Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Nondoped blue fluorescent organic light-emitting diodes based on benzonitrile-anthracene derivative with 10.06 % external quantum efficiency and low efficiency roll-off

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Content

1.Solvatochromic effect

Lippert−Mataga equation:

$$hc(\vartheta_a - \vartheta_f) = hc(\vartheta_a^{\circ} - \vartheta_f^{\circ}) - \frac{2(\mu_e - \mu_g)^2}{a^3} f(\varepsilon, n) \qquad \text{Equation 1}$$

$f(\varepsilon,n)$: the orientational polarizability of solvents.

ε: the solvent dielectric.

n: the solvent refractive index.

μ_e: the excited state dipole moment.

μ_g: the ground state dipole moment.

a: the solvent cavity (Onsager) radius

$$f(\varepsilon, n) = \frac{\varepsilon - 1}{2\varepsilon + 1} - \frac{n^2 - 1}{2n^2 + 1}; a = (3M/4N\pi d)^{1/3} \qquad \text{Equation 2}$$

N: avogadro number.

M: molecular weight.

d: density (d = 1.0 g cm^{-3}).

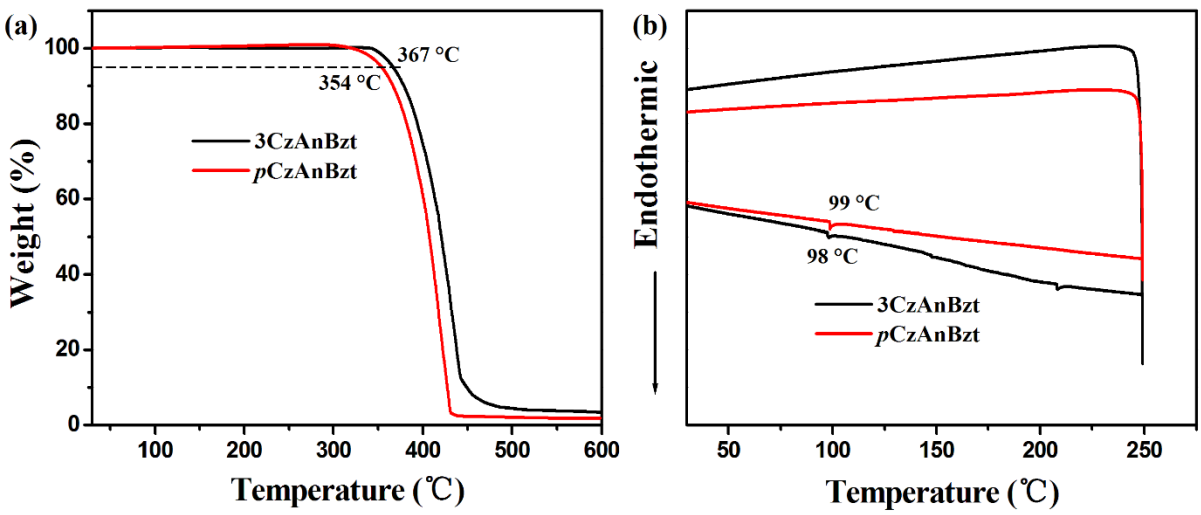


Fig. S1. (a) Thermogravimetric analysis (TGA) and (b) Differential scanning calorimetry (DSC) curves of **3CzAnBzt** and ***p*CzAnBzt**.

Table S1. Nondoped electroluminescent performances for some representative blue-emitting materials.

Compound	$CE_{max/1000}$[a] (cd A^{-1})	$EQE_{max/1000}$[a] (%)	λ_{EL} (nm)	CIE (x, y)	Ref.
3CzAnBzt	11.72/10.17	10.06/8.97	463	(0.14, 0.14)	This work
***p*CzAnBzt**	8.22/6.07	9.23/7.10	454	(0.14, 0.10)	This work
PIAnCN	13.16/-	9.44/9.44	470	(0.14, 0.19)	47
DMAC-DPS	-	19.5/14.6	480	(0.16, 0.29)	30
Blu2	3.34	7.40/-	493	(0.15, 0.29)	12
PPI-2TPA	4.4/-	7.20/6.30	440	(0.15, 0.06)	45
TPA-PA	4.07/-	7.23/-	428	(0.16, 0.07)	14
TAT	3.64/-	7.18/-	444	(0.16, 0.09)	9
N1-1-PhTPA	6.35/5.70	6.08/5.46	458	(0.14, 0.12)	38
BBTPI	5.48	5.77/5.41	448	(0.15, 0.10)	15
TPAXAN	-	4.62/-	428	(0.16, 0.05)	16

[a] CE and EQE of maximum / at 1000 cd m^{-2}.

Table S2. Detailed information of absorption and emission peak positions of **3CzAnBzt** and ***p*CzAnBzt** in different solvents at an identical concentration of 10^{-5} M.

