# Supporting Information

# Triphenylsilyl-Promoted Iridium Complex for High-Performance Green-Yellow Phosphorescent Organic Light-Emitting Diodes

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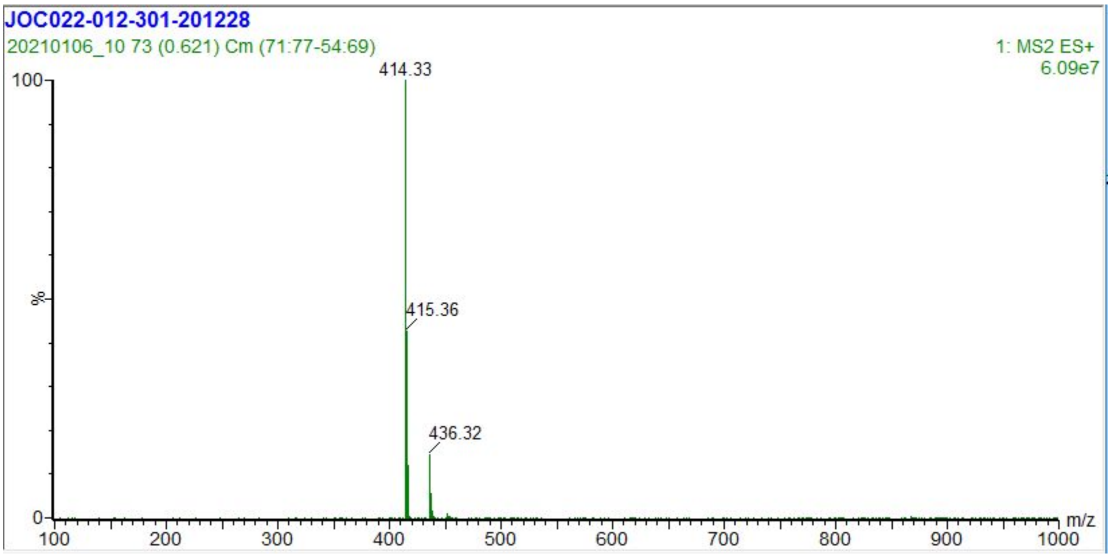


