectrometer. The ionization potential (I_p) was determined by an photoelectron yield spectroscopy (PYS)² under the vacuum (~10⁻³ Pa). The phosphorescent spectra were measured by using a streak camera (C4334 from Hamamatsu Photonics) at 5 K. The current density–luminance–voltage characteristics of the OLEDs were measured by Keithley source meter 2400 and Konica Minolta CS-200, respectively. Electroluminescence (EL) spectra were taken by an optical mutichannel analyzer, Hamamatsu PMA 11.

(1) M. J. Frisch et al. Gaussian 09; Gaussian Inc.: Pittsburgh, PA 2009.

(2) H. Ishii, D. Tsunami, T. Suenaga, N. Sato, Y. Kimura, M. Niwano, *J. Surf. Sci. Soc. Jpn.* **2007**, 28, 264.

Synthesis of BTPS.



Scheme 1. Synthetic route of BTPS.

Synthesis of bis(3,5-dichlorophenyl)sulfide (BCPS **3**)³

3,5-dichloriodobenzene **1** (22.6 g, 82.8 mmol) and dimethylformamide (200 ml) were added to a round bottom flask. After nitrogen flow for 2 hours, 3,5-dichlorothiophenol **2** (14.80 g, 82.6 mmol), potassium carbonate (22.80 g, 165 mmol) and copper(I)iodide (1.57 g, 8.24 mmol) were added. The resultant mixture was stirred for 3 hours at 100 °C under N₂ flow and cooled to room temperature. The precipitate was filtered. The filtrate was evaporated to dryness and poured into water (200 ml). The resulting off-white solid was filtered and purified by chromatography on silica gel (eluent: hexane = 10) to afford BCPS **3** (25.0 g, 94 %) as a off-white solid: ¹H-NMR (400 MHz, CDCl₃): δ = 7.31 (t, 2H, *J* = 1.8 Hz), 7.22 (d, 4H, *J* = 1.8 Hz) ppm; MS: *m/z* 324 [M]⁺.

Synthesis of bis(3,5-dichlorophenyl)sulfone(BCPSO **4**)³

At 0 °C, BCPS **3** (14.3 g, 44.1 mmol) in dichloromethane (125 ml) was added dropwise to a slurry of *m*-chloroperbenzoic acid (25.8 g, 97.2 mmol) in dichloromethane (200 ml) keeping the temperature at 0–10 °C. The resultant mixture was stirred for 12 hours at room temperature. Then, saturated NaHCO₃ solution (300 ml) was added to the mixture and stirred for 30 minutes. The organic layer was separated and dried over anhydrous MgSO₄, filtered, and evaporated to dryness. The resulting white solid was dissolved in reflux toluene (100 ml), filtered through a silica-gel pad (50 g). The clear filtrate was evaporated to dryness. The resulting white solid was purified by recrystallization from toluene/ethanol (25 ml/5 ml) to afford BCPSO **4** (12.8 g, 82 %) as a white solid: ¹H-NMR (400 MHz, CDCl₃): δ = 7.80 (d, 4H, *J* = 1.8 Hz), 7.60 (t, 2H, *J* = 1.8 Hz) ppm; MS: *m/z* 356 [M]⁺.

Synthesis of 5',5'''-sulfonyl-di-1,1':3',1''-terphenyl (BTPS)

BTPSO **4** (4.50 g, 12.4 mmol) and phenylboronic acid (8.01 g, 65.7 mmol) were added to a round bottom flask. 1,4-Dioxane (375 ml) and aqueous K₃PO₄ (1.35 M, 65.4 ml) were added and nitrogen bubbled through the mixture for 1 hour. Then, Pd₂(dba)₃ (570 mg, 616 μmol) and PCy₃ (450 mg, 1.60 mmol) were added and the resultant mixture was vigorously stirred for 24 hours at reflux temperature under N₂ flow. The resulting mixture was cooled to room temperature. The precipitate was filtered, and washed with 1,4-dioxane, water and methanol. The resulting off-white solid was dissolved in reflux toluene (300 ml), filtered through a silica-gel pad (30 g). The clear filtrate was evaporated to dryness. The resulting white solid was purified by recrystallisation from toluene to afford BTPS (4.66 g, 71 %) as a white solid: ¹H-NMR (400 MHz, CDCl₃): δ = 8.18 (d, 4H, *J* = 1.6 Hz), 7.97 (t, 2H, *J* = 1.6 Hz), 7.65-7.63 (m, 8H), 7.52-7.40 (m, 12H) ppm; MS: *m/z* 523 [M]⁺ ; Anal. Calcd for C₃₆H₂₆O₂S: C, 82.73, H 5.01, S 6.14 %; found: C 82.81, H 4.89, S 6.34 %.