				3CzAnBzt			***p*CzAnBzt**		
Solvent	ε	n	Δf	λ_a (nm)	λ_f (nm)	υ_a-υ_f (cm^{-1})	λ_a (nm)	λ_f (nm)	υ_a-υ_f (cm^{-1})
n-Hexane	1.58	1.381	0.001	394	434	2339.2	393	426	1971.1
Touene	2.38	1.494	0.014	398	442	2501.2	396	434	2211.1
Dioxane	2.21	1.422	0.021	396	442	2628.1	395	433	2221.8
Triethylamine	2.42	1.401	0.048	394	438	2549.7	393	428	2080.8
Choloroform	4.81	1.443	0.149	397	449	2917.2	396	438	2421.5
Ethyl ether	4.34	1.352	0.167	394	446	2959.2	392	436	2574.4
Ethyl aceyate	6.02	1.372	0.200	394	446	2959.2	393	433	2350.6
Tetrahydrofuran	7.58	1.407	0.210	397	448	2867.5	395	436	2380.7
Methylene chloride	8.93	1.424	0.217	398	454	3099.2	396	438	2421.5

Dimethyl formamide	37.0	1.427	0.276	398	464	3573.9	396	442	2628.1
Acetone	20.7	1.359	0.284	394	452	3256.8	393	437	2562.0

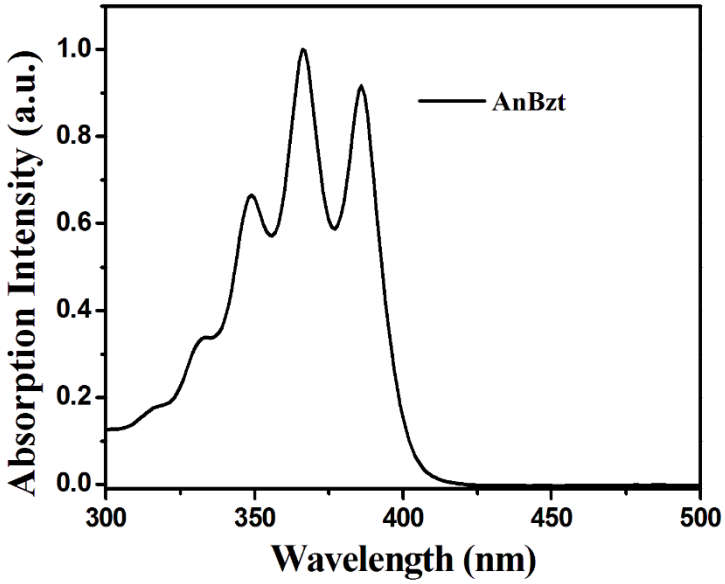


Fig. S2. The absorption (UV) spectra of **AnBzt** in dichloromethane (10^{-5} M).

