Electronic Supplementary Information (ESI)

Novel aggregation-induced delayed fluorescent materials for efficient OLEDs with high stabilities of emission color and efficiency

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Materials and Instruments

All the chemicals and reagents were purchased from commercial sources and used as received without further purification. The final products were subjected to vacuum sublimation to further improve purity before photoluminescence (PL) and electroluminescence (EL) properties investigations. ^{1}H and ^{13}C NMR spectra were measured on a Bruker AV 400 spectrometer in CD_3Cl or CD_2Cl_2 at room temperature. High-resolution mass spectra (HRMS) were recorded on a GCT premier CAB048 mass spectrometer operating in MALDI-TOF mode. UV-vis absorption spectra were measured on a Shimadzu UV-2600 spectrophotometer. PL spectra were recorded on a Horiba Fluoromax-4 spectrofluorometer. PL quantum yields were measured using a Hamamatsu absolute PL quantum yield spectrometer C11347 Quantaurus_QY. Transient PL decay spectra were measured under nitrogen atmosphere for solutions and neat films, using Quantaurus-Tau fluorescence lifetime measurement system (C11367-03, Hamamatsu Photonics Co., Japan). Cyclic voltammograms were performed in dichloromethane (HOMO energy level) and dimethylformamide (LUMO energy level) containing 0.1 M tetrabutylammonium hexafluorophosphate with the scan rate of 50 mV s^{-1}, using a platinum wire as the auxiliary electrode, a glass carbon disk as the working electrode and Ag/Ag^{+} as the reference electrode, standardized for the redox couple ferricenium/ferrocene (Fc/Fc^{+}). The effective emitting area of the devices was 9 mm^{2}, determined by the overlap between anode and cathode. The ground-state geometries were calculated using the density function theory (DFT) method with the PBE0 hybrid functional at the basis set level of 631G(d,p). All the calculations were performed using Gaussian 09 package.

Device fabrication and measurement

The glass substrates precoated with a 90 nm layer of indium tin oxide (ITO) with a sheet resistance of 15~20 Ω per square were successively cleaned in ultrasonic bath of acetone, isopropanol, detergent and deionized water, respectively, taking 10 minutes for each step. Then, the substrates were totally dried in a 70 °C oven. Before the fabrication processes, in order to improve the hole injection ability of ITO, the substrates were treated by O_2 plasma for 10 minutes. The vacuum-deposited OLEDs were fabricated under a pressure of < 5 × 10^{-4} Pa in the Fangsheng OMV-FS380 vacuum deposition system. Organic materials, LiF and Al were deposited at rates of 1~2 Å s^{-1}, 0.1 Å s^{-1} and 5 Å s^{-1}, respectively. The luminance-voltage-current density characteristics and EL spectra were obtained via a Konica Minolta CS-200 Color and Luminance Meter and an Ocean Optics USB 2000+ spectrometer, along with a

Keithley 2400 Source Meter. The external quantum efficiencies were estimated utilizing the normalized EL spectra and the current efficiencies of the devices, assuming that the devices are Lambertian emitters. All the characterizations were conducted at room temperature in ambient conditions without any encapsulation, as soon as the devices were fabricated.
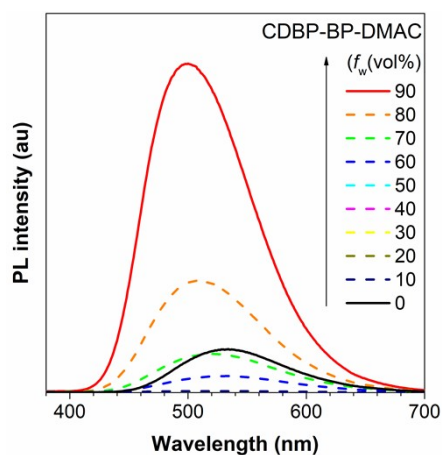
Additional Spectra and Tables

Fig. S1 PL spectra of CDB-BP-DMAC in THF/water mixtures with different water fractions (f_w), where the concentration is 10^{-5} mol L^{-1}.
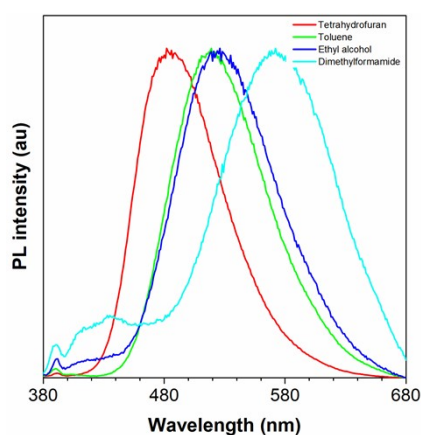