(3) P. C. Taylor, M. D. Wall, P. R. Woodward, *Tetrahedron* **2005**, *61*, 12314.

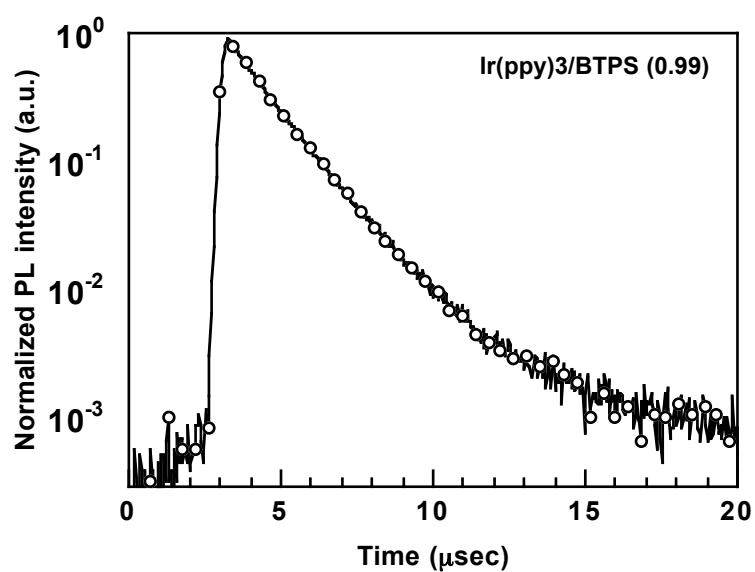
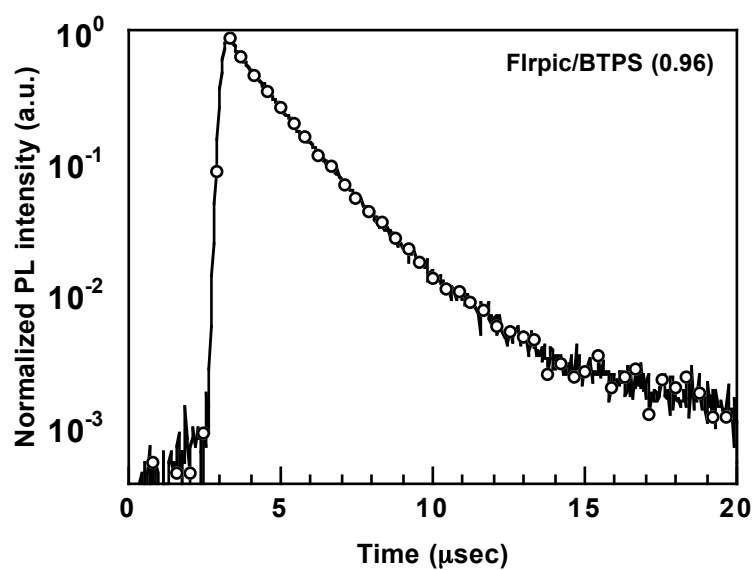


Figure S-1. Transient photoluminescence decay curve of (a) 5 wt% Flrpic/BTPS film (top) and (b) 5 wt% Ir(ppy)₃/BTPS film (bottom) at room temperature (film thickness: 30 nm).