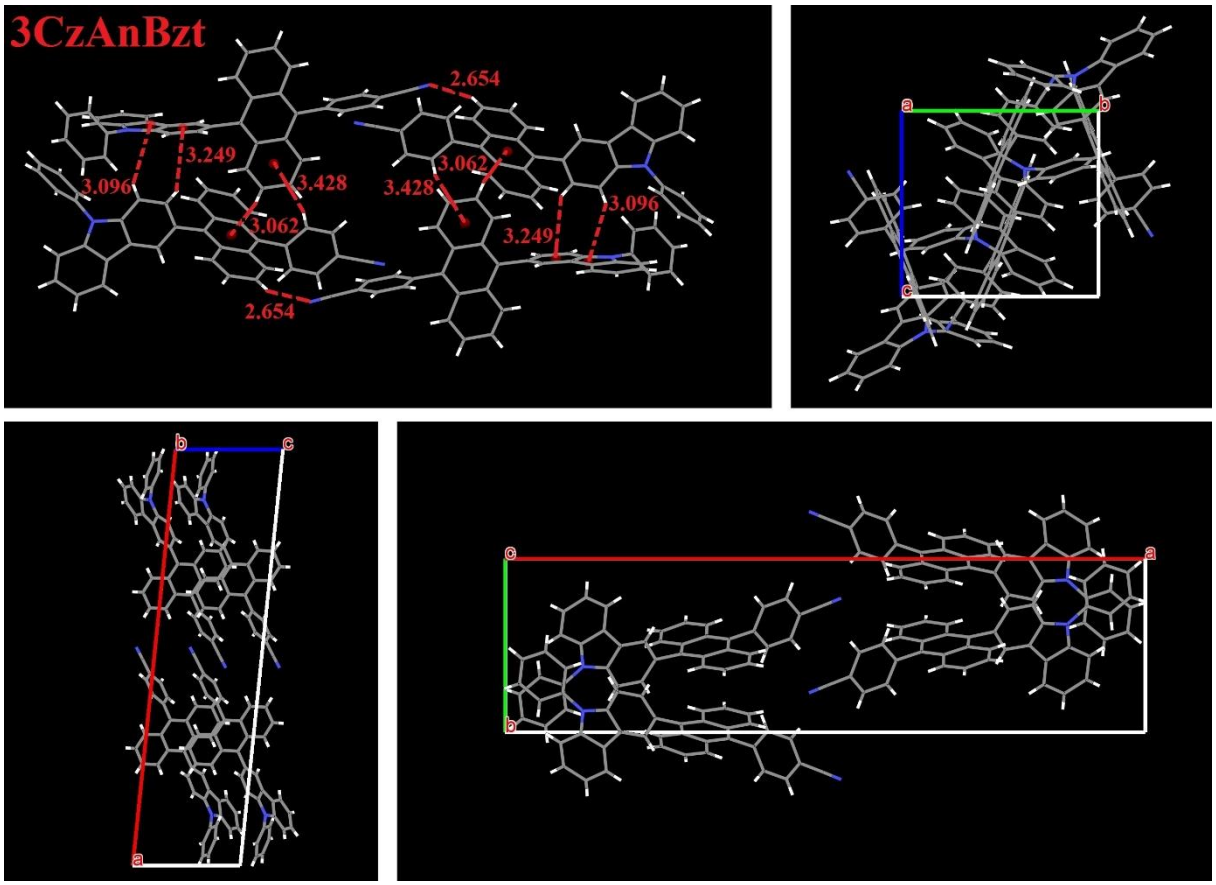


Fig. S3. Schematic molecular conformations and interactions of **3CzAnBzt** in the crystal.

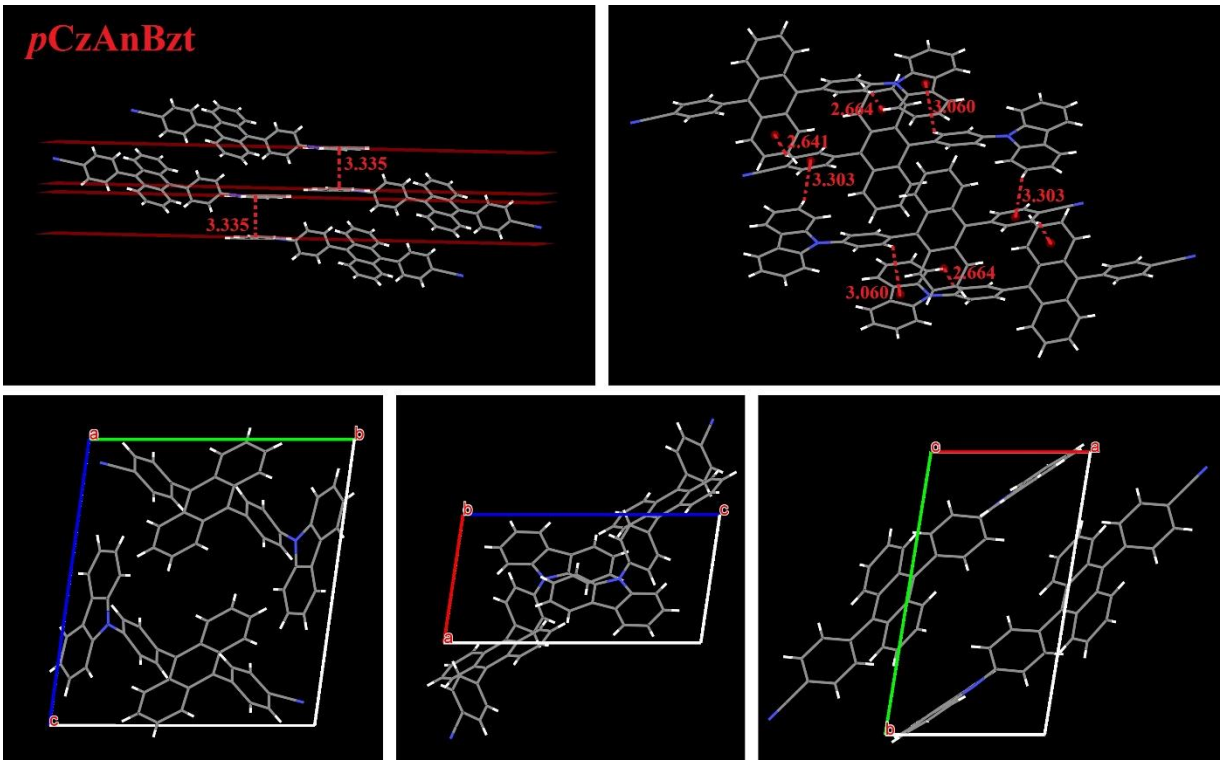


Fig. S4. Schematic molecular conformations and interactions of ***p*CzAnBzt** in the crystal.

