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Supporting Information

High-efficiency deep-blue organic light-emitting diodes based on a thermally activated delayed fluorescence emitter

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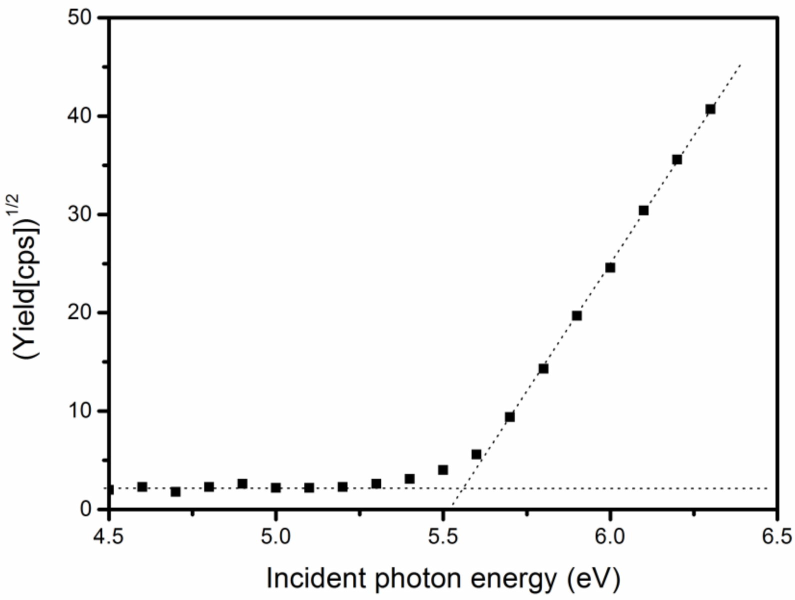

Fig. S1 The photoelectron yield spectrum of the neat film of DMOC-DPS. The HOMO level of DMOC-DPS is at 5.55 eV, in contrast to 5.81 eV for DTC-DPS.[1]

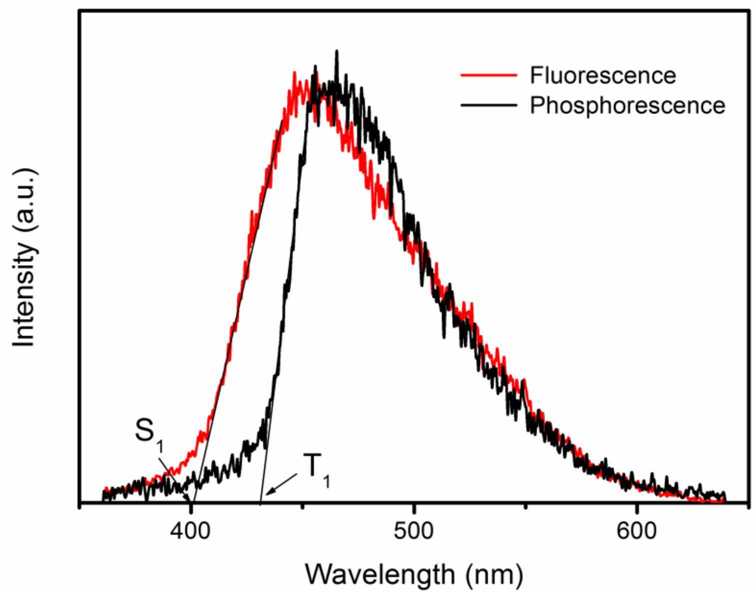

Fig. S2 Fluorescence (< 0.1 μs) and phosphorescence (> 0.1 μs) spectra of a DPEPO film doped with 10 wt% DMOC-DPS at 10 K.