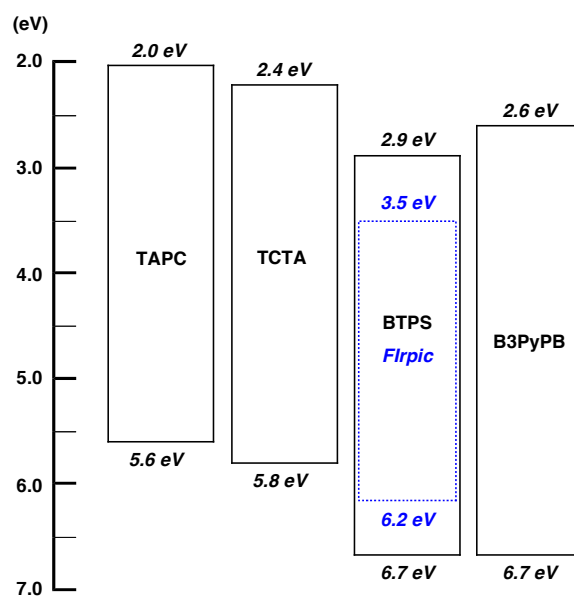


Figure S-2. Energy diagram of FIrpic-based device.

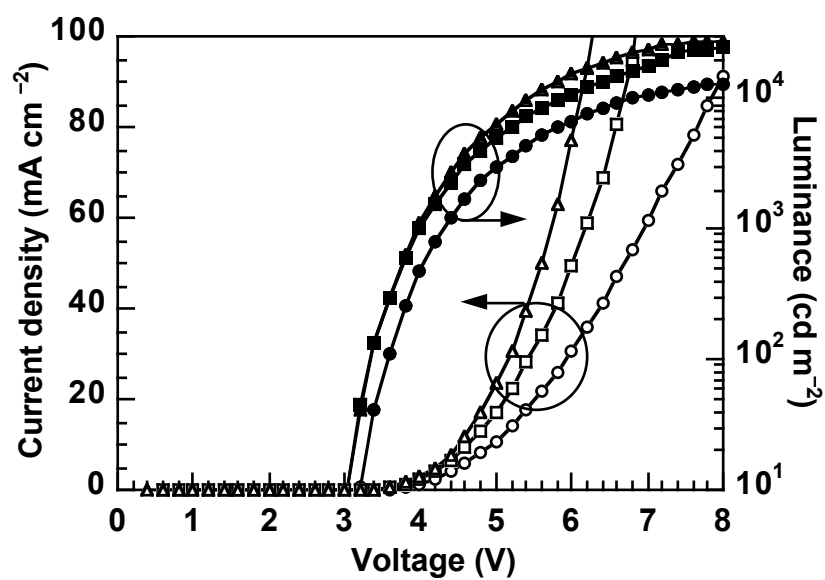


Figure S-3. $J-V-L$ characteristics of FIrpic-based device. 5 wt% (circle), 10 wt% (square) and 15 wt% (triangle) doped device, respectively.

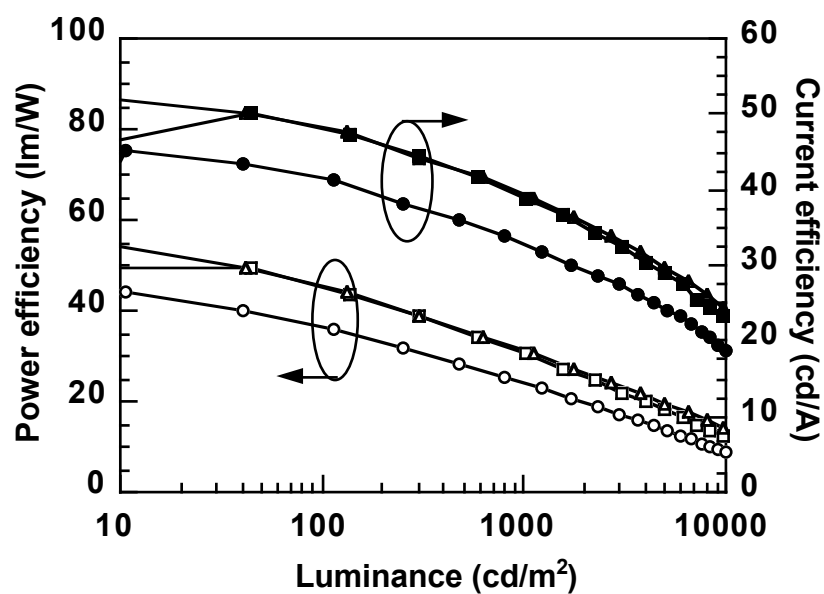


Figure S-4. *CE-L-PE* characteristics of FIrpic-based device. 5 wt% (circle), 10 wt% (square) and 15 wt% (triangle) doped device, respectively.