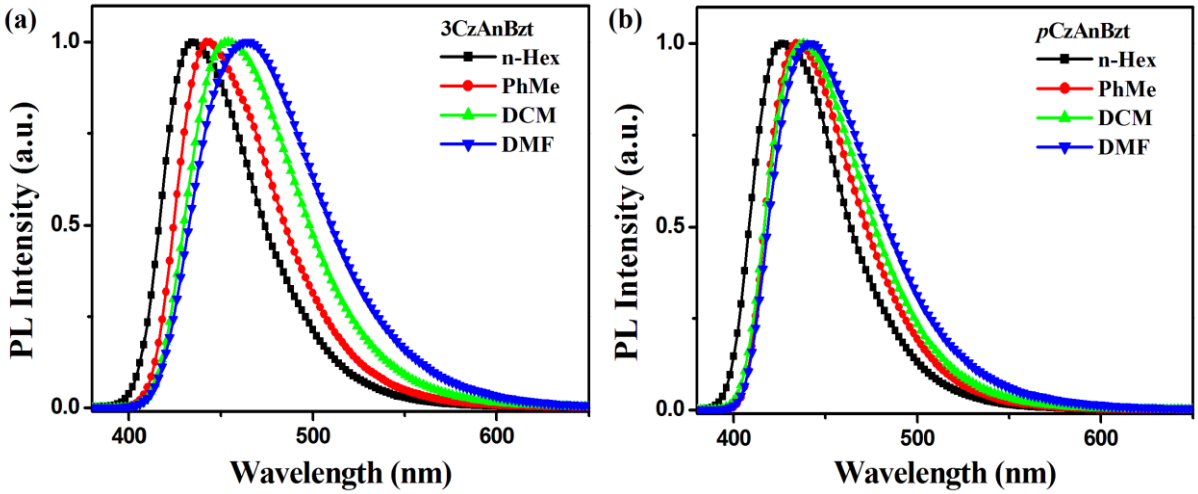


Fig. S5. The emission of **3CzAnBzt** (a) and ***p*CzAnBzt** (b) in different solvents.

Table S3 Crystal data and structure refinement for **3CzAnBzt** and ***p*CzAnBzt**.

Identification code	**3CzAnBzt**	***p*CzAnBzt**
Empirical formula	$C_{39}H_{24}N_2$	$C_{39}H_{24}N_2$
Formula weight	520.64	520.64
Temperature	100 K	100 K
Crystal system, space group	Monoclinic, P-1	Triclinic, P-1

a, Å	33.7852(9)	7.4203(2)
b, Å	9.1188(2)	13.3663(3)
c, Å	8.6590(3)	14.5908(4)
Alpha, deg	90	96.694(2)
Beta, deg	95.866(3)	97.320(2)
Gamma, deg	90	98.178(2)
Volume	2653.70(13) Å^3	1407.32(6) Å^3
Calculated density	1.303 g/cm^3	1.229 g/cm^3
F(000)	1088	544
CCDC number	1857041	1857042

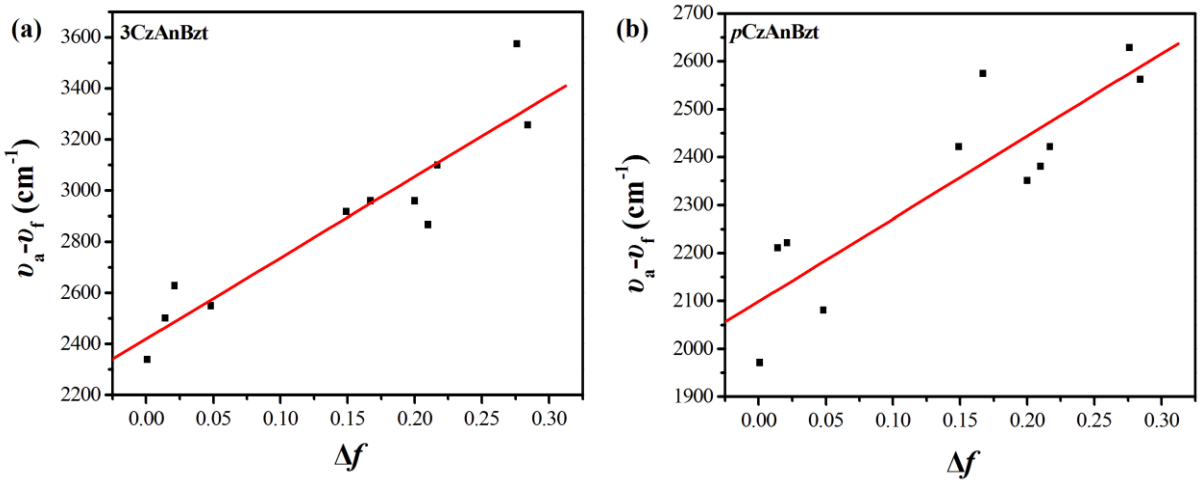


Fig. S6. Linear correlation of orientation polarization (Δf) of solvent media with the Stokes shift ($\nu_a - \nu_f$) for **3CzAnBzt** (a) and ***p*CzAnBzt** (b).