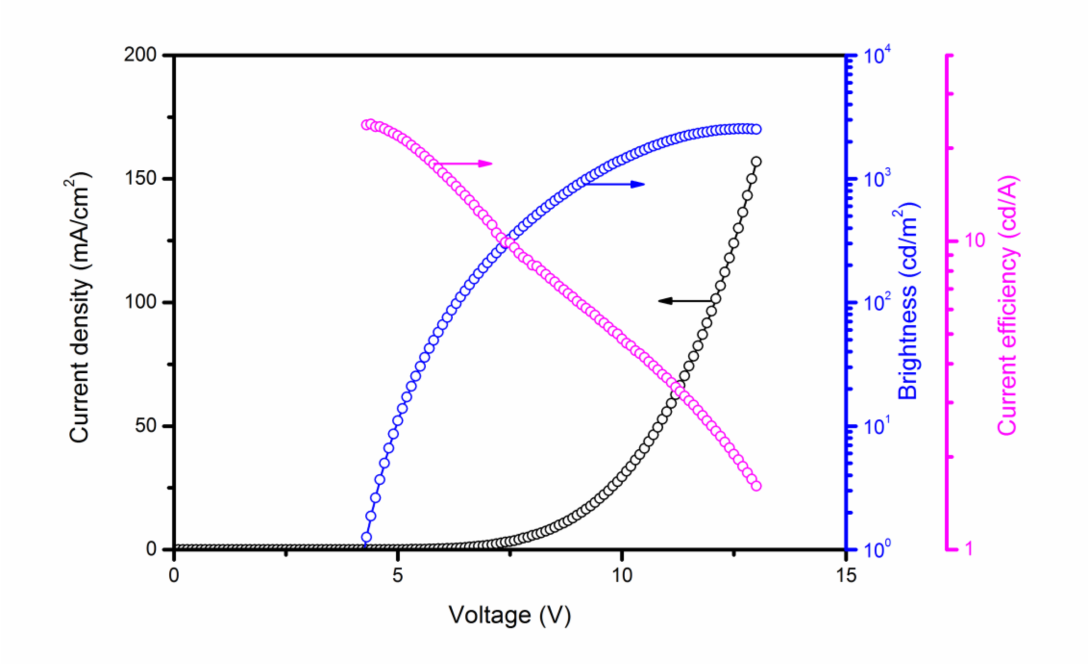

Fig. S3 Relationship between brightness, current density, and voltage for the OLED based on DMOC-DPS.

Table S1 Emission maximun (λ_{max}), turn-on voltage (V_T), maximum brightness (B_{max}), current efficiency (η_c), and external quantum efficiency (η_{ext}) of the OLEDs with different DMOC-DPS concentration in the emitting layer.

Concentration (wt%)	λ_{max} (nm)	V_T (V)	B_{max} (cd/m^2)	η_c [a] (cd/A)	η_{ext} [a] (%)	η_{ext} [b] (%)	η_{ext} [c] (%)
5	458	4.3	2154	18.1	10.4	6.8	1.2
10	460	4.0	2544	24.0	14.5	8.2	1.5
20	461	4.0	2001	19.4	11.2	5.8	1.1

[a] Measured at 0.01 mA/cm^2; [b] Measured at 1.0 mA/cm^2; [c] Measured at 100 mA/cm^2.

Experimental

1. Materials: Spectral grade solvents and all starting materials were purchased from commercial resources and were used as received. DPEPO was prepared by procedures given in the literature [2] and was further purified twice by sublimation. Other OLED materials were purchased from Luminescence Technology Corporation (Taiwan) and were used without further purification.

2. General: ^{1}H nuclear magnetic resonance (NMR) and ^{13}C NMR spectra were determined using a Bruker Avance 500 spectrometer. Elemental analyses were performed on a Yanaco MT-5 CHN analyzer. Mass spectra were measured in positive ion atmospheric pressure chemical ionization (APCI) mode on a Waters 3100 mass detector. The HOMO energy level of DMOC-DPS film was determined by atmospheric ultraviolet photoelectron spectroscopy (AC-3, Riken-Keiki).

