Electronic Supplementary Information

Fluorinated 9,9′-bianthracene Derivatives with Twisted Intramolecular Charge Transfer Excited States as Blue Host Materials for High-Performance Fluorescent Electroluminescence

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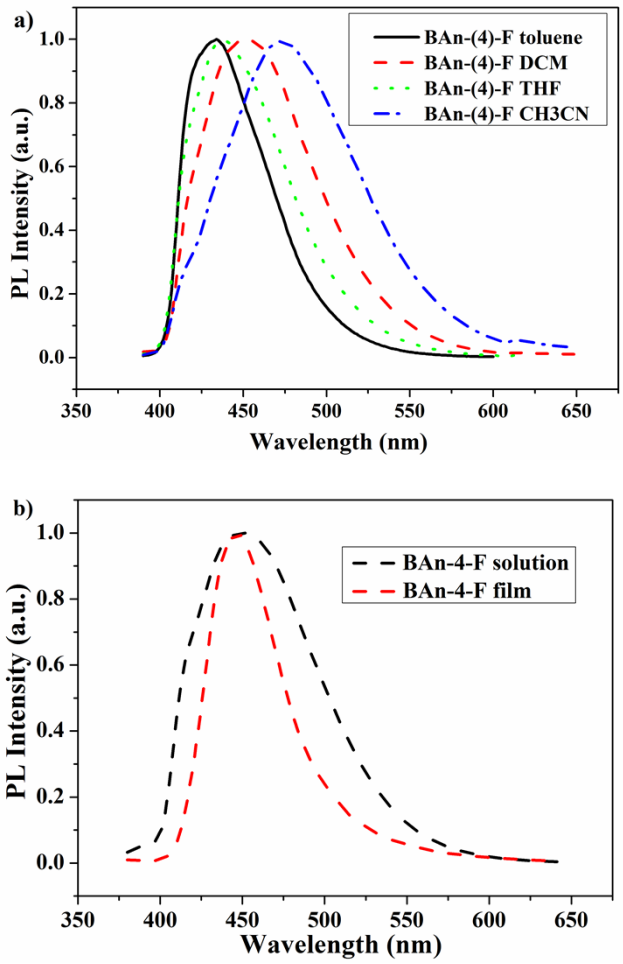

Fig. S1 (a) PL spectra of BAn-(4)-F in various solvents. (b) PL spectra of BAn-(4)-F in CH_2Cl_2. and in film

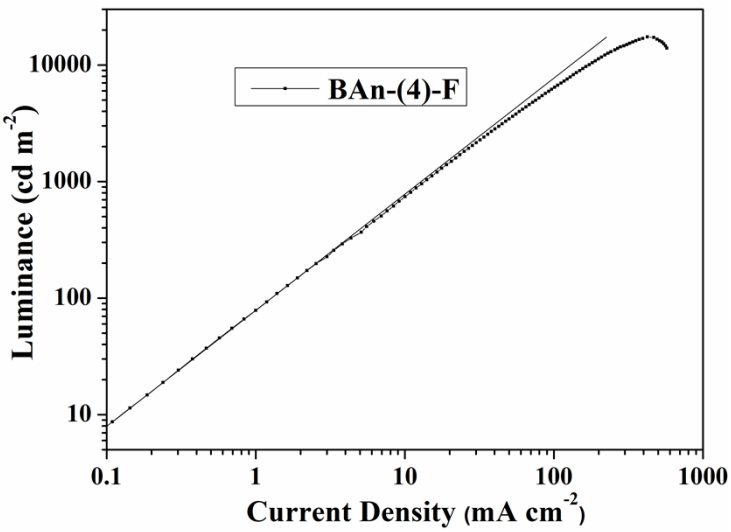

Fig. S2 The current–brightness characteristic of the device based on the host BAn-(4)-F.

Electroluminescent properties

we have fabricated non-doped blue devices, consisting of indium tin oxide (ITO)/ poly(3,4-ethylenedioxythiophene) : poly(styrenesulfonate) (PEDOT : PSS) (30 nm)/4,4',4''-Tris(carbazol-9-yl)-triphenylamine (TcTa) (40 nm)/blue emitting layer (EML) (20 nm)/1,3,5-Tris(1-phenyl-1H-benzimidazol-2-yl)benzene (TPBi) (40 nm)/LiF (1 nm)/Al (100 nm). PEDOT : PSS was used as hole injection layer (HIL), TcTa was used as hole transporting layer (HTL), BAnFs were used as emitting layer (EML), TPBi was used as electron transporting layer (ETL), and LiF was used as electron injection layer (EIL), respectively. As shown in Fig. S3, the non-doped OLEDs utilizing BAnFs as the emitters exhibited blue emissions with Commission Internationale de l'Éclairage (CIE) coordinates in a range of (0.169–0.201, 0.142–0.240), of which the device using BAn-(4)-F as blue emitter gets excellent CIE coordinates of (0.169, 0.142) with blue emissions peaking at 436 nm. The current density–voltage–luminance–efficiency (*J–V–L–η*) measurements of the blue fluorescent OLEDs with BAnFs as the EMLs were performed under ambient conditions and the results are summarized in Table S2. *J–V–L–η* characteristic of the devices are shown in Fig.S4 and Fig.S5. The blue OLEDs show the current efficiency in the range of 1.37–2.38 cd A^{-1} (Fig. S4). It is noteworthy that there is little roll-off of luminance efficiency as a function of current density in the SFs blue device. For example, the device using BAn-(4)-F gives the highest efficiency of 1.78 cd A^{-1} at 20 mA cm^{-2} and 1.75 cd A^{-1} at 100 mA cm^{-2}, respectively. The high EL efficiencies indicate rather effective and balanced hole/electron injection into the large-energy-gap blue emitting BAnF in the present device structure.