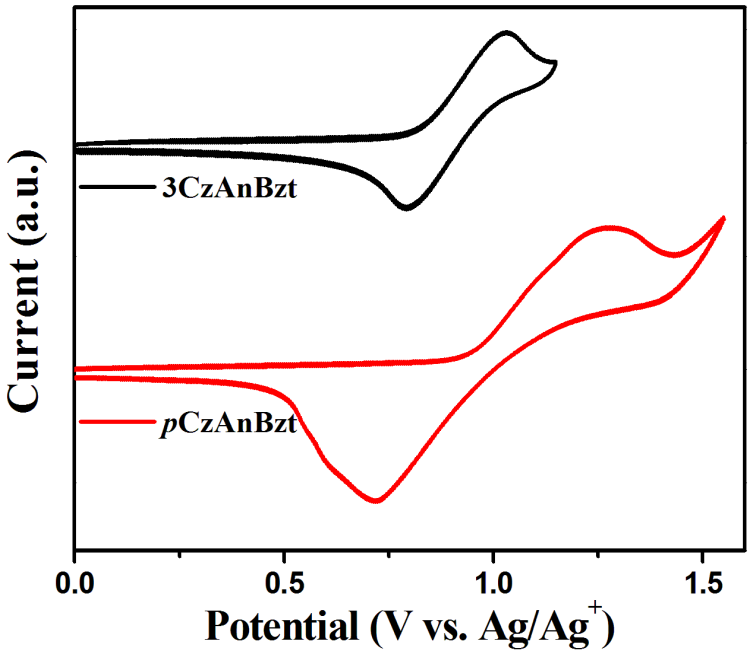


Fig. S7. Cyclic voltammetric scans of **3CzAnBzt** and ***p*CzAnBzt**.

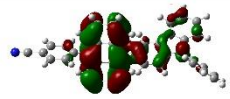
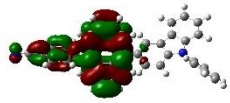
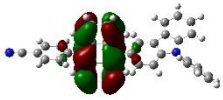
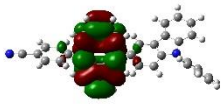
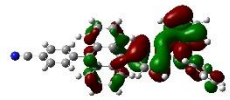
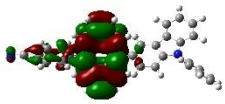
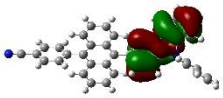
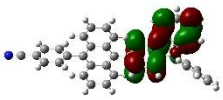
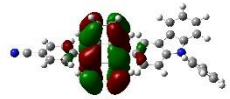
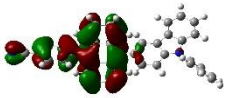
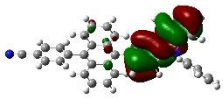
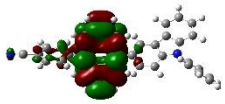
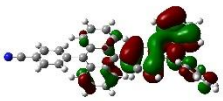
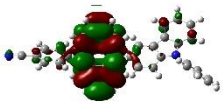
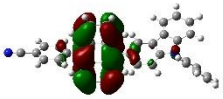
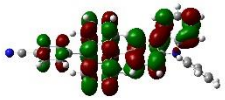
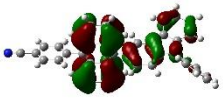
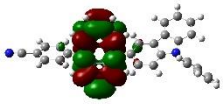
	Hole	Particle		Hole	Particle
S_1			T_1		
S_2			T_2		
S_3			T_3		
S_4			T_4		
S_5			T_5		

Fig. S8. NTOs of singlet and triplet excited states for **3CzAnBzt**.

