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Tailoring the structural rigidity utilizing lock/unlock donor strategy for highly efficient Solution processed Blue and Green HLCT OLEDs

Md Intekhab Alam[a,b], Mangey Ram Nagar[c], Debika Barman[d], Parameswar Krishnan Iyer[d], Jwo-Huei Jou[c], and Sivakumar Vaidyanathan[b]*

[a]Department of Chemistry, National Institute of Technology Rourkela, Rourkela, Odisha-769008, India.

[b]Department of Chemistry, Indian Institute of Technology Hyderabad, Sangareddy, Kandi, Telangana- 502285, India.

[c]Department of Materials Science and Engineering, National Tsing Hua University, Hsinchu, Taiwan-30013.

[d]Department of Chemistry, Indian Institute of Technology Guwahati, Guwahati, Assam- 781038, India.

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1. Experimental section.

1.1 General Information and Measurements.

Unless otherwise indicated, all reagents were purchased from commercial resources and used without further purification. All air-sensitive reactions were carried out under nitrogen. Solvents were carefully dried and distilled from suitable drying agents prior to use where needed. TLC was performed with 0.25 mm coated commercial silica gel plates (DC-kiesel gel

60 F254) and stained by Iodine, vanillin solution. Chromatographic separation was done by using (200-400 and 100-200 mesh) silica gel.

Nuclear Magnetic Resonance (NMR): NMR spectra were recorded on an AV 400 Avance-III 400 MHz FT-NMR Spectrometer (Bruker Biospin International, Switzerland) with tetramethylsilane (TMS) as standard reference. ^{1}H was recorded on 400 MHz & ^{13}C NMR was recorded on 100 MHz at 21 ^{o}C. NMR chemical shift (δ) value is reported in ppm. Multiplicity was reported as follows: s (singlet); d (doublet); t (triplet); q (quartet); m (multiplet); dd (doublet of doublets); td (triplet of doublets); dq (doublet of quartets); qd (quartet of doublets) etc. Coupling constants are given in Hz.

High resolution Mass Spectra (HRMS): HRMS was measured in a QTOF I (quadrupolehexapole-TOF) mass spectrometer with an orthogonal Z-spray-electrospray interface on micro (YA-263) mass spectrometer.

Themogravimetric analysis (TGA): TGA were performed using TA Instrument TGAQ50 thermal analysis system under N_2.

UV-Vis Absorption: UV-Vis absorption spectra were recorded using UV-vis spectrophotometer (Shimadzu Corporation, japan/UV-2450 pekin Elmer, USA/Lamda 25).

Photophysical measurements: Photoluminescence (PL) spectra were recorded using an Edinburgh instrument FLS980 spectrofluorometer. Time-resolved PL spectra were recorded by FLS980 spectrometer (Edinburgh Instruments Ltd.) The absolute PL Quantum yields (PLQY) were measured using an Edinburgh instrument spectrofluorometer, Integrating sphere SC-30 model. The quantum yield of the emitters is calculated by using equation (S1).[1]

$$\Phi = \frac{L_0(\lambda) - L_i(\lambda)}{L_0(\lambda)} \qquad \text{……..…(S1)}$$

$$\eta = \frac{E_i(\lambda) - (1 - \Phi)E_0(\lambda)}{E_0(\lambda)\Phi}$$

…….(S2)

Where, $L_0(\lambda)$ is the integrated excitation profile (sample is directly excited by the incident beam) and $L_i(\lambda)$ are the integrated excitation profile attained from the empty integrated sphere. $E_0(\lambda)$ is the integrated luminescence of solid caused by direct excitation and Ei(λ) is indirect illumination from the sphere, respectively.