**Figure S1.** Mass spectrum of tpsp.

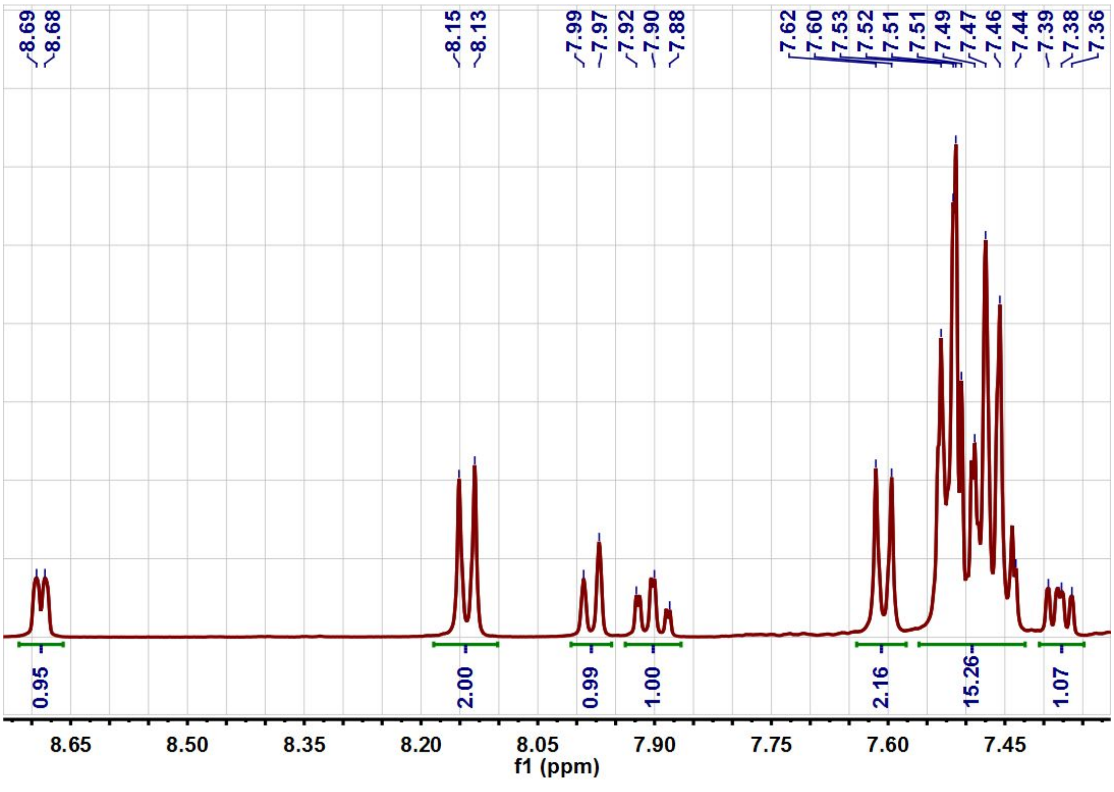


**Figure S2.** The $^{1}$H NMR spectrum of tpsp in DMSO-$d_6$.

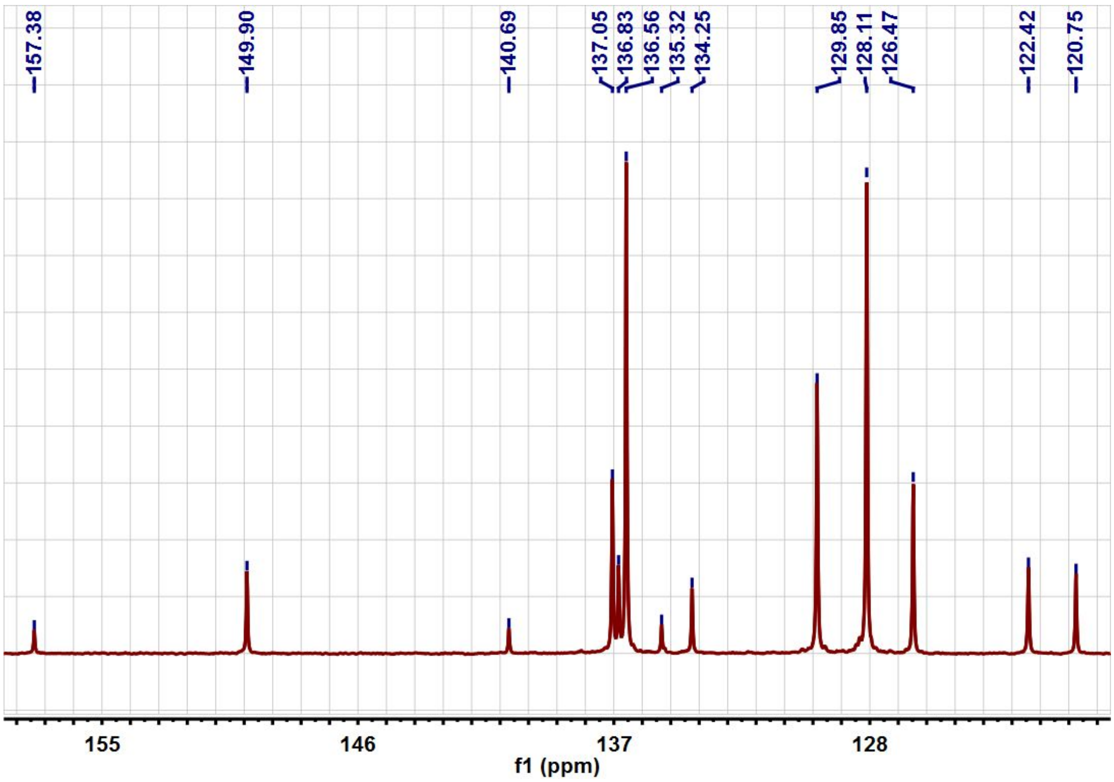


**Figure S3.** The $^{13}C$ NMR spectrum of tpsp in $CDCl_3$.

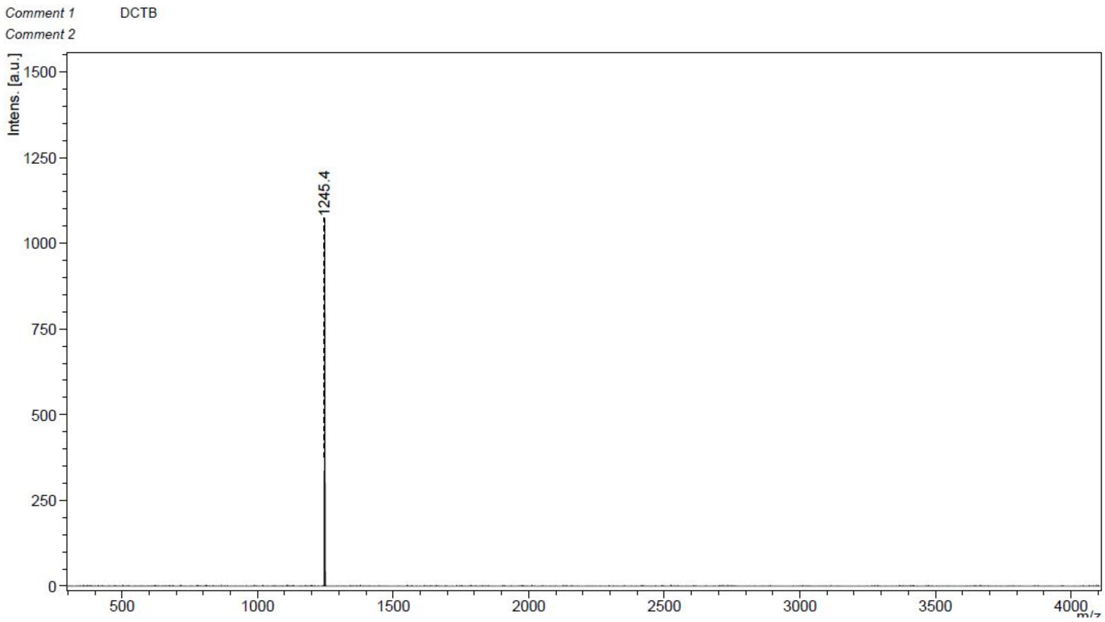


**Figure S4.** Mass spectrum of $Ir(tpsp)_2(bpp)$.

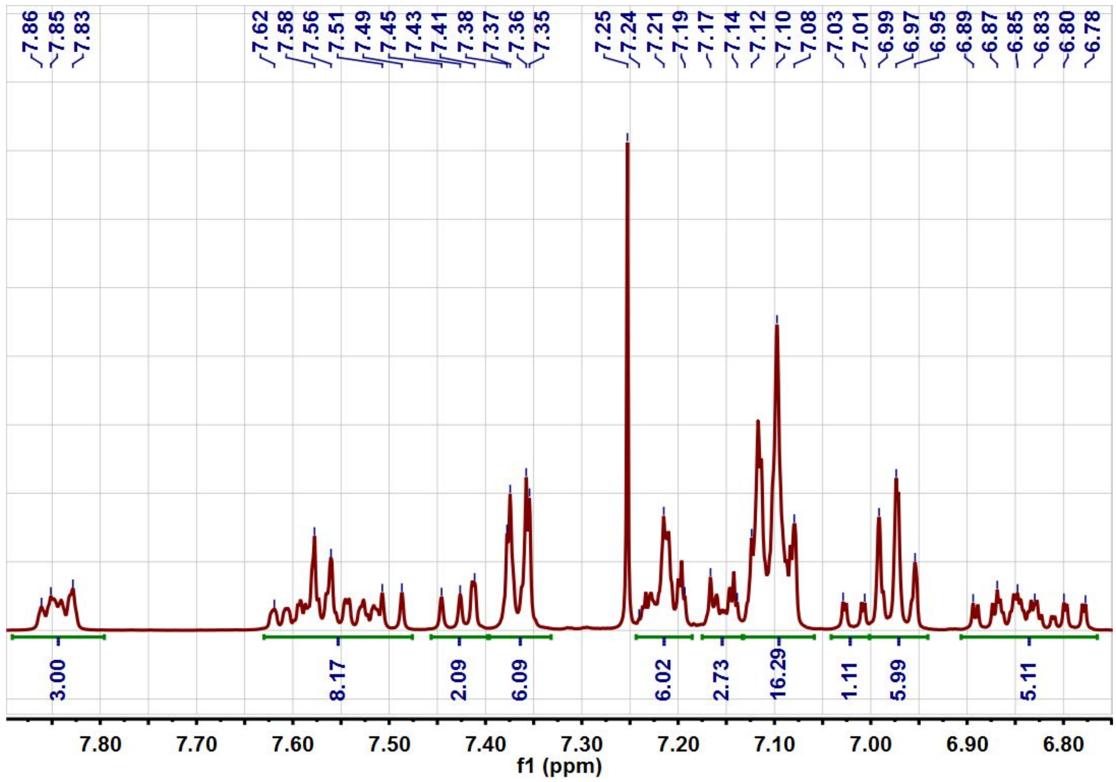


**Figure S5.** The $^{1}H$ NMR spectrum of $Ir(tpsp)_2(bpp)$ in $CDCl_3$.

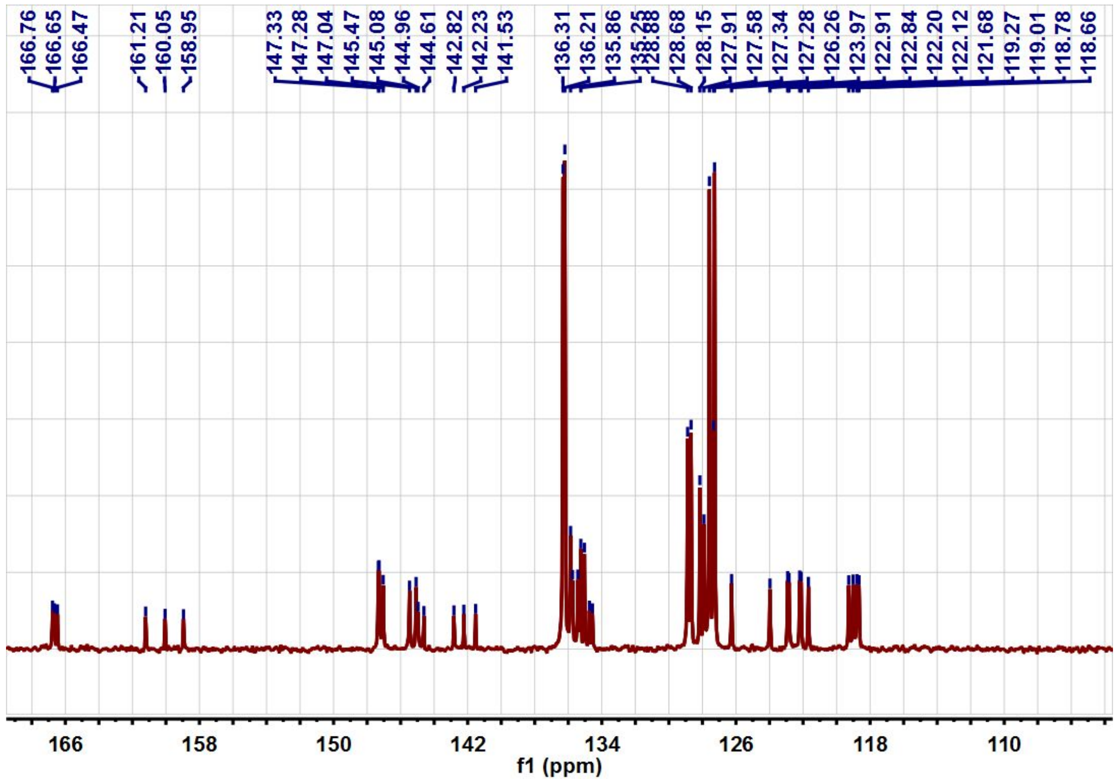


**Figure S6.** The $^{13}C$ NMR spectrum of $Ir(tpsp)_2(bpp)$ in $CDCl_3$.

**Table S1.** The frontier orbital energy levels and energy-level compositions of fac-Ir(tpsp)$_2$(bpp) from DFT calculations.

| Orbital | Energy (eV) | Ir | tpsp-1 | tpsp-2 | bpp | Main bond type |
