Electronic Supplementary Information

High-performing D- π -A- π -D Benzothiadiazole-based hybrid local and charge-transfer emitters in solution-processed OLEDs

Indu Bala,^a Rohit Ashok Kumar Yadav,^{b,†} Manisha Devi,^{a,†} Joydip De,^a Nitya Singh,^a Kamalakannan Kailasam,^d Jayachandran Jayakumar,^c Jwo-Huei Jou,^b Chien-Hong Cheng^c and Santanu Kumar Pal^{*a}

^aDepartment of Chemical Sciences, Indian Institute of Science Education and Research (IISER) Mohali, Sector-81, SAS. Nagar, Knowledge City, Manauli-140306, India

^bDepartment of Materials Science and Engineering, National Tsing Hua University, Hsinchu 30013, Taiwan ^cDepartment of Chemistry, National Tsing Hua University, Hsinchu 30013, Taiwan

^dEnergy and Environment Unit, Institute of Nano Science and Technology (INST), Sector-64, Phase X, Mohali 160062, India

Page No.

[†]Joint second author

* Correspondence: E-mail: skpal@iisermohali.ac.in; santanupal.20@gmail.com

Table of Contents

1 1. Experimental section 2. Synthesis and Characterization Details 1-3 3. NMR Spectral Data 4-6 4. Photophysical Properties (UV-vis, fluorescence and sensing studies) 7-12 5. DFT Study (HOMO-LUMO calculations) 12 6. Electrochemical Measurements (Cyclic voltammetry) 12-13 7. NTO Calculations 13-14 8. Device Fabrication and Testing 15-18 9. Fluorescence Decay Studies 18

1. Experimental Section

Materials and reagents: Commercially purchased chemicals were used without any 1.1 further purification. o-Phenylenediamine, triethylamine (NEt₃), bromine (Br₂), 4-(N-Bocamino)phenylboronic acid, tetrakis(triphenylphosphine)palladium(0) $(Pd(PPh_3)_4),$ trifluoroacetic acid (CF₃COOH), sodium bicarbonate (Na₂CO₃), tetrahydrofuran (THF) were purchased from Sigma-Aldrich. The solvents dichloromethane (DCM) and 1,2dimethoxyethane (DME) used in synthesis were bought from Merck. For photophysical studies, HPLC quality solvents viz. THF, hexane, triethylamine (NEt₃), chloroform (CHCl₃), diethyl ether, ethyl acetate (EtOAc), dichloromethane (DCM), dimethylformamide (DMF) and acetonitrile (ACN) were bought from Sigma-Aldrich. Silica gel (60-120) and neutral alumina gel were used to purify the intermediates and target materials by column chromatographic techniques. Thin-layer chromatography (TLC) was performed on alumina sheets pre-coated with silica gel (Merck, Kieselgel 60, F254). Poly-(ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) and 4,4'-Bis(N-carbazolyl)-1,1'-biphenyl (CBP) were purchased from H.C. Starck Clevios and Luminance Technology, respectively, and used as received. 2,2',2"-(1,3,5-Benzinetriyl)-tris(1-phenyl-1-Hbenzimidazole) (TPBi) were purchased from Merck.

1.2 Instrumentation: The detailed instrumental used for structural characterization (NMR: 400 MHz for ¹H NMR and 100 MHz for ¹³C NMR, Mass, FT-IR), photophysical studies (UV-vis & fluorescence), electrochemical characterization (cyclic voltammetry), are similar as mentioned in our previous papers.¹⁻³ The electroluminescence⁻ instrumental and device fabrication details are similar as described in our previous paper.³ The NMR instrumental details for 500 MHz for ¹H NMR and 125 MHz for ¹³C NMR is Bruker Biospin Switzerland Avance-Nu spectrometer.