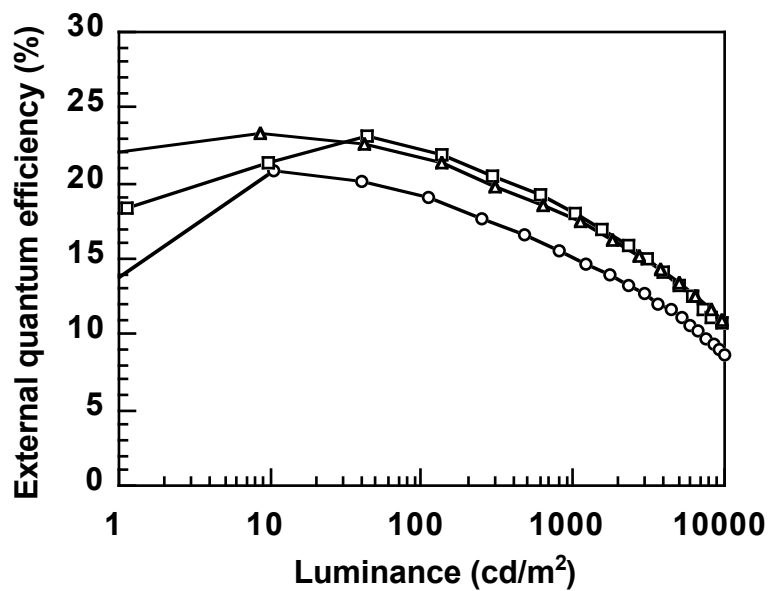


Figure S-5. *EQE-L* characteristics of FIrpic-based device. 5 wt% (circle), 10 wt% (square) and 15 wt% (triangle) doped device, respectively.

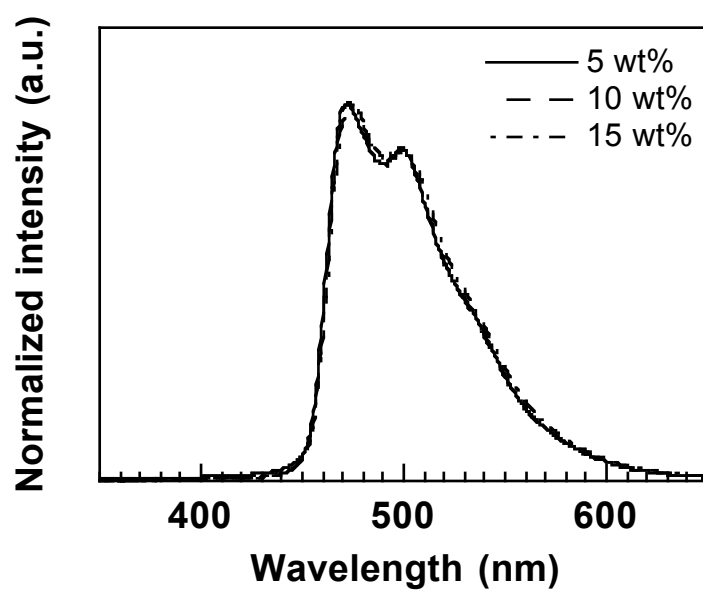


Figure S-6. EL spectra of FIrpics-based device.