|---|---|---|---|---|---|---|
| 290 | -0.98 | 0.43 | 56.45 | 31.99 | 11.13 | π*(Si) |
| 289 | -1.20 | 3.01 | 3.41 | 6.43 | 89.14 | π*(Ph) |
| 288 | -1.36 | 3.59 | 50.82 | 45.07 | 0.52 | π*(Si) |
| 287lumo | -1.42 | 0.84 | 44.95 | 46.19 | 8.02 | π*(Si) |
| 286homo | -4.80 | 37.09 | 7.85 | 19.01 | 36.05 | d+π(Si)+π(Ph) |
| 285 | -5.16 | 39.98 | 37.87 | 8.64 | 14.52 | d+π(Si)+π(Ph) |
| 284 | -5.50 | 8.12 | 3.78 | 18.44 | 69.77 | π(Si)+π(Ph) |
| 283 | -5.60 | 11.94 | 35.79 | 40.77 | 11.51 | d+π(Si)+π(Ph) |

**Table S2.** Calculated excited energies, dominant orbital excitation and oscillator strength(f) from TD-DFT calculations for complex fac-Ir(tpsp)$_2$(bpp).

| State | Excitation | $E_{calcd}$ eV | $\lambda_{calcd}$ nm | f | character |
|---|---|---|---|---|---|
| S1 | 286→287(0.61636) | 2.68 | 462 | 0.0193 | MLCT/LLCT/ILCT |
| S3 | 286→289(0.67976) | 2.90 | 428 | 0.0189 | MLCT/LLCT/ILCT |
| S5 | 285→288(0.65207) | 3.06 | 406 | 0.0227 | MLCT/LLCT/ILCT |
| S7 | 285→289(0.66322) | 3.30 | 375 | 0.0355 | MLCT/LLCT/ILCT |
| S9 | 283→287(0.49115) | 3.44 | 361 | 0.0192 | MLCT/LLCT/ILCT |
| S10 | 286→292(0.64002) | 3.45 | 359 | 0.0101 | MLCT/LLCT/ILCT |
| S22 | 284→289(0.36841) | 3.94 | 314 | 0.1331 | LLCT/ILCT |
| S39 | 284→291(0.53789) | 4.29 | 288 | 0.1224 | LLCT/ILCT |