2. Synthesis and Characterization Details

4,7-bis[4-(diphenylamino)phenyl]-2,1,3-benzothiadiazole **5** was obtained in three steps as per the reported procedure.^{4,5} The first step involves the formation of benzo[c][1,2,5]thiadiazole **3** by treating benzene-1,2-diamine with NEt₃ and SOCl₂ in dichloromethane.⁵ In the second step, the bromination of **3** gives rise to the synthesis of 4,7-dibromo substituted thiadiazole compound **4**.⁵ The Suzuki coupling of **4** with 4-(N-Boc-amino)phenylboronic acid leads to the formation of Boc-protected aminophenyl-substituted BTD derivative which on deprotection in

acidic medium forms aminophenyl-BTD derivative **5**.⁴ On the other hand, tri-alkoxy benzoyl chloride **6** was synthesized by following the earlier reported procedures.⁶⁻⁷ Finally, the target compounds **1** & **2** were simply afforded by condensation of trialkoxy benzoyl chloride **6** (1 equiv.) with 4,7-bis[4-(diphenylamino)phenyl]-2,1,3-benzothiadiazole **5** (2 equiv.) in dry THF using Et₃N as a base to form amide linked BTD derivatives **1** ($R = C_{10}H_{21}$) and **2** ($R = C_{12}H_{25}$). Both the derivatives differ only in the length of alkoxy chains and are characterized by ¹H NMR, ¹³C NMR, FT-IR and mass spectroscopy.



Scheme S1. (a) SOCl₂, Et₃N, DCM, RT; (b) Br₂, HBr, 12h, 120 °C; (c) i. 4-(N-Bocamino)phenylboronic acid, Pd(PPh₃)₄, Na₂CO₃, aq. DME ii. CF₃COOH, CH₂Cl₂; (d) Et₃N, THF, RT, 12h. Yield: 1: 62%; 2: 73%.

Intermediate: 4,7-bis[4-(diphenylamino)phenyl]-2,1,3-benzothiadiazole 5:

FT-IR (cm⁻¹): 3468, 3365, 1620, 1602, 1544, 1519, 1475, 1346, 1327, 1301, 1273, 1186, 1132, 1114, 855, 823.

¹**H** NMR (500 MHz*, CDCl₃, δ in ppm): δ 7.82-7.81 (d, 4H, J = 8.65 Hz), 7.68 (s, 2H), 6.86-6.84 (d, 4H, J = 8.55 Hz), 3.83 (s, 4H). *Note: This NMR spectrum has been recorded on a 500 MHz NMR spectrometer.

¹³C NMR (125 MHz[⊥], CDCl₃, δ in ppm): δ 154.45, 146.76, 132.39, 130.39, 128.04, 127.04,
 115.23. [⊥]Note: This NMR spectrum has been recorded on a 125 MHz NMR spectrometer.

Target BTD derivative: compound 1

FT-IR (cm⁻¹): 3300, 2951, 2923, 2853, 1645, 1582, 1520, 1495, 1468, 1426, 1336, 1238, 1215, 892, 827.

¹**H** NMR (400 MHz, CDCl₃, δ in ppm): δ 8.05-8.03 (d, 4H, J = 8.28 Hz), 7.85-7.81 (dd, 8H), 7.09 (s, 4H), 4.08-4.02 (m, 12H), 1.86-1.75 (m, 12H), 1.51-1.46 (m, 12H), 1.32-1.28 (m, 72H), 0.90-0.87 (t, 18H, J = 6.36 Hz).

¹³C NMR (100 MHz, CDCl₃, δ in ppm): δ 165.90, 154.19, 153.38, 141.67, 138.35, 133.51, 132.49, 130.04, 129.91, 127.88, 120.27, 105.96, 73.72, 69.58, 32.09, 32.07, 29.90, 29.84, 29.80, 29.75, 29.57, 29.51, 26.24, 22.84, 14.28.

HRMS-MALDI $(M+H)^+$ for C₉₂H₁₄₂N₄O₈S: calculated - 1464.0627, observed - 1464.0251

Target BTD derivative: compound 2

FT-IR (cm⁻¹): 3267, 2954, 2921, 2850, 1738, 1645, 1582, 1524, 1495, 1467, 1426, 1378, 1339, 1241, 1188, 1120, 1081, 969, 894, 824.