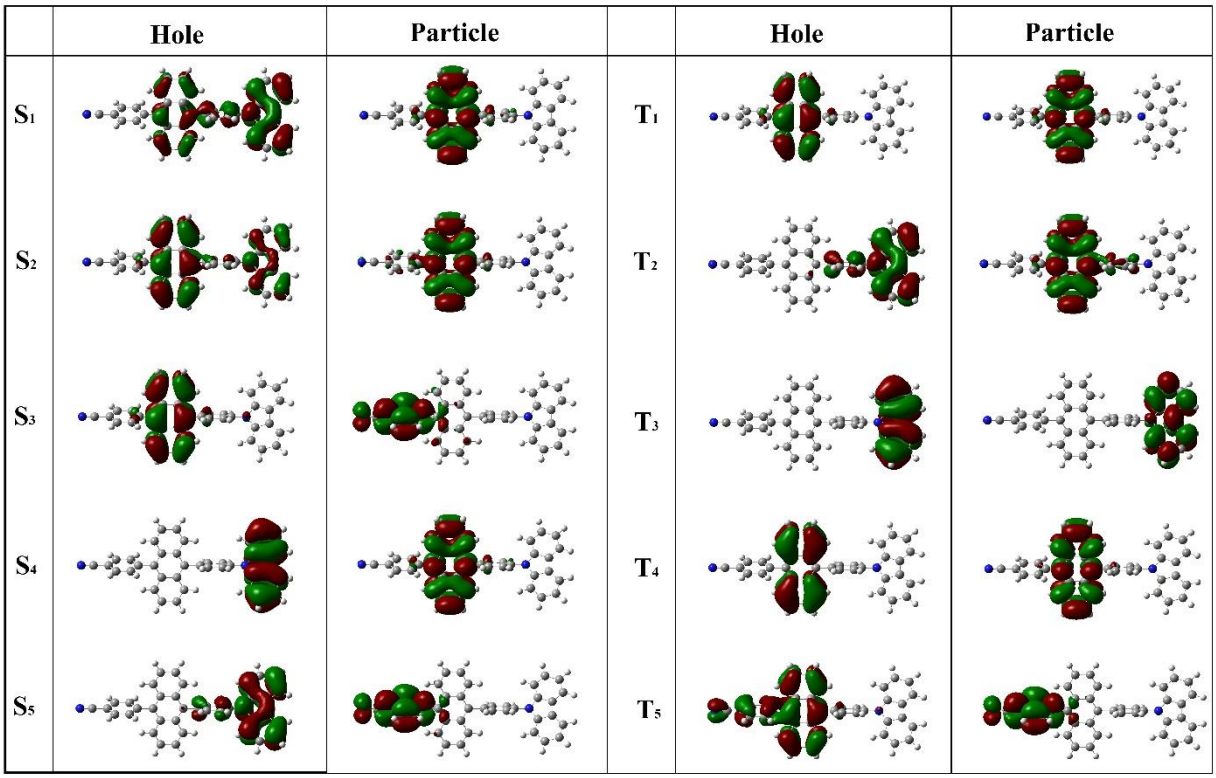


Fig. S9. NTOs of singlet and triplet excited states for ***p*CzAnBzt**.

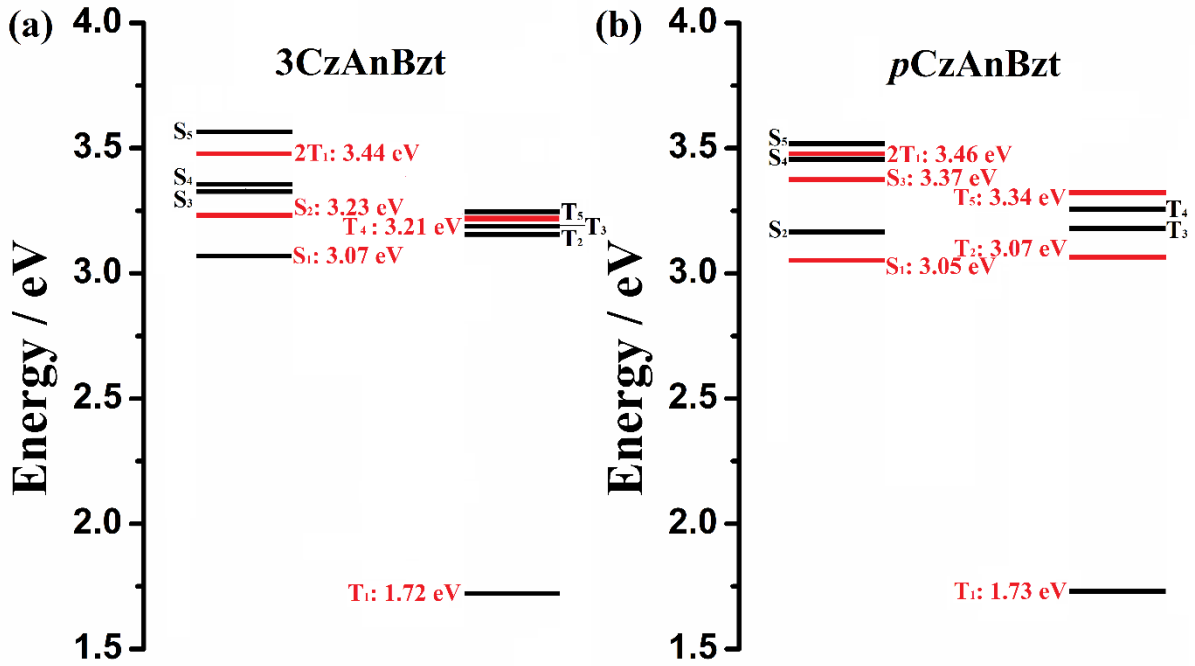


Fig. S10. Energy diagram of calculated singlet and triplet excited states for **3CzAnBzt** (a) and ***p*CzAnBzt** (b).