**Table S3.** The frontier orbital energy levels and energy-level compositions of $Ir(ppy)_3$ from DFT calculations.

| Orbital | Energy(eV) | Ir | ppy-1 | ppy-2 | ppy-3 |
|---|---|---|---|---|---|
| 134 | -0.85 | 0.97 | 32.94 | 33.04 | 33.05 |
| 133 | -1.10 | 4.01 | 32.37 | 4.68 | 58.94 |
| 132 | -1.10 | 4.01 | 31.85 | 59.19 | 4.95 |
| 131lumo | -1.20 | 0.69 | 32.86 | 33.23 | 33.22 |
| 130homo | -4.85 | 49.46 | 16.87 | 16.8 | 16.87 |
| 129 | -4.98 | 41.39 | 34.64 | 8.58 | 15.39 |
| 128 | -4.98 | 41.4 | 4.41 | 30.54 | 23.65 |
| 127 | -5.83 | 2.71 | 54.21 | 2.06 | 41.02 |

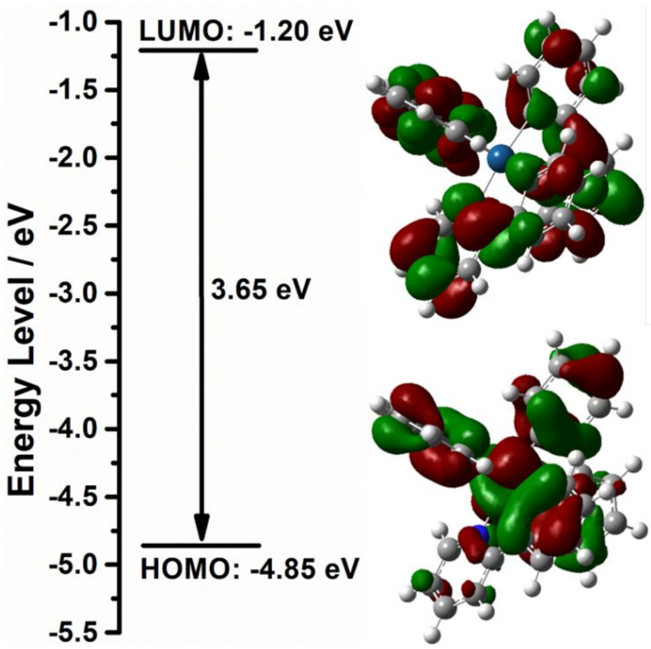


**Figure S7.** Frontier-molecular-orbital distributions, energy levels, and HOMO-LUMO energy gap for $Ir(ppy)_3$ characterized by DFT calculations.

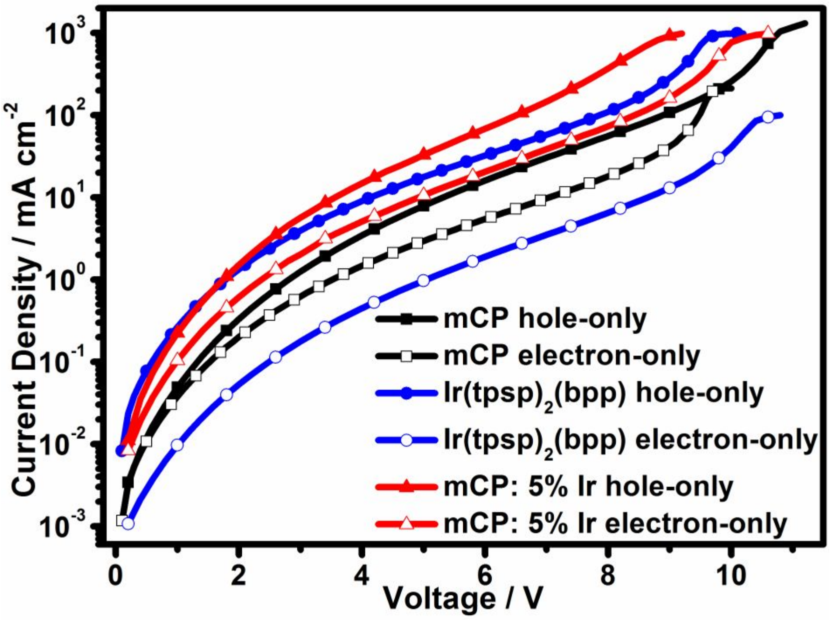


**Figure S8.** Current density versus voltage characteristics of the hole-only and electron-only devices of mCP, fac-Ir(tpsp)$_2$(bpp) and doped film (mCP: 5% fac-Ir(tpsp)$_2$(bpp)).