¹**H NMR** (400 MHz, CDCl₃, δ in ppm): δ 8.04-8.02 (d, 4H, *J* = 8.68 Hz), 7.88-7.81 (m, 8H), 7.09 (s, 4H), 4.07-4.01 (m, 12H), 1.85-1.74 (m, 12H), 1.49-1.45 (m, 12H), 1.26 (s, 96H), 0.89-0.86 (t, 18H, *J* = 6.44 Hz).

¹³C NMR (100 MHz, CDCl₃, δ in ppm): δ 165.85, 154.22, 153.43, 141.75, 139.44, 138.34, 132.53, 130.08, 127.91, 120.22, 114.21, 106.01, 73.74, 69.64, 32.09, 30.49, 29.86, 29.82, 29.67, 29.58, 29.53, 29.32, 26.25, 22.86, 14.29.

HRMS-MALDI $(M+H)^+$ for $C_{104}H_{166}N_4O_8S$: calculated – 1633.2538, observed – 1633.2627

3. NMR Spectral Data



Fig. S2 ¹³C NMR of compound **5**.



Fig. S4 ¹³C NMR of compound 1.



Fig. S6 13 C NMR of compound **2**.

4. Photophysical Properties





Fig. S7 Absorption and emission spectra of compound 1: (a) in solution state (THF, 10^{-5} M) and (b) in thin-film state (prepared by drop-casting the millimolar solution of compound 1 in DCM). Inset images presented the green and yellow colored luminescence showed by 1 under 365 nm UV light in solution and thin-film state, respectively.



Fig. S8 (a) TD-DFT simulated (black solid line) (no. of states considered = 40) and experimental (red dotted line) UV-vis absorption spectra of compound 2 in THF solvent. (b) Solvent-dependent fluorescence spectra of compound 2 in different solvents.

Calculation of dipole moment. The dipole moment in the excited states was calculated by using Lippert-Mataga equation⁸ given by:

$$\Delta v = \frac{2\Delta f}{4\pi\varepsilon_0 \hbar ca^3} (\mu_e - \mu_g)^2 + b$$
$$\Delta f = \frac{\varepsilon - 1}{2\varepsilon + 1} - \frac{n^2 - 1}{2n^2 + 1}$$

where $\Delta v = v_a - v_f$ represents the Stokes shift, v_a and v_f stands for absorption and emission frequency (cm⁻¹), Δf is the orientation polarizability of the solvent, ε_0 is the permittivity of the vacuum, $\hbar = h/2\pi$, where h is the Planck's constant, c is the velocity of light in vacuum, a is the Onsager radius and b is a constant, ε is the solvent dielectric, n is the solvent refractive index, μ_e and μ_g are the dipole moments of the excited and ground states, respectively, and $(\mu_e - \mu_g)^2$ is proportional to the slope of the Lippert-Mataga plot.

		Compound 1			
Solvents	Δf^a	$\lambda_{abs} (nm)^b$	$\lambda_{em} (nm)^c$	v_a - v_f (cm ⁻¹) ^d	
Hexane	0.0012	417	520	4750	
Triethylamine (NEt ₃)	0.048	419	530	4999	
Chloroform (CHCl ₃)	0.147	422	546	5381	
Diethyl ether	0.167	416	542	5277	
Ethyl acetate (EtOAc)	0.200	411	540	5812	
Dichloromethane (DCM)	0.217	410	536	6075	
Dimethylformamide (DMF)	0.276	417	566	6313	
Acetonitrile (ACN)	0.305	410	554	6340	
^{<i>a</i>} Orientational polarizability of the solvent. ^{<i>b</i>} λ_{abs} = absorption maximum. ^{<i>c</i>} λ_{em} =					
emission maximum. ${}^{a}v_{a}-v_{f}$ = the Stokes shift.					