Cyclic voltammetry (CV): CV of the emitters were carried out by using AUTOLAB 302 Modular Potentiostat electrochemical analyzer at 298 ± 1 K. The tests were carried out in dimethylformamide (DMF) containing 0.1 M tetrabutylammonium perchlorate (Bu_4NClO_4) as a supporting electrolyte, and the scan rate were maintained at 100 mVs^{-1} with three conventional electrode configurations viz, a glassy carbon working electrode, a platinum plate auxiliary electrode, and an Ag/AgCl reference electrode. The HOMO and LUMO energies of both the emitters were estimated from the onset oxidation and reduction potentials, using the equation (S3) and (S4) reported by Leeuw *et.al.* [2 3]

$$E_{HOMO} = -\left(E_{ox}^{onset} + 4.4\right)\ eV \quad \text{..... (S3)}$$

$$E_{LUMO} = -\left(E_{red}^{onset} + 4.4\right)\ eV \quad \text{..... (S4)}$$

Theoretical Calculations: Molecular geometrical properties, optimized structure and HOMO-LUMO, singlet-triplet energy levels and natural transition orbitals of the emitters were theoretically calculated by using DFT/TD-DFT with B3LYP/6-31G (d, p) basic set using Gaussian09 program package.

1.2 Device fabrication and measurements.

To check the electroluminescent properties of KCPhDPA and KCPhCz emitters, the organic light-emitting diodes were fabricated on indium-tin oxide (ITO) coated glass substrates. The device fabrication involved both cost-effective solution process. The monochromatic device structures are consisting of following device configurations: ITO/ PEDOT:PSS/ PVK/ KCPhDPA or KCPhCz/ TPBi/ LiF/Al for non-doped device and ITO/ PEDOT:PSS/ PVK/ CBP: emitters of X wt %/TPBi/LiF/Al for doped devices. Where X is 5, 7.5, 10, and 15 wt%. Initially, the glass substrates were cleaned with soap-solution, deionized water, acetone, and alcohol at optimized temperature and time. The cleaning process was carried-out in water-bath-tub sonicator. After cleaning, these substrates were treated with ultraviolet-ozone (UVO) light to remove residual solvents and remaining impurities. UVO treated substrates were transferred into nitrogen filled glovebox for further layer processing. First, the aqueous solution of poly(3,4-ethylenedioxythiophene) polystyrene-sulfonate (PEDOT:PSS) was spin-coated at 4,000 rpm for 20s to form a thin-film of hole-injection layer followed by annealing at 120 ^{o}C for 30 min. After that PVK was deposited to form a hole-transport layer. The emissive layer (EML) solution was prepared by dispersing host and guest molecules in tetrahydrofuran (THF) at 50 ^{o}C for 30 min in water-bath-tub. The EML was spin-coated at 2,500 rpm for 20s. After that, these samples were loaded into thermal evaporator chamber for further layer deposition. Then, a 40 nm TPBi as electron transport layer, a 1 nm LiF as electron injection layer, and 200 nm Al as cathode, were deposited sub sequentially via thermal evaporation method at 4.0×10^{-6} Torr base pressure. After that, Fabricated devices were kept in the mini vacuum chamber during testing process and then measured at room temperature conditions. To analyze the device, the electroluminescence (EL) spectrum, luminance, and the CIE coordinates were obtained using a photo research (PR-655) spectrometer. The current density-voltage-

luminance (J-V-L) characteristics were obtained by a computer mounted voltmeter (Keithley 2400) and spectrophotometer CS-100 Minolta.

2. Synthesis and characterizations.

Scheme 1 shows the structure and synthesis route of KCPhCz and KCPhDPA.

Initially, 4'-bromo-4-(4-bromobenzoyl)-3,5-dimethyl-[1,1'-biphenyl]-2-carbonitrile (KC) was synthesized.[4] [5] Next, 4-(4'-(9*H*-carbazol-9-yl)-[1,1'-biphenyl]-4-carbonyl)-4"-(9*H*-carbazol-9-yl)-3,5-dimethyl-[1,1':4',1"-terphenyl]-2-carbonitrile (KCPhCz) and 4"-(diphenylamino)-4-(4'-(diphenylamino)-[1,1'-biphenyl]-4-carbonyl)-3,5-dimethyl-[1,1':4',1"-terphenyl]-2-carbonitrile (KCPhDPA) were synthesized by Suzuki coupling reaction using $Pd(PPh_3)_4$ as catalyst in presence of K_2CO_3 as base in THF/EtOH solvent.