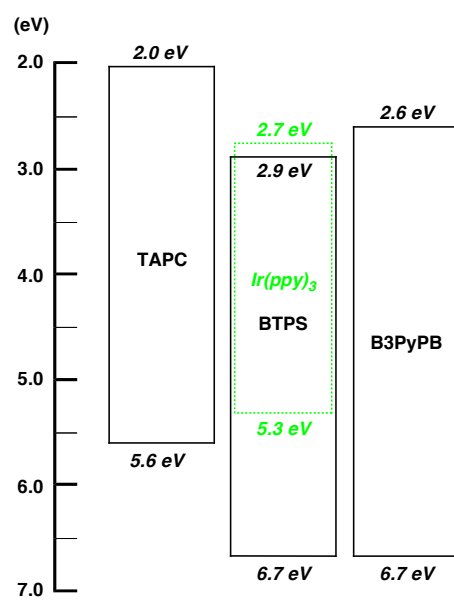


Figure S-7. Energy diagram of FIrpics-based device.

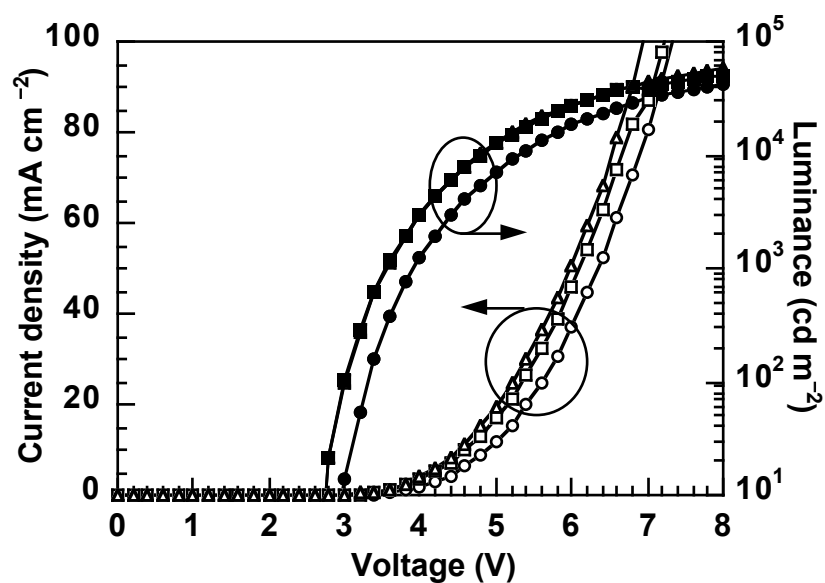


Figure S-8. J - V - L characteristics of Ir(ppy)_3 -based device. 5 wt% (circle), 10 wt% (square) and 15 wt% (triangle) doped device, respectively.

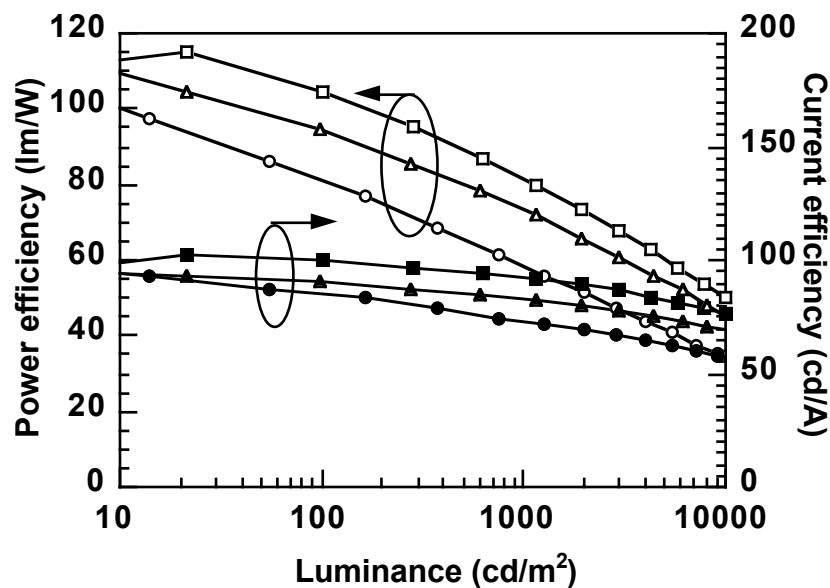


Figure S-9. CE - L - PE characteristics of Ir(ppy)_3 -based device. 5 wt% (circle), 10 wt% (square) and 15 wt% (triangle) doped device, respectively.