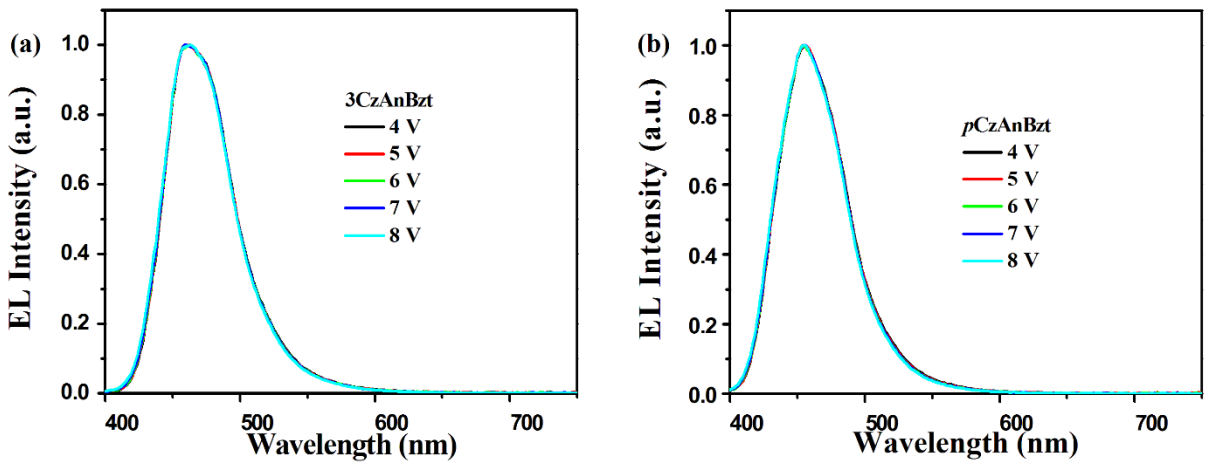


Fig. S11. The EL spectrum with different applied bias of **3CzAnBzt** (a) and ***p*CzAnBzt** (b).

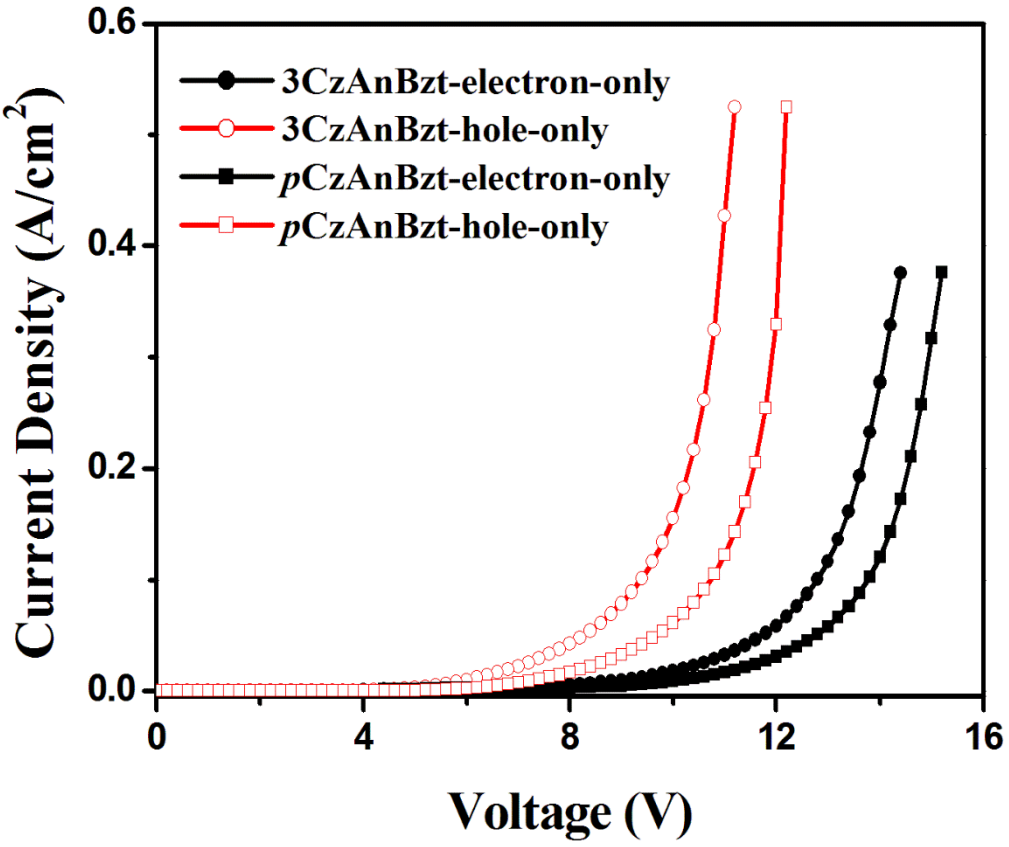


Fig. S12. *J-V* characteristics of hole-only and electron-only of **3CzAnBzt** and ***p*CzAnBzt**. The devices structure of hole-only: ITO/HATCN (15 nm)/TAPC (50 nm)/TCTA (5 nm)/EML (20 nm) /TCTA (5 nm)/ /TAPC (50 nm) /HATCN (15 nm) /Al(150 nm), and the devices structure of electron-only: ITO/LiF(1 nm)/TmPyPB (40 nm)/EML (20)/ TmPyPB (40 nm)/ LiF(1 nm)/Al(150 nm).