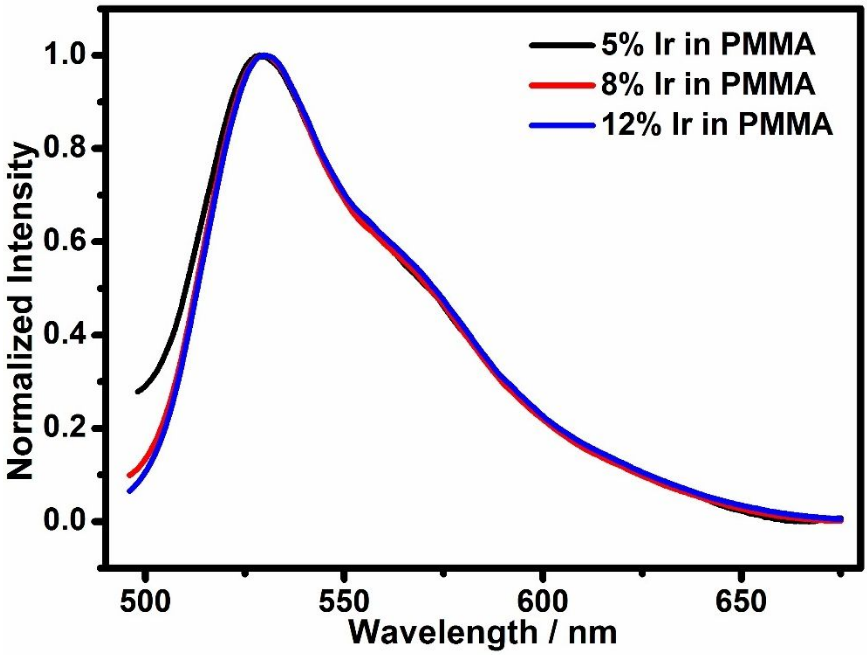


**Figure S9.** Room-temperature photoluminescence spectra of fac-Ir(tpsp)$_2$(bpp)-doped PMMA film (doped concentrations: 5%, 8% and 12%) on quartz.