***Synthesis of 1-(4-Bromophenyl)but-3-yn-1-ol*:**

On activated zinc (3.6 g, 50.0 mmol) in THF (15 mL) at room temperature, propargyl bromide (2.4 mL, 80 wt % in toluene, 15.0 mmol) was added. This generated zinc-ylide. At room temperature, 4-Bromobenzaldehyde (1.85 grams, 10 mmol) in THF was added to this ylide suspension, followed by a saturated NH_4Cl solution (10mL). This was followed by filtering through a pad of Celite once the reaction was completed (as monitored by TLC). Using ethyl acetate (2 x 15 mL), the aqueous layer was extracted from the organic layer. Afterward, the resulting organic layers were washed with brine (30 mL) and dried over anhydrous Na_2SO_4. The crude 1-(4-bromophenyl)but-3-yn-1-ol was then concentrated under reduced pressure. Column chromatography was used to purify the crude product (ethyl acetate/Petroleum ether =1/20). Light yellow liquid (Yield = 75%). **^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm):** δ 7.50–7.44 (m,2H), 7.29–7.22 (m, 2H), 4.85 (q, *J* = 6.4 Hz, 1H), 2.67–2.56 (m, 2H), 2.39 (s, 1H),

2.08 (t, *J* = 2.8 Hz, 1H); **$^{13}C\{^{1}H\}$ NMR: (100 MHz, $CDCl_3$), δ (ppm):** δ 141.32, 131.68, 127.51, 121.83, 80.14, 71.62, 71.43, 29.43.

***Synthesis of 1-(4-bromophenyl)buta-2,3-dien-1-one*:**

A solution of 1-(4-bromophenyl)but-3-yn-1-ol (1.12 gm, 5 mmol) in acetone/DCM (1:1) (30 mL) was cooled to 0 ºC. Jones reagent (2 mL, 3.0 M solution, 6.25 mmol) was added dropwise *via* syringe with stirring. Upon complete consumption of the starting material as monitored by TLC, the reaction was quenched by the addition of isopropanol (0.2 mL). The mixture was filtered and the filtrate was concentrated under a vacuum. The residue was purified by column chromatography on silica gel eluting with ethyl acetate/hexane (1:10) to give 1-(4-bromophenyl)buta-2,3-dien-1-one. Dark red liquid (Yield = 48%). **^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm):** 7.81–7.75 (m, 2H), 7.63–7.60 (m, 2H), 6.40 (t, *J* = 6.4 Hz, 1H), 5.29 (d, *J* = 6.4 Hz, 2H); **$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$), δ (ppm):** 217.24, 190.09, 136.13, 132.47, 132.11, 131.89, 131.70, 130.25, 93.25, 79.54.

***Synthesis of 4'-bromo-4-(4-bromobenzoyl)-3,5-dimethyl-[1,1'-biphenyl]-2-carbonitrile (KC)*:**

A mixture of 1-(4-bromophenyl)buta-2,3-dien-1-one (2.23 gm, 10 mmol), Ethyl cyanoacetate (0.53 ml, 5 mmol), and K_2CO_3 (1.38 gm, 5 mmol) in acetone (35 mL) was refluxed for 15 min. Upon completion, the reaction mixture was cooled to room temperature, added with water (70 mL), and extracted with ethyl acetate. The combined organic phases were washed with brine, dried, filtered, and concentrated under a vacuum. The residue was purified by column chromatography on silica gel eluting with ethyl acetate/hexane (1:20) to give white solid compound (Yield = 78%). **^{1}H NMR (400 MHz, DMSO-d_6), δ (ppm):** 7.82 (d, *J* = 8.4 Hz, 2H) , 7.77 (d, *J* = 8.4 Hz, 2H), 7.72 (d, *J* = 8.4 Hz, 2H), 7.59 (d, *J* = 8.4 Hz, 2H), 7.48 (s, 1H), 2.28

(s, 3H), 2.15 (s, 3H); **$^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-d_6), δ (ppm):** 197.12, 144.79, 140.04, 139.26, 139.09, 137.43, 135.04, 133.21, 132.15, 131.52, 131.39, 130.05, 129.79, 123.08, 117.46, 110.03, 19.7, 18.7.