Table S1 Solvatochromic absorption and emission data for Lippert-Mataga model.

4.2 Chemical sensing studies:

The BTD derivatives are highly emissive and upon excitation at 407 nm showed an emission band at 537 nm (in THF:H₂O, 90:10 (ν/ν), H₂O: 1mM tris-buffered saline (TBS), pH = 7.4) and displayed green fluorescence in the solution state. Thereby, the sensing ability of 1 towards various metal ions and anions was investigated by monitoring the change in fluorescence intensity upon the addition of various ions in 5×10^{-6} M parent solution (THF:H₂O, 90:10 (ν/ν), H₂O: 1mM tris-buffered saline (TBS), pH = 7.4). No change in the fluorescence intensity was observed on the addition of various metal ions tested (Co²⁺, Zn²⁺, Al³⁺, Pb²⁺, Mn²⁺, Cd²⁺, Cu²⁺, Fe^{2+} and Ni²⁺) except Fe^{2+} (Fig. S9a). On the addition of 78 μ M of Fe^{2+} into the parent solution of 1, fluorescence intensity gets quenched (Fig. S9b). Quenching of fluorescence intensity in the presence of Fe^{2+} is may be due to the complex formation of 1 with Fe^{2+} . As shown in the inset of Fig. S9b, fluorescence intensity decreased linearly on increasing the concentration of Fe^{2+} up to 72 µM and the detection limit was calculated as low as 41 ppb (Fig. S10a). Quenching constant was calculated using a Stern-Volmer plot as 2.23×10³ M⁻¹ (Fig. S10b). Non-linear fitting of Stern-Volmer plot shows that fluorescence quenching is due to the combination of both dynamic and static mechanisms.⁹ Using Benesi-Hildebrand plot, the binding constant was calculated as 4.53×10^4 M⁻¹ (Fig. S10c). Further to confirm the binding of 1 with Fe^{2+} , we have performed the ¹H NMR titration in CDCl₃ (Fig. S9c). It was observed that protons correspond to the amide hydrogen of 1 at 8.04 ppm get shifted to the 8.77 ppm without deprotonating. It means Fe²⁺ binds to -NH of **1**. It is evident from Fig. S9d, **1** is highly selective and sensitive for the detection of Fe^{2+} and the competitive experiment showed that there is no interference of other ions for the detection of Fe^{2+} .



Fig. S9 (a) Fluorescence spectra of 1 on the addition of various metal ions. Inset (top) consists of photographs of 1 on the addition of different metal ions under normal and UV (365 nm) light. (b) Fluorescence titration spectra of 1 (5 μ M) with Fe²⁺ ions (0-78 μ M) in THF:H₂O (90:10, ν/ν , H₂O: 1mM tris-buffered saline (TBS), pH = 7.4). Inset shows the change in fluorescence intensity on the addition of various concentrations of Fe²⁺ ions; $\lambda_{ex} = 407$ nm and $\lambda_{em} = 537$ nm for THF:H₂O (90:10, ν/ν , H₂O: 1mM tris-buffered saline (TBS), pH = 7.4) parent solution of compound 1. (c) Comparative ¹H NMR spectra of compound 1 (10⁻² M) upon addition of 6 μ l of Fe²⁺ ion (10⁻³ M). (d) The blue bars represent the fluorescence intensity of 1 in presence of different cations (78 μ M) followed by the addition of 78 μ M of Fe²⁺.



Fig. S10 (a) Plot between fluorescence intensity vs concentration of Fe²⁺ for the calculation of detection limit. (b) Stern-Volmer plot of 1 on addition of Fe²⁺ at $\lambda_{em}^* = 537$ nm for calculating quenching constant. (c) Benesi-Hildebrand plot of 1.Fe²⁺ association at $\lambda_{em} = 537$ nm for calculating binding constant. *Note: $\lambda_{em} = 537$ nm is for THF:H₂O (90:10, *v/v*, H₂O: 1mM trisbuffered saline (TBS), pH = 7.4) parent solution of compound 1.