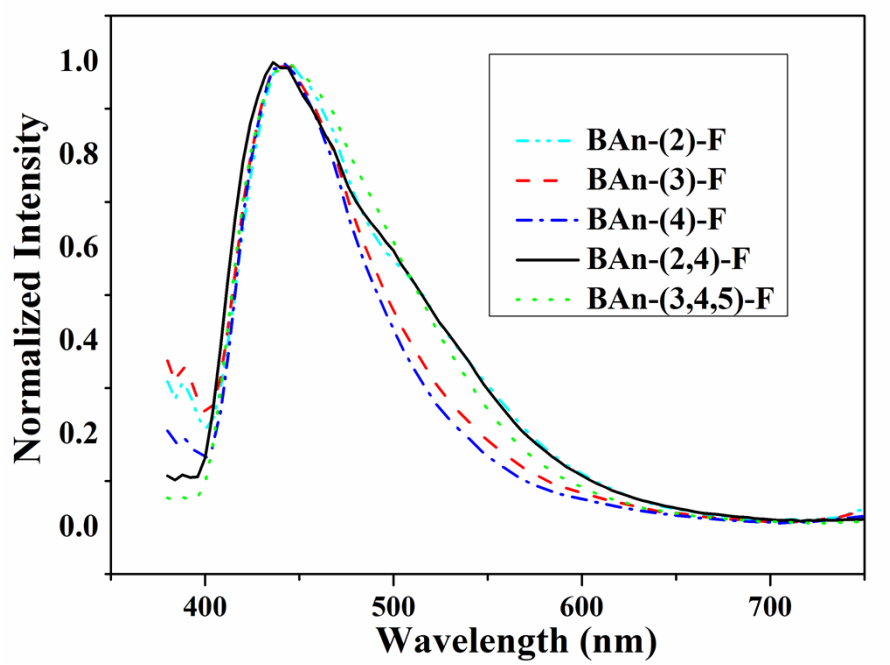

Fig. S3 EL spectrum of non-doped devices at 10 mA cm^{-2}.

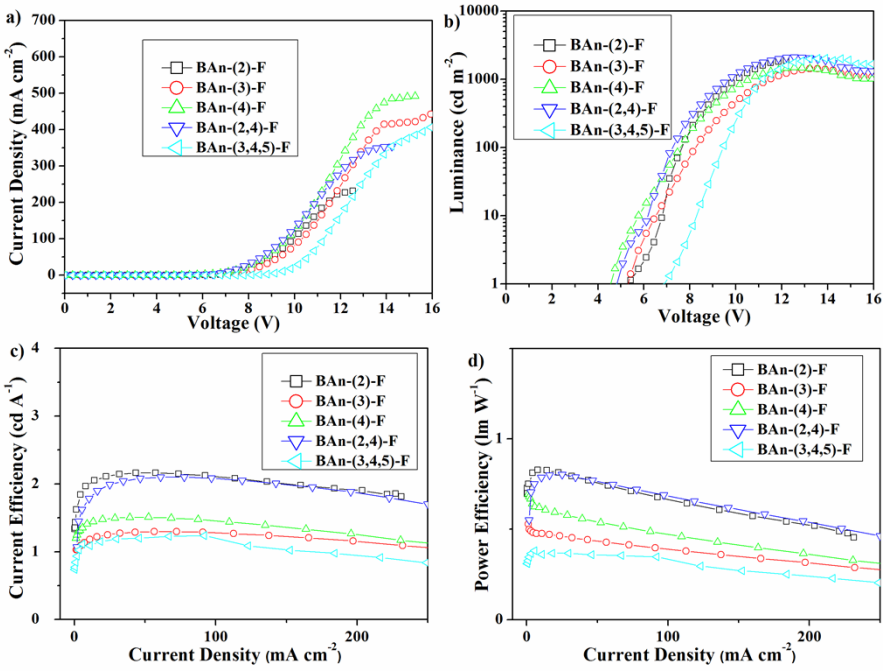

Fig. S4 a) Current density–voltage curves, b) Brightness–voltage curves, c) Current efficiency–current density curves, and d) Power efficiency–current density curves for the devices employing BAnFs as a non-doped emitter.