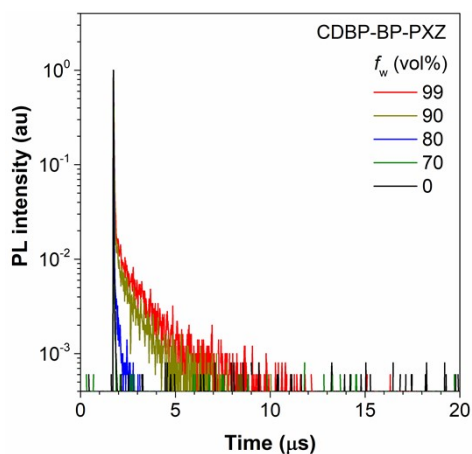**Fig. S2** PL spectra of CDBP-BP-DMAC in different solvents with varied polarity.

Fig. S3 Transient PL decay curves of CDBP-BP-PXZ in THF/water mixtures with different water fractions (f_w), where the concentration is 10^{-5} mol L^{-1}.
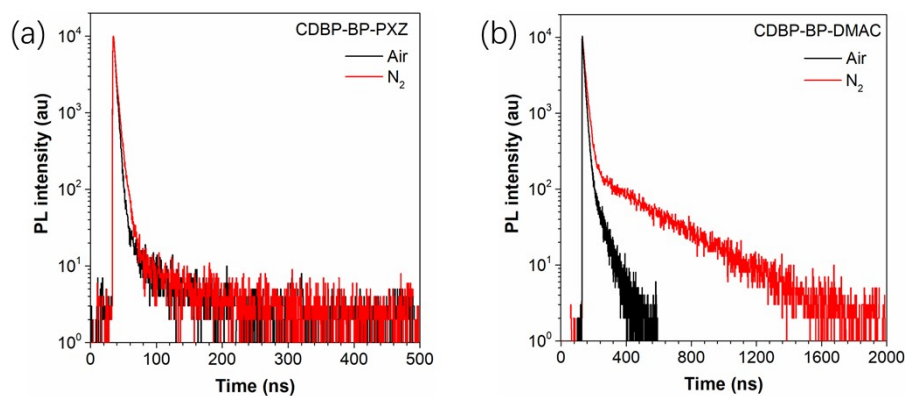
Fig. S4 PL decay curves in THF solutions (10^{-5} M) under air and N_2 atmospheres for (a) CDBP-BP-PXZ and (b) CDBP-BP-DMAC.
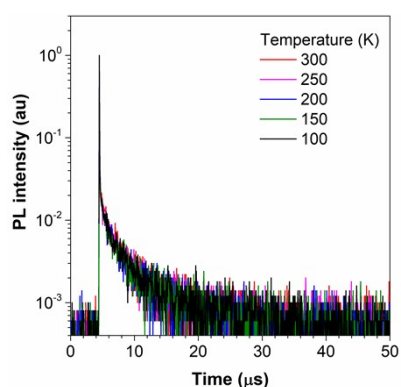