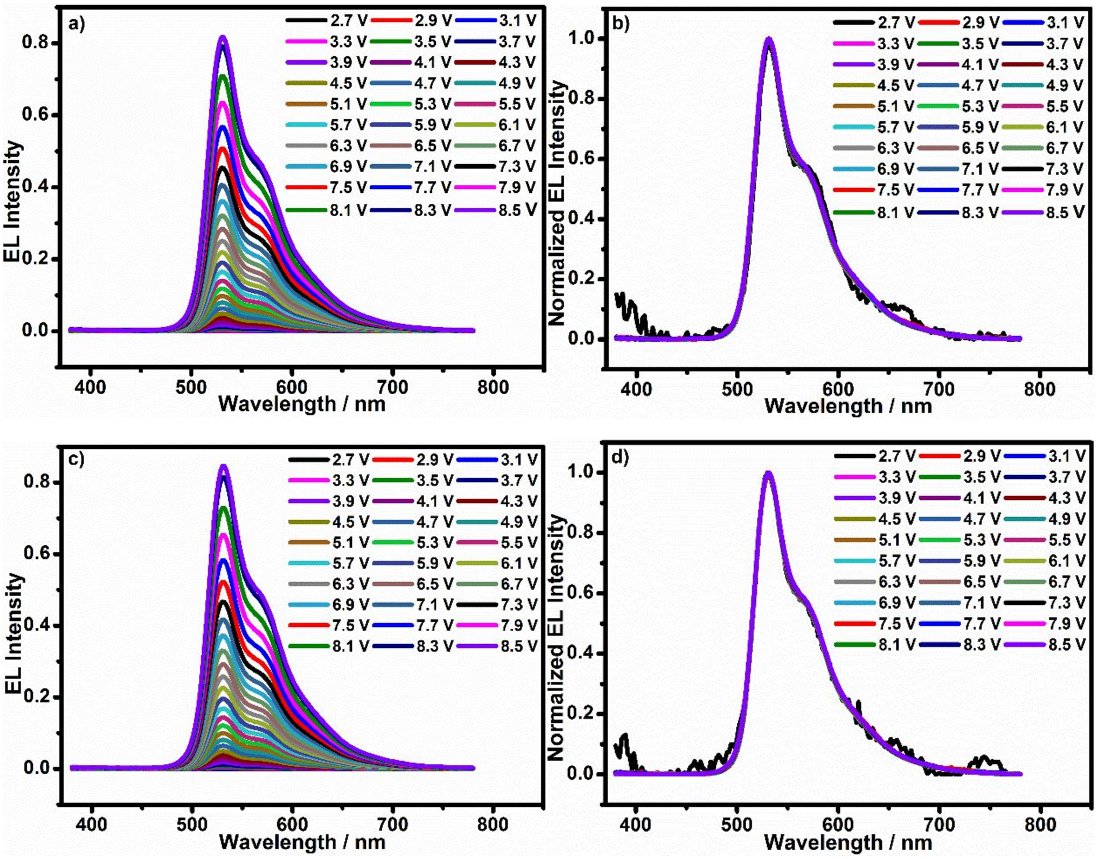


**Figure S10.** (a) EL spectra of device D1 at different voltages (from 2.7 to 8.5 V; interval: 0.2 V). (b) Normalized EL spectra of device D1 at different voltages (from 2.7 to 8.5 V; interval: 0.2 V). (c) EL spectra of device D3 at different voltages (from 2.7 to 8.5 V; interval: 0.2 V). (d) Normalized EL spectra of device D3 at different voltages (from 2.7 to 8.5 V; interval: 0.2 V).