3. Photoluminescence characterization: UV-VIS absorption spectrum of DMOC-DPS was measured in toluene using a Perkin-Elmer Lambda 950-PKA UV/VIS spectrophotometer. The photoluminescence (PL) spectra of the samples in toluene were measured using a FP-6500 spectrofluorometer (JASCO) equipped with liquid nitrogen attachment. The transient photoluminescence decay of the solution samples were recorded using a Quantaurus-Tau fluorescence lifetime measurement system (C11367-03, Hamamatsu Photonics Co.). The normal fluorescence component was recorded in the TCC900 mode used along with a 340 nm LED excitation source, while the TADF component was recorded in the M9003-01 mode used along with a flash lamp source. The PL spectra, transient PL decay, and streak image of the film samples at 300 K and 10 K were investigated under vacuum conditions by using a streak camera (C4334, Hamamatsu Photonics Co.) equipped with a Nd:YaG pulsed laser (λ=266 nm, pulse width≈10 ns, repetition rate=10 Hz) as the excitation source. PL quantum yield of all samples was obtained with an absolute photoluminescence quantum yield measurement system (C9920-02, Hamamatsu Photonics Co.).

4. OLED Fabrication and Measurements: All of the film layers including organic layers and metal layer were thermally evaporated on the cleaned Indium-tin-oxide (ITO) glass substrate under a vacuum of $< 4\times10^{-4}$ Pa. The active area of the device was 4 mm^2. The deposition rates of the organic layers and the Al layer were 0.1–0.2 nm/s, while for the LiF layer the deposition rate was 0.01 nm/s. The current density-voltage-luminance characteristics of OLEDs were measured using a semiconductor parameter analyzer (Agilent E5273A) and an optical power meter (Newport 1930C). The electroluminescence spectra were determined by multi-channel analyzer (Ocean Optics SD2000).

5. Synthesis of bis[4-(3,6-dimethoxycarbazole)phenyl]sulfone

3,6-Dimethoxy-9H-carbazole (0.90 g, 4 mmol) [3] was added to a solution of sodium hydride (0.20 g, 8 mmol) in dehydrated dimethylformamide（DMF) (15 mL). After the solution was stirred at room temperature for 30 min, bis(p-fluorophenyl)sulfone (0.50 g, 2.0 mmol) in dehydrated DMF (15 mL) was added, following which the mixture was stirred at 100 ℃ for an additional 1 h. After cooling, the mixture was poured into 300 mL of water, and the yellow precipitate was filtered and dried. The crude product was recrystallized from chloroform and diethyl ether to produce pale yellow crystals (1.2 g) in 89% yield. ^{1}H NMR ($CDCl_3$, 500 MHz): δ [ppm] 8.21 (d, J = 9.0 Hz, 4H), 7.77 (d, J = 9.0 Hz, 8H), 7.53 (s, 4H), 7.04 (d, J = 9.0 Hz, 4H), 3.95 (s, 12H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ [ppm] 154.8, 143.2, 138.7, 135.2, 129.6, 126.4, 124.6, 115.4, 110.7, 103.2, 56.1. FD-MS m/z: 668 $[M+1]^+$. Anal. Calcd for $C_{40}H_{32}N_2O_6S$: C, 71.84; H, 4.82; N, 4.19. Found: C, 71.09; H, 4.82; N, 4.10.

6. Quantum Chemical Calculations: All of the calculations were performed using the Gaussian 09 program package.[4] The geometries in the ground state were optimized via DFT calculations. The calculations for the excited state properties were based on TD-DFT level calculations. Both the ground and excited state calculations were performed with the B3LYP functional[5] using 6-31G(d) basis sets.[6]

Geometry Data for **DMOC-DPS** (S_0 optimization: unit Å)

C	1.48393800	−2.77279200	−0.20431900
S	0.08248900	−3.89945100	−0.15509100
C	−1.36371300	−2.83674400	−0.02709600
C	2.12794700	−2.42128600	0.98369500
C	3.20655600	−1.54309000	0.94623300
C	3.65803200	−1.02657700	−0.27961400
C	3.01184900	−1.40533300	−1.46862000