Further, we have tested the sensing ability of **1** towards the anions under similar conditions (Fig. S11-S12). Among the various anions tested here (F⁻, Cl⁻, Br⁻, I⁻, NO₃⁻, CH₃COO⁻, SO₄^{2-,} and CO₃²⁻), only I⁻ showed the fluorescence quenching. Fig. S11 revealed the high selectivity and sensitivity towards the I⁻ anion. Detection limit was calculated as 32 ppb (Fig. S12a) and from the Stern-Volmer plot, quenching constant was obtained as 5.85×10^3 M⁻¹ (Fig. S12b). Using Benesi-Hildebrand method binding constant was calculated as 1.85×10^4 M⁻¹ (Fig. S12c).



Fig. S11 (a) Photographs of 1 on addition of different anions under normal and UV (365 nm) light. (b) Fluorescence spectra of 1 on addition of various anions. (c) Fluorescence titration spectra of 1 (5 μ M) with I⁻ ions (0-54 μ M) in THF:H₂O (90:10, *v*/*v*, H₂O: 1mM tris-buffered saline (TBS), pH = 7.4). Inset: change in fluorescence intensity on addition of various concentrations of I⁻ ions. $\lambda_{ex} = 407$ nm and $\lambda_{em} = 537$ nm for THF:H₂O (90:10, *v*/*v*, H₂O: 1mM tris-buffered saline (TBS), pH = 7.4) parent solution of compound 1. (d) The blue bars represent the fluorescence intensity of 1 in presence of different anions (54 μ M), the orange bars represent the fluorescence intensity of the above solution upon further addition of 54 μ M of I⁻.



Fig. S12 (a) Plot between fluorescence intensity at $\lambda_{em}^* = 537$ nm vs concentration of I⁻ for the calculation of detection limit. (b) Stern-Volmer plot of 1 on addition of I⁻ at $\lambda_{em} = 537$ nm for calculating quenching constant. (c) Benesi-Hildebrand plot of ligand 1.I⁻ association at $\lambda_{em} = 537$ nm for calculating binding constant. *Note: $\lambda_{em} = 537$ nm is for THF:H₂O (90:10, *v/v*, H₂O: 1mM tris-buffered saline (TBS), pH = 7.4) parent solution of compound 1.

Calculations of quenching constant, detection limit and binding constant: Quenching constant

The quenching constant of compound 1 for Fe^{2+}/I^- ion was determined from the non-linear Stern-Volmer curve. The exponential quenching equation given below was used to fit the non-linear Stern-Volmer curve¹⁰:

$$\frac{I_o}{I} = Ae^{Kx} + B$$

Where A, B, and K are constants. Quenching constant can be calculated as A×K.

Detection limit

The detection limit (DL) of compound 1 towards Fe^{2+}/I^- ions was determined from the following equation¹¹:

$$DL = \frac{3 \times SD}{S}$$

Where SD is the standard deviation of the blank solution detected 5 times; S is the slope of the calibration curve.

Binding constant

The binding constant, K_a , for compound 1 towards Fe^{2+}/I^- ions was determined using the Benesi-Hildebrand equation 1 for Fe^{2+} and 2 for I^- respectively¹²:

$$\log(\frac{I-I_0}{I_f-I_0}) = \log[M^{x-}] + \log K_a \qquad -----(1)$$

$$\frac{1}{(I-I_0)} = \frac{1}{[K_a(I_{max}-I_0)[M^{x+}]n]} + \frac{1}{I_{max}-I_0} \qquad -----(2)$$

where I_o is the emission intensity of the host in the absence of guest, I represent the emission intensity of the host recorded in the presence of an added guest, I_f or I_{max} is the emission intensity in the presence of added analyte ($[M^{x+/-}]_{max}$) and K_a represents the binding/association constant.



