m-Terphenyl-modified carbazole host material for highly efficient blue and green PHOLEDs

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General Procedures. The optimized structures and single-point energies were calculated by Gaussian03[1] at the RB3LYP 6-31G(d) and 6-311+G(d,p) levels for the ground state, and at the UB3LYP 6-31G(d) and 6-311+G(d,p) levels for the excited triplet state respectively. The E_{T1} energies of CzTP, mCP and CBP were calculated by using the reported method.[2] ^{1}H 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. HOMO levels were determined by atmospheric photoelectron spectroscopy (AC-3, Riken Keiki Co.). The phosphorescent spectra were measured by using a streak camera (C4334 from Hamamatsu Photonics) at 4.2 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 03; Gaussian Inc.: Pittsburgh, PA 2003.

(2) P. Marsal, I. Avilov, D. A. da Silva Filho, J. L. Brédas and D. Beljonne, *Chem. Phys. Lett.* 2004, **392**, 521.

Data for CzTP: colorless solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.52 (d, *J*=1.4 Hz, 2H), 7.93 (d, *J*=1.8 Hz, 4H), 7.80–7.74 (m, 12H), 7.66–7.64 (m, 4H), 7.54–7.47 (m, 11H), 7.41–7.37 (m, 4H) ppm; MS: *m/z* 700 $[M]^+$; Anal. Calcd for $C_{54}H_{37}N$: C, 92.67; H, 5.33; N, 2.00%. Found: C, 92.73; H, 5.27; N, 1.95%; UV-vis (film): λ_{max} = 262, 305 nm; PL (film): λ_{max} = 395 nm.

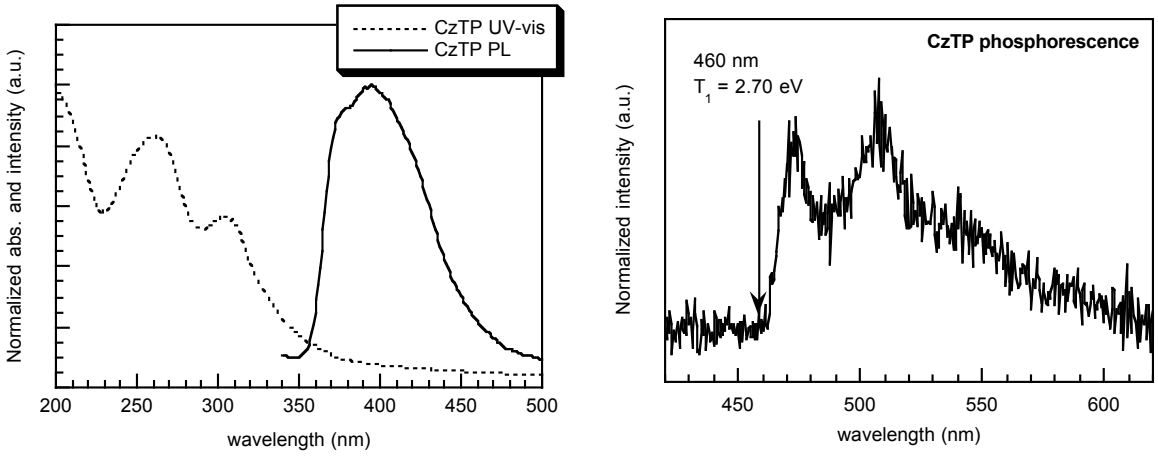

Figure S-1. UV–vis and PL spectra of vacuum deposited film of CzTP (left). Phosphorescent spectrum of vacuum-deposited film of CzTP at 4.2 K, measured by streak camera with a N_2 gas laser (337 nm) as an excitation light (right).