C	1.92385600	-2.27118100	-1.43149100
C	-1.81719400	-2.43584600	1.23172100
C	-2.93833700	-1.61804000	1.32872700
C	-3.60341400	-1.18628300	0.16880400
C	-3.13813900	-1.60162500	-1.08965100
C	-2.02613400	-2.43233200	-1.18782400
N	4.75390600	-0.14190000	-0.31789200
N	-4.73279000	-0.34868500	0.26818600
C	5.98677200	-0.31951500	0.33852500
C	6.82584700	0.78718000	0.05411500
C	6.07293700	1.67924600	-0.80604200
C	4.80673300	1.07798900	-1.01809300
C	-4.82501600	0.82648100	1.03530600
C	-6.11151000	1.39556200	0.85296000
C	-6.83126700	0.52905600	-0.05733000
C	-5.95851800	-0.52698600	-0.39913000
C	6.44926500	-1.38347400	1.10960200
C	7.74707100	-1.32314500	1.62294600
C	8.57858900	-0.21811600	1.36244600
C	8.11965900	0.83774800	0.57024100
C	6.36636700	2.91629800	-1.37741400
C	5.39529700	3.55652500	-2.15223100
C	4.13322400	2.96317500	-2.34068100
C	3.82971400	1.72375800	-1.77203900
C	-3.87081400	1.46091500	1.82752100
C	-4.21583700	2.65521500	2.46393200
C	-5.49727100	3.21604000	2.30487100
C	-6.44569400	2.58882400	1.49326100
C	-8.13467600	0.57283300	-0.57462100
C	-8.54918400	-0.45217300	-1.42328200
C	-7.67552100	-1.51472900	-1.73942700

C	-6.38467100	-1.56727500	-1.23276200
O	-9.78740800	-0.53314800	-2.00158500
O	-5.90560600	4.38096400	2.90049100
O	5.76371300	4.76521600	-2.68213600
O	9.85789000	-0.08961700	1.83575000
C	10.39231400	-1.13722500	2.62531800
C	4.81927900	5.47346100	-3.46468200
C	-4.98312700	5.07809900	3.71849300
C	-10.72048800	0.49528200	-1.72128800
O	0.17965300	-4.65826500	1.10286100
O	0.01443500	-4.56859600	-1.46473300
H	1.78656000	-2.83751700	1.92561800
H	3.69567300	-1.24084600	1.86598100
H	3.38652600	-1.04066000	-2.41903100
H	1.44107700	-2.58981000	-2.34937700
H	-1.31836900	-2.79571100	2.12547300
H	-3.32308200	-1.33257000	2.30196800
H	-3.64292500	-1.25828100	-1.98625200
H	-1.67284600	-2.77093600	-2.15608500
H	5.83240100	-2.25338700	1.30720100
H	8.10473800	-2.15031700	2.22469200
H	8.78484300	1.67124300	0.36753800
H	7.32662700	3.40093500	-1.23145700
H	3.37314000	3.46277200	-2.92976200
H	2.84543100	1.29158800	-1.91612100
H	-2.87294600	1.05382800	1.94987900
H	-3.47378100	3.14589000	3.08268500
H	-7.42090900	3.05043600	1.37320700
H	-8.79602900	1.38813200	-0.30495000
H	-8.04525000	-2.29959900	-2.39135900
H	-5.73786700	-2.40334500	-1.47541100

H	11.40833200	-0.83063900	2.88160400
H	10.43058800	-2.08522800	2.07150800
H	9.81685400	-1.28489800	3.54954800
H	5.31827000	6.39308000	-3.77661200
H	3.92111000	5.72938300	-2.88592400
H	4.52112200	4.90535200	-4.35657200
H	-5.51054700	5.96448300	4.07654700
H	-4.09421500	5.39127200	3.15385600
H	-4.66617400	4.47519900	4.58054500
H	-11.62564600	0.23984500	-2.27558600
H	-10.35498200	1.47573300	-2.05634100
H	-10.95509800	0.54794400	-0.64928100

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