Fig. S13 Fluorescence microscopic photographs of pollen grains of *Hibiscus rosa-sinensis* in presence of compound **1** (a) bright field and (b) dark field.

5. DFT Studies for HOMO-LUMO Calculations

The geometrical optimization of the compounds 1 & 2 was carried out by DFT calculations using B3LYP functional with 6-31G(d,p) basis set. Excited states were calculated by time-dependent DFT (TD-DFT) calculations within the Tamm–Dancoff approximation (TDA)¹³⁻¹⁵ using the ground state optimized geometries.



Fig. S14 Frontier molecular orbitals of compounds (a) **1** and (b) **2** as obtained by DFT method at B3LYP/6-31G (d,p) level.

6. Electrochemical Measurements

The experimental setup for CV measurements consists of a single compartment cell equipped with Ag/AgNO₃ as a reference electrode, a platinum wire as a counter electrode, and glassy carbon as a working electrode. Millimolar solutions of all the compounds were used for CV measurements. A 0.1 M solution of tetrabutylammonium hexafluorophosphate was used as a supporting electrolyte.

The half-wave potential of the ferrocene/ferrocenium (Fc/Fc⁺) was calculated as:

 $E_{1/2,Fc/Fc^+} = (E_{anodic peak potential} + E_{cathodic peak potential})/2$

 $E_{LUMO} = -(4.8 - E_{1/2,Fc,Fc^+} + E_{red,onset}) eV. E_{HOMO} = -(4.8 - E_{1/2,Fc,Fc^+} + E_{oxd,onset}) eV.$

Electrochemical band gap: $\Delta E_{CV} = E_{LUMO}$ - E_{HOMO} .



Fig. S15 Cyclic voltammogram of compounds (a) 1 and (b) 2 in HPLC dichloromethane solution of tetrabutylammonium hexafluorophosphate (0.1 M) performed at a scanning rate 50 mVs⁻¹.

7. Natural Transition Orbital (NTO) Calculations



Table S2 Calculated natural transition orbitals (NTO) of first five singlet excited states.



Table S3 Calculated natural transition orbitals (NTO) of first five triplet excited states.

8. Device Fabrication and Testing

The solution-processed OLEDs were fabricated with a simple structure of ITO/PEDOT:PSS (35 nm)/ emissive layer (22 nm)/ TPBi (40 nm)/ LiF (1.5 nm)/ Al (150 nm). The patterned indium tin oxide (ITO) substrates were pre-cleaned with the routine procedure; acetone (30 min, 50 °C), isopropyl alcohol (30 min, 60 °C) and deionized water (15 min, RT) under sonication and further treated by UV-ozone for 30 min. A 30 nm layer of PEDOT:PSS (4000 rpm) was deposited on the ITO substrate *via* spin-coating to form a hole injection layer (HIL). The PEDOT:PSS coated substrates were baked in an oven at 120 °C for 15 min. The emissive layer (EML) consisting of CBP host matrix doped with **1** and **2** (1, 3, 5, or 100 wt%) was spin-coated (2500 rpm) from a fresh THF solution. A device structure of TPBi (40 nm)/ LiF (1.5 nm)/Al (150 nm) was thermally deposited in sequence in a vacuum chamber at a base pressure of less than 4×10^{-6} Pa. The current density-luminance-voltage characteristics were measured by a Keithley source measurement unit (Keithley 2400). The EL spectra of the devices were measured by SpectraScan PR650 spectrophotometer. All measurements were carried out at room temperature under ambient conditions.



Fig. S16 The topography image of thin film of compound 2 (1.0 wt%) doped with CBP host, measured by AFM in tapping mode.



Fig. S17 (a) & (c) Luminance-voltage-current density curve, (b) & (d) current efficiencyluminance-power efficiency curves for compounds 1 (a and b) and 2 (c and d) based solutionprocessed OLED devices using CBP host with 1, 3 and 5 wt% of emitter concentration.