Fig. S5 Temperature-dependent transient PL decay spectra of CDBP-BP-PXZ in neat film, measured under nitrogen atmosphere.
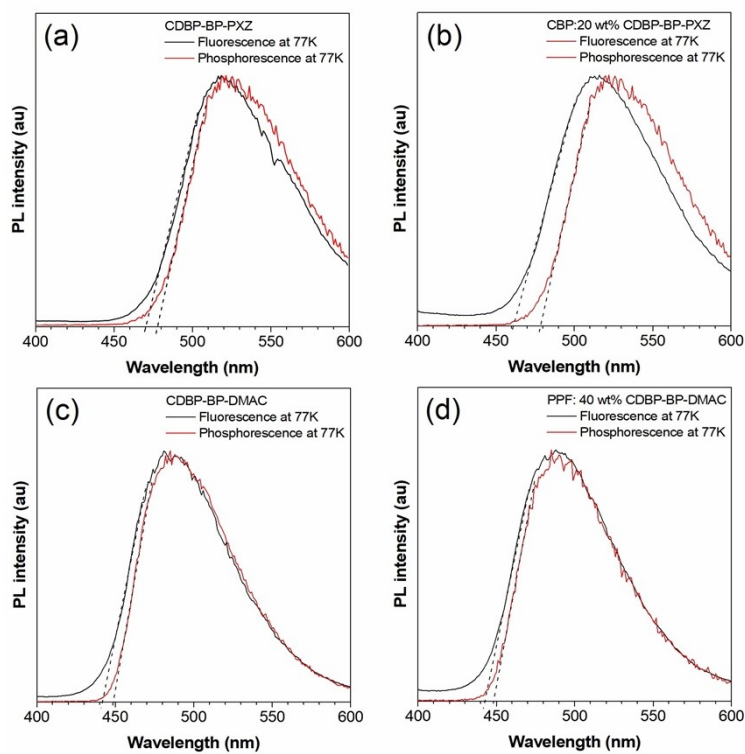

Fig. S6 Fluorescence spectra at 77 K and phosphorescence spectrum at 77 K of (a) CDBP-BP-PXZ in neat film, (b)

CDBP-BP-PXZ in in doped film (20 wt% doping concentration with CBP as host), (c) CDBP-BP-PXZ in neat film, (d) CDBP-BP-DMAC in in doped film (40 wt% doping concentration with PPF as host).
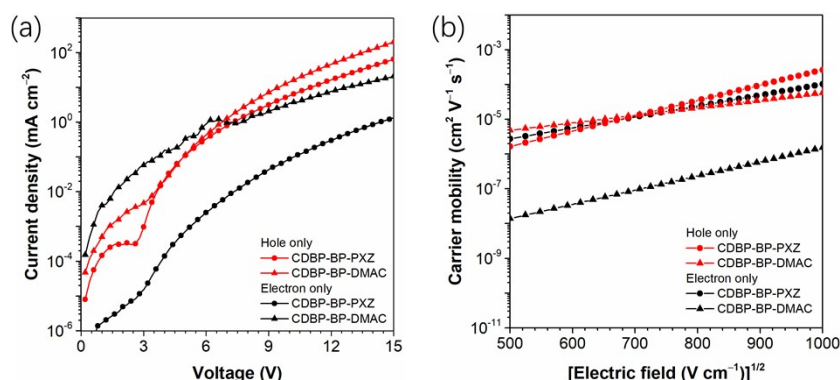

Fig. S7 (a) Plots of current density versus applied voltage of the hole only and electron only devices, and (b) electric field-dependent hole and electron mobilities of both luminogens.

Table S1. The performance of CDBP-BP-PXZ and CDBP-BP-DMAC in doped OLEDs with different hosts.

Emitter	Host	V_{on} (V)	L_{max} (cd m^{-2})	η_C (cd A^{-1})	η_P (lm W^{-1})	η_{ext} (%)	CIE (x, y)	λ_{EL} (nm)
				maximum value / at 1000 cd m^{-2}				
20 wt% CDBP-BP-PXZ	*m*CP	3.2	51121	60.1/55.3	45.7/34.7	18.9/17.4	524	(0.314, 0.570)
	CBP	3.0	60899	67.1/65.4	56.5/46.7	20.8/20.3	528	(0.322, 0.575)
	PPF	3.0	48018	29.6/29.4	23.0/22.0	9.0/8.9	536	(0.364, 0.577)
40 wt% CDBP-BP-DMAC	*m*CP	3.0	21403	34.2/31.1	32.0/22.2	13.8/12.5	490	(0.208, 0.423)
	CBP	3.2	12009	27.8/24.2	23.0/15.2	11.4/10.0	490	(0.207, 0.406)
	PPF	2.8	31007	44.9/41.0	50.4/29.3	16.8/15.4	504	(0.227, 0.466)

[a] Abbreviation: V_{on} = turn-on voltage at 1 cd m^{-2}; L_{max} = maximum luminance; η_C = current efficiency; η_P = power efficiency; η_{ext} = external quantum efficiency; CIE = Commission Internationale de l'Eclairage coordinates at 1000 cd m^{-2}; λ_{EL} = electroluminescence peak at 1000 cd m^{-2}.