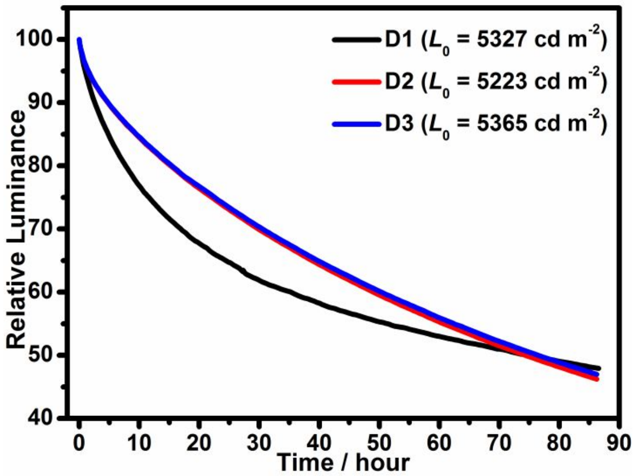


**Figure S11.** The operation lifetimes of devices D1, D2, D3 with an initial luminance of 5200-5400 cd m$^{-2}$.

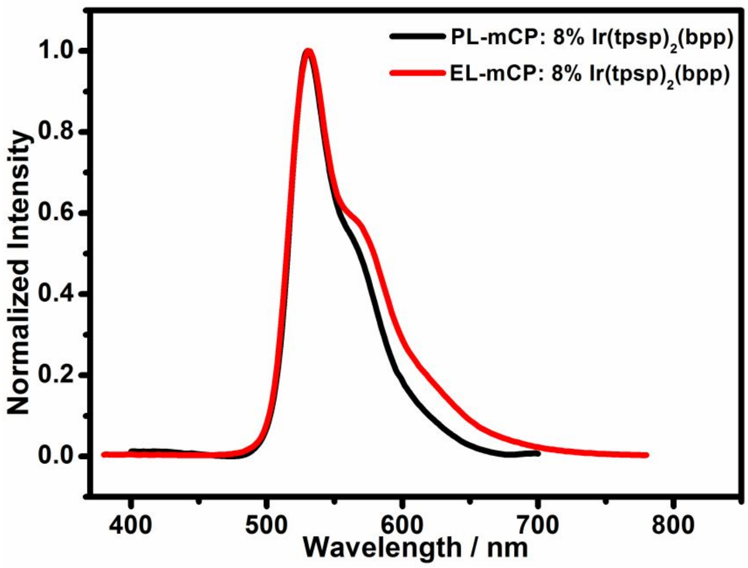


**Figure S12.** The photoluminescence and electroluminescent spectra of emitting layer (mCP: 8% fac-Ir(tpsp)$_2$(bpp)).

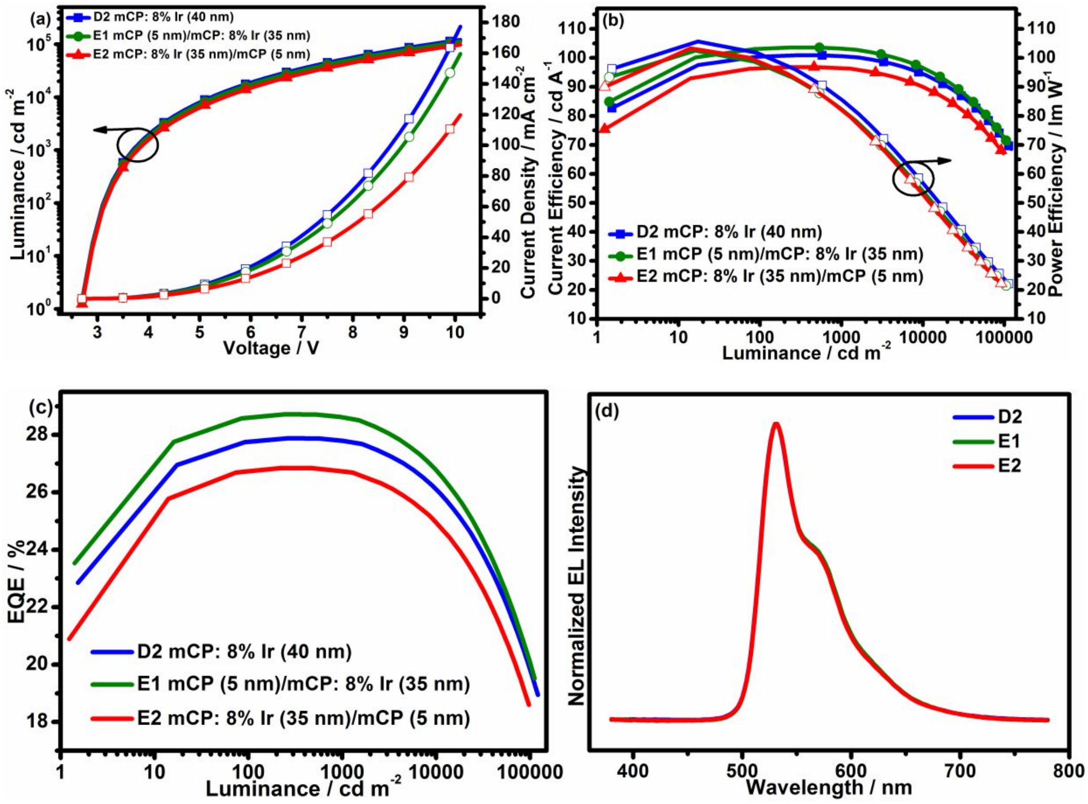


**Figure S13.** (a) Luminance-voltage-current density (L-V-J) curves of devices D2, E1, E2. (b) Current efficiency-luminance-power efficiency (CE-L-PE) curves of devices D2, E1, E2. (c) External quantum efficiency-luminance curves of devices D2, E1, E2. (d) Normalized EL spectra of devices D2, E1, E2 at the luminance of 100 cd/m$^2$.

**Table S4**. The electroluminescent performance of devices D2, E1, E2.

| Device | $V_{on}$ a) [V] | $L_{max}$ b) [cd m$^{-2}$] | $\eta_c$ c) [cd A$^{-1}$] | $\eta_p$ c) [lm W$^{-1}$] | $\eta_{ext}$ c) [%] | CIE (x,y) d) |
|---|---|---|---|---|---|---|
| D2 | 2.7 | 121600 | 100.9, 100.4, 100.6, 95.1 | 105.6, 101.8, 85.4, 58.6 | 27.9, 27.7, 27.8, 26.3 | 0.37, 0.60 |
| E1 | 2.7 | 112358 | 103.6, 103.1, 103.3, 96.6 | 102.5, 98.7, 82.8, 54.1 | 28.7, 28.6, 28.6, 26.8 | 0.37, 0.60 |
| E2 | 2.7 | 97629 | 96.8, 96.3, 96.5, 89.9 | 103.3, 100.1, 84.1, 52.7 | 26.9, 26.7, 26.8, 24.9 | 0.37, 0.60 |

a) $V_{on}$: Voltage recorded at 1 cd m$^{-2}$. b) $L_{max}$: Maximum luminance. $\eta_c$: Current efficiency. $\eta_p$: Power efficiency. $\eta_{ext}$: External quantum efficiency. c) In the order of maximum, then values at 100, 1000 and 10000 cd m$^{-2}$. d) Measured at 100 cd m$^{-2}$.

**Table S5.** The data of Ir(tpsp)$_2$(bpp) crystal.

| | |
|---|---|
| empirical formula | $C_{75}H_{56}IrN_3Si_2$ |
| formula wt | 1247.60 |
| crystal system | triclinic |
| T (K) | 293(2) |
| space group | P-1 |
| a/Å | 14.2766(18) |
| b/Å | 14.3194(19) |
| c/Å | 15.349(2) |
| α/ ° | 98.224(2) |
| β/ ° | 98.049(2) |
| γ/ ° | 91.321(2) |
| V/Å$^3$ | 3072.1(7) |
| Z | 2 |

| | |
|---|---|
| density, Mg/m$^3$ | 1.349 |
| absorption coefficient, mm$^{-1}$ | 2.258 |
| F (000) | 1264.0 |
| θ range/Å | 1.438-26.402 |
| no. of reflcns collected | 12240 |
| no. of unique reflcns | 8518 |
| R(int) | 0.0895 |
| wR2 (all data) | 0.1496 |
| R1 (all data) | 0.0610 |
| wR2(reflections) | 0.1746(12240) |