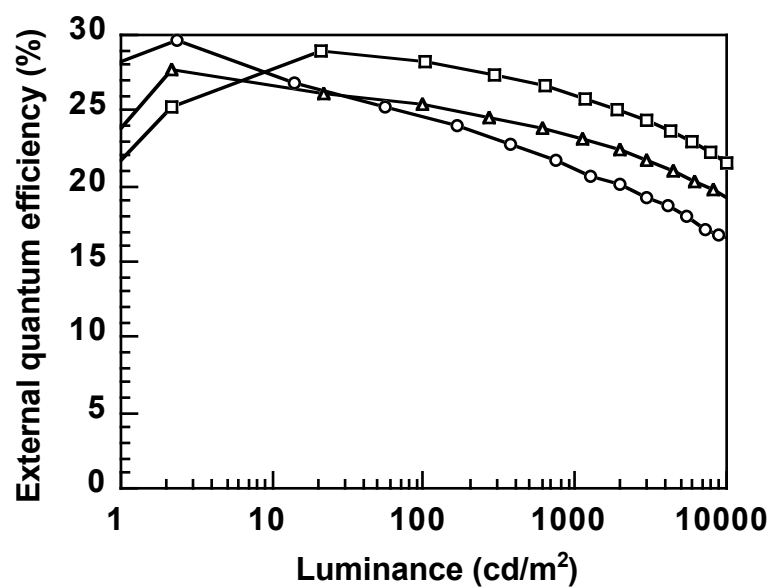


Figure S-10. *EQE-L* characteristics of Ir(ppy)₃-based device. 5 wt% (circle), 10 wt% (square) and 15 wt% (triangle) doped device, respectively.

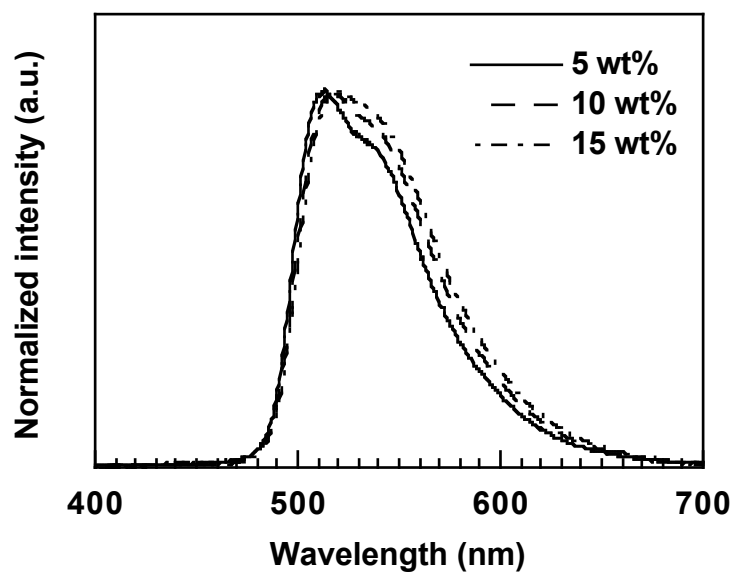


Figure S-11. EL spectra of Ir(ppy)₃-based device.