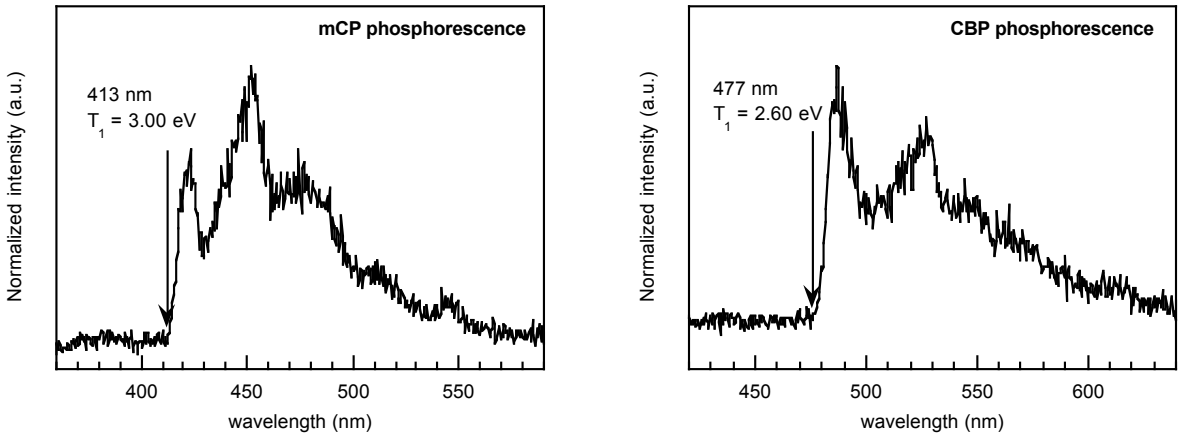

Figure S-2. Phosphorescent spectra of vacuum-deposited film of mCP (left) and CBP (right) at 4.2 K, measured by streak camera with a N_2 gas laser (337 nm) as an excitation light.

Table S-1. HOMO, LUMO, E_g, E_{T1} and ΔE_{ST} energies of materials.

Compound	HOMO/eV[a]	LUMO/eV[b]	E_g/eV[c]	E_{T1}/eV (onset)[d]	E_{T1}/eV (first peak)[d]	ΔE_{ST}/eV[e]
CzTP	5.91	2.48	3.43	2.70	2.63	0.73
mCP	6.09	2.60	3.49	3.00	2.95	0.49
CBP	6.10	2.66	3.44	2.60	2.55	0.84
TmPyPB[3]	6.68	2.73	3.95	2.78	–	1.17
B3PyPB[4]	6.67	2.62	4.05	2.77	2.67	1.28

[a]Measured by atmospheric photoelectron spectroscopy (AC-3). [b]Calculated using HOMO and E_g values. [c]Taken as the point of intersection of the normalized absorption spectra. [d]Measured by using a streak camera (C4334 from Hamamatsu Photonics) at 4.2 K. [e]$\Delta E_{ST} = E_g - E_{T1}$ (onset).

(3) S.-J. Su, T. Chiba, T. Takeda and J. Kido, *Adv. Mater.* 2008, **20**, 2125.

(4) H. Sasabe, E. Gonmori, T. Chiba, Y.-J. Li, D. Tanaka, S.-J. Su, T. Takeda, Y.-J. Pu, K. Nakayama and J. Kido, *Chem. Mater.* 2008, **20**, 5951.

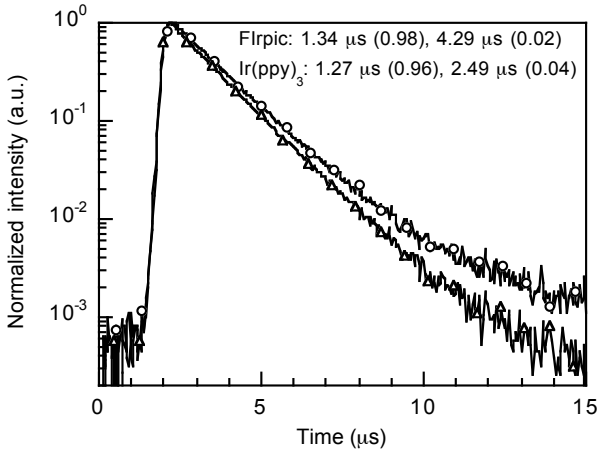

Figure S-3. Transient photoluminescence decay curves of CzTP/FIrpic film (circles) and CzTP/$Ir(ppy)_3$ film (triangles) at room temperature.