Emitter	Emitter conc. (wt%)	$\frac{\text{PE}_{\text{max}}/\text{CE}_{\text{max}}}{\text{EQE}_{\text{max}}^{a}}$ (Im W ⁻¹ / cd A ⁻¹ / %)	$\frac{PE_{100}/ CE_{100}}{EQE_{100}^{b}}$ (lm W ⁻¹ / cd A ⁻¹ / %)	CIE _{xy} ^c	L_{max}^{d} (cd m ⁻²)
1	1	14.5/ 23.1/ 7.0	10.0/ 16.0/ 6.1	(0.31, 0.55)	1910
	3	9.7/ 15.5/ 4.7	9.3/ 14.9/ 4.5	(0.31, 0.55)	2995
	5	2.8/ 5.7/ 1.7	2.7/ 5.0/ 1.5	(0.35, 0.57)	3798
2	1	15.6/24.9/8.1	11.8/ 19.1/ 6.2	(0.29, 0.51)	2476
	3	10.5/ 16.7/ 5.1	7.2/ 11.5/ 4.8	(0.32, 0.56)	1978
	5	5.7/ 10.0/ 2.1	5.7/ 10.0/ 1.8	(0.31, 0.50)	2758

Table S4 Electroluminescent data of the BTD derivatives 1 and 2.

^{*a*}Maximum power efficiency (PE_{max}), current efficiency (CE_{max}) and external quantum efficiency (EQE_{max}). ^{*b*}Power efficiency (PE₁₀₀), current efficiency (CE₁₀₀) and external quantum efficiency (EQE₁₀₀) at 100 cd m⁻². ^{*c*}CIE coordinates at 100 cd m⁻². ^{*d*}Maximum measured luminance (L_{max}) of the device.



Fig. S18 Electroluminescence (EL) and photoluminescence (PL) spectrum of compounds (a) **1** and (b) **2** in the thin-film state. EL spectra were recorded for compounds **1** and **2** at 1 wt% doping concentration of emitters with CBP host.



Fig. S19 Low-temperature (at 77 K) phosphorescence (Phos) spectra of compounds (a) 1 (λ = 537 nm; triplet energy (E_T) = 2.31 eV) and (b) 2 (λ = 508 nm; E_T = 2.44 eV) in THF.

	PE _{max} / CE _{max} / EQE _{max} (Im W ⁻¹ / cd A ⁻¹ / %)	$\begin{array}{l} {\rm PE}_{100}/~{\rm CE}_{100}/\\ {\rm EQE}_{100}\\ {\rm (Im}~W^{-1}/~cd\\ {\rm A}^{-1}/~\%) \end{array}$	PE _{max} ~PE ₁₀₀ ^{<i>a</i>} (%)	CE _{max} ~CE ₁₀₀ ^b (%)	EQE _{max} ~EQE ₁₀₀ ^c (%)
1	14.5/23.1/7.0	10.0/ 16.0/ 6.1	31.0	30.7	12.8
2	15.6/24.9/8.1	11.8/ 19.1/ 6.2	24.3	23.3	23.4
aDe	war officiancy rol	11 off (DE DE	E) ^b Current	officianay roll	$\operatorname{off}(CE \to CE \operatorname{co})$

Table S5 Summary of EL performance and roll-off ratio of the best OLED devices.

^{*a*}Power efficiency roll-off ($PE_{max} \sim PE_{100}$). ^{*b*}Current efficiency roll-off ($CE_{max} \sim CE_{100}$). ^{*c*}External quantum efficiency roll-off ($EQE_{max} \sim EQE_{100}$).



Fig. S20 EQE (%) versus voltage (V) plots of the devices displaying an efficiency roll-off profile for compounds (a) **1** and (b) **2** based solution-processed OLED devices using CBP host with 1, 3 and 5 wt% of emitter (**1** and **2**) concentration.

9. Fluorescence Decay Study



Fig. S21 Fluorescence decay spectra of compound 2 in diethylether (solvent of moderate polarity), χ^2 value= 1.27; τ = 6.53 ns.

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