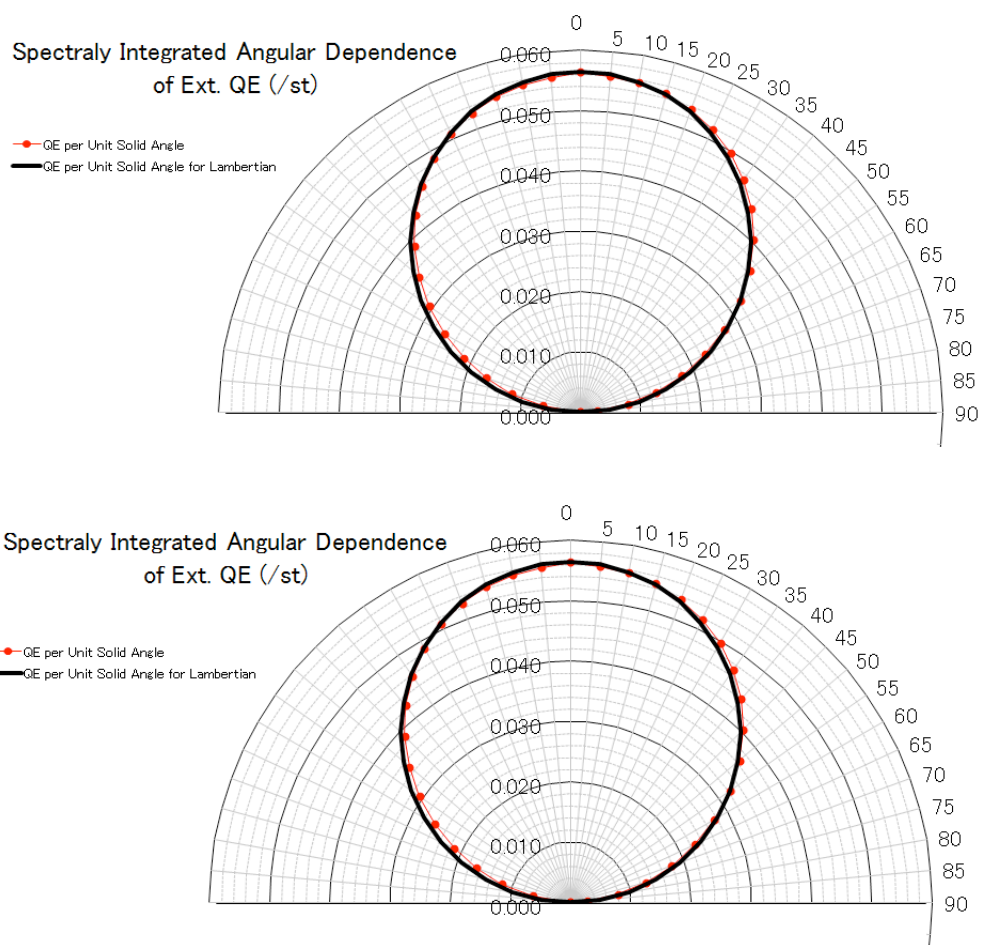


Figure S-10. The angular dependence of luminous intensity in OLED with (a) 10 wt%-doped OLED (top: Lambertian factor = 0.968), (b) 15 wt%-doped OLED (bottom: Lambertian factor = 0.956).

Table S1. Summary of OLED performances.

Device	$\eta_{p,100}/\eta_{e,100}/V_{100}/EQE$ [a] [lm W ⁻¹ /cd A ⁻¹ /V/%]	$\eta_{p,1000}/\eta_{p,1000}/V_{1000}/EQE$ [b] [lm W ⁻¹ /cd A ⁻¹ / V/%]	CIE _{x,y} [c]	$J_{1/2}$ [d] [mA cm ⁻²]
Green(5 wt%)	82.0/85.6/3.28/24.8	59.1/73.2/3.89/21.2	(0.30,0.63)	44.5
Green(10 wt%)	105/100/3.00/28.2	82.0/92.4/3.54/26.1	(0.31,0.63)	71.9
Green(15 wt%)	94.4/90.2/3.00/25.3	73.4/82.8/3.55/23.2	(0.32,0.62)	90.1
Blue(5 wt%)	36.7/41.6/3.56/19.2	24.1/32.9/4.29/15.2	(0.16,0.38)	25.9
Blue(10 wt%)	45.8/48.4/3.32/22.3	30.8/39.1/3.99/18.1	(0.16,0.38)	28.0
Blue(15 wt%)	46.0/48.6/3.33/21.8	31.4/39.4/3.95/17.7	(0.17,0.39)	30.8

[a] Power efficiency (PE), current efficiency (CE), voltage (V) and external quantum efficiency (EQE) at 100 cd m⁻². [b] PE, CE, V and EQE at 1000 cd m⁻². [c] Commission Internationale de L'Eclairage coordinates at 100 cd m⁻². [d] Current density at half the maximum EQE.