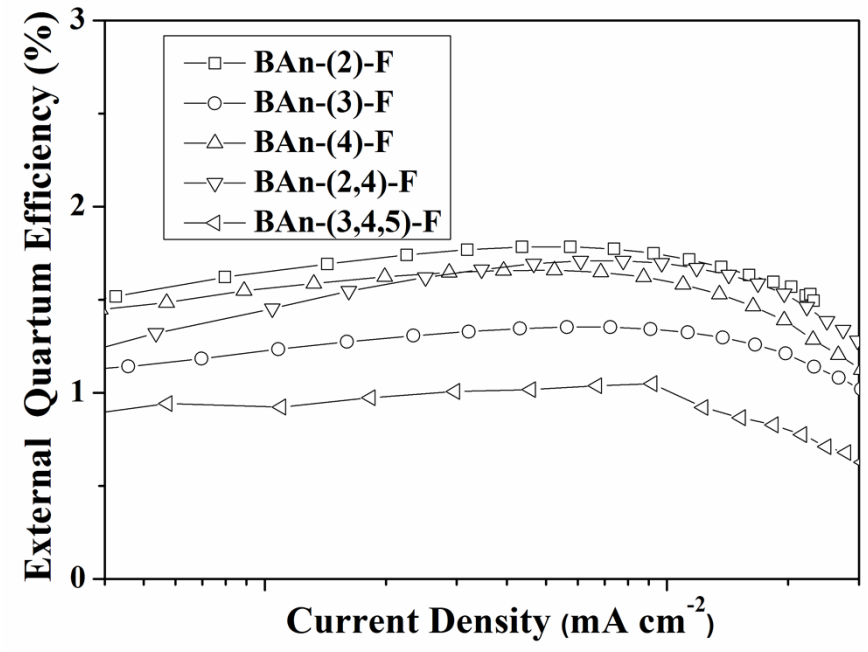

Fig. S5 External quantum efficiency (EQE) at different current densities for non-doped devices.

Table S1 Physical properties of BAnFs

Compound	$\lambda_{max}^{Abs\,a/b}$ (nm)	$\lambda_{max}^{PL\ a/b}$ (nm)	$\Phi_f{}^c$	$T_g/T_m{}^d$ (°C)	$E_{ox}{}^e$ (V)	HOMO/LUMO^{exp} (E_g^{opt})^f (eV)	HOMO/LUMO^{cal} ($\Delta E_{HOMO\text{-}LUMO}$)^g (eV)
BAn-(2)-F	259, 340, 358 , 378, 400 /270, 342, 361, 382, 404	449/448	0.55	168/299, 328	0.90	–5.70/–2.66 (3.04)	–5.26/–1.77 (3.49)
BAn-(3)-F	260, 340, 359, 379, 400 /269, 343, 362, 383, 405	445/447	0.48	167/362	0.93	–5.73/–2.67 (3.06)	–5.29/–1.81(3.48)
BAn-(4)-F	260, 340, 359, 379, 401 /266, 343, 362, 383, 405	449/447	0.41	167/347	0.88	–5.68/–2.63 (3.05)	–5.25/–1.77(3.48)
BAn-(2,4)-F	259, 338, 358, 378, 400 /270, 342, 362, 382, 405	448/443	0.69	156/248, 322	0.97	–5.77/–2.69 (3.08)	–5.28/–1.82 (3.46)
BAn-(3,4,5)-F	259, 339, 358, 378, 400 /264, 342, 360, 380, 403	449/445	0.93	NA/387	0.94	–5.74/–2.67 (3.07)	–5.47/–1.99 (3.48)

[a] Measured in CH_2Cl_2. [b] Measured in solid thin film on quartz plates. [c] Determined in CH_2Cl_2 using quinine sulfate (Φ_{PL} = 0.56 in 1.0 M H_2SO_4 solution) as standard. [d] T_g: glass-transition temperature; T_m: melting point; na: not available. [e] Determined from the onset of oxidation potentials; measured in CH_3CN; all of the potentials are reported relative to ferrocene, which was used as the internal standard in each experiment. The ferrocene oxidation potential was located at 0.16V, relative to the Pt-wire reference electrode. [f] The HOMO and LUMO energies were determined from cyclic voltammetry and the absorption onset. $E_{HOMO} = -(qE_{ox} + 4.8)$ eV; $E_{LUMO} = E_{HOMO} + E_g^{opt}$. [g] Values from DFT calculation.

Table S2 EL performance of blue devices with a non-doped EML

EML	λ_{max}^{EL} [a] (nm)	L^b (cd m^{-2})	η_c^c (cd A^{-1})	η_p^c (lm W^{-1})	η_{ext}^c (%)	CIE (x, y)[a]
BAn-(2)-F	444	2067	2.38	0.92	1.80	(0.192, 0.204)
BAn-(3)-F	444	1569	1.43	0.59	1.36	(0.171, 0.122)
BAn-(4)-F	436	1629	1.83	0.77	1.71	(0.169, 0.142)
BAn-(2,4)-F	445	2328	2.31	0.89	1.70	(0.201, 0.240)
BAn-(3,4,5)-F	444	2231	1.37	0.42	1.05	(0.183, 0.195)

[a] Values collected at 8 V. [b]Maximum luminance. [c]Values collected at a peak efficiency.