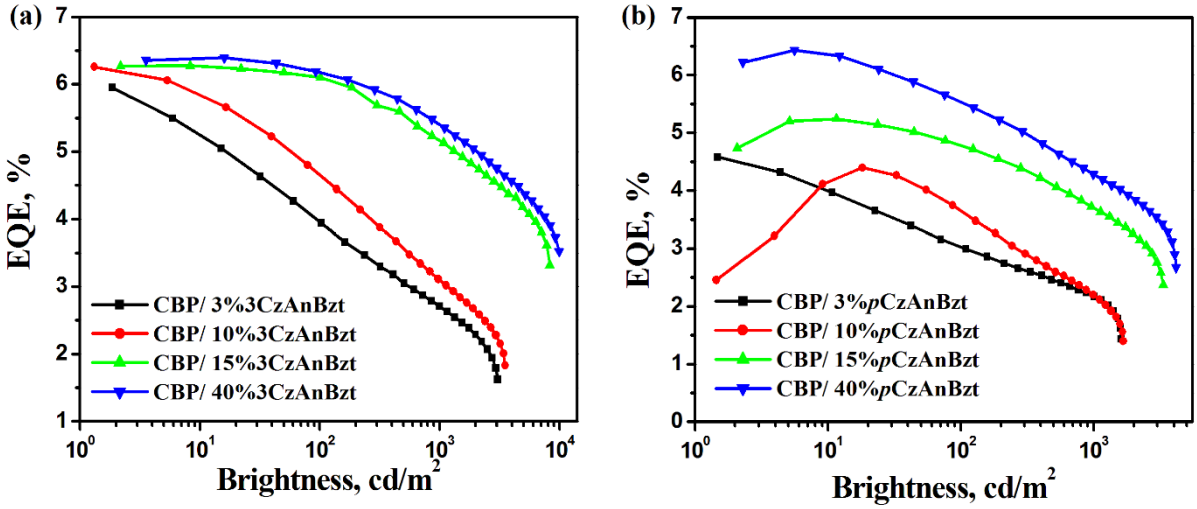


Fig. S13. EQE as a function of brightness of doped devices for **3CzAnBzt** (a) and ***p*CzAnBzt** (b).

Table S4. Summary of the doped EL performances of OLEDs based on **3CzAnBzt** and ***p*CzAnBzt**.

device[a]	V_{on}[b] (V)	L_{max}[c] (cd m^{-2})	CE_{max}[d] (cd A^{-1})	PE_{max}[e] (lm W^{-1})	EQE_{max}[f] (%)	λ_{EL}[g] (nm)	CIE[h] (x, y)
CBP/3% 3CzAnBzt	3.4	3049	4.92	4.54	5.95	452	(0.15, 0.08)
CBP/10% 3CzAnBzt	3.2	3507	5.77	5.66	6.25	454	(0.14, 0.09)
CBP/15% 3CzAnBzt	3.0	8298	6.67	6.98	6.27	458	(0.14, 0.12)
CBP/40% 3CzAnBzt	3.0	9918	6.94	7.14	6.39	457	(0.14, 0.13)
CBP/3% *p*CzAnBzt	3.6	1599	2.70	2.36	4.58	450	(0.15, 0.06)
CBP/10% *p*CzAnBzt	3.4	1659	3.01	2.58	4.39	452	(0.15, 0.07)
CBP/15% *p*CzAnBzt	3.2	3318	4.37	4.04	5.24	453	(0.14, 0.08)
CBP/40% *p*CzAnBzt	3.2	4168	5.62	5.41	6.43	453	(0.14, 0.09)

[a] The uniform device structure: ITO/HAT-CN (15 nm)/TAPC (50 nm)/TCTA (5 nm)/CBP:3%**3CzAnBzt** or **CBP:3%*p*CzAnBzt** (20 nm)/TmPyPB (40 nm)/LiF (1 nm)/Al (150 nm). [b] Voltage at 1 cd m^{-2}. [c] Maximum luminance. [d] Maximum current efficiency. [e] Maximum power efficiency. [f] Maximum external quantum efficiency. [g] EL emission peak at 6 V. [h] Commission Internationale de l'Éclairage coordinates at 6 V.