Synthesis of 9-(4-bromophenyl) Carbazole:

In one neck round bottom flask, mixture of CuI (0.569 gm, 2.99 mmol), K_2CO_3 (8.264 gm, 59.8 mmol), 18-crown-6 (0.26 gm, 0.986 mmol), 1,3-dimethyl-3,4,5,6-tetrahydro-2(1H)-pyrimidinone (DMPU) (1 ml), carbazole (5 gm, 29.9 mmol) and dibromo benzene (7.05 gm, 29.9 mmol) were added and refluxed at 170°C for 12 hours under nitrogen atmosphere. After completion of the reaction as indicated by TLC, the temperature cooled down to room temperature then the reaction mixture was quenched with 1 N HCl. Then the reaction mixture was extracted from DCM by water-DCM work-up and dried over sodium sulfate (Na_2SO_4). The grey color solid mixture was purified with column chromatography using petroleum ether as an eluent to get the white product (Yield = 71%). **^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm):** 8.17 (d, *J* = 7.5 Hz, 1H), 7.79 – 7.73 (m, 1H), 7.52 – 7.37 (m, 3H), 7.32 (dd, *J* = 16.6, 9.5 Hz, 1H).

Synthesis of 9-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-9H-carbazole, (CBZ PhPin):

In one neck round bottom flask, a mixture of 9-(4-bromophenyl) Carbazole (2.5 gm, 7.787 mmol), Bis(pinacolato)diboron (2.37 gm, 9.344 mmol), Potassium acetate (2.29 gm, 23.361 mmol), $Pd(dPPF)_2Cl_2$ (0.19 gm, 0.2336 mmol) in dioxane solvent was refluxed at 90°C for 24 hours under nitrogen atmosphere. After completion of the reaction as indicated by TLC, the reaction was stopped and the temperature was allowed to go down to room temperature. The reaction mixture was then extracted from DCM solution from water-DCM work-up and dried over sodium sulfate (Na_2SO_4). The reaction mixture was purified with column chromatography

using petroleum ether as an eluent to get the white product (Yield = 71%). **^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm):** 8.17 (d, *J* = 7.8 Hz, 2H), 8.08 (d, *J* = 8.2 Hz, 2H), 7.62 (d, *J* = 8.3 Hz, 2H), 7.44 (ddd, *J* = 10.9, 9.3, 4.6 Hz, 4H), 7.34 – 7.27 (m, 2H), 1.43 (s, 12H); **^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$), δ (ppm):** 140.50, 136.39, 126.03, 123.53, 120.19, 109.86, 84.10, 24.94.

Synthesis of 4-(4'-(9H-carbazol-9-yl)-[1,1'-biphenyl]-4-carbonyl)-4''-(9H-carbazol-9-yl)-3,5-dimethyl-[1,1':4',1''-terphenyl]-2-carbonitrile (KCPhCz):

A mixture of KC (200 mg, 0.426 mmol), CBZPhPin (409 mg, 1.108 mmol), and $Pd(PPh_3)_4$ (492.34 mg, 0.426 mmol) was dissolved in Tetrahydrofuran (THF) (20ml) at 40°C under nitrogen atmosphere. After this solution mixture became clear, was added a mixture of ethanol (5ml) and 2M aq. K_2CO_3 and the resulting mixture was heated to 70°C and refluxed for 24 hours under a nitrogen atmosphere. After completion of the reaction as indicated by TLC, stirring was stopped and the reaction mixture was allowed to cool to room temperature. The reaction mixture was then extracted from the DCM solution by water-DCM work-up and dried over sodium sulfate (Na_2SO_4). The product was purified by column chromatography. White powder (Yield = 78%) **^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm):** 7.90 (d, *J* = 7.9 Hz, 2H), 7.71 (dt, *J* = 17.3, 7.5 Hz, 6H), 7.55 (dd, *J* = 10.0, 8.8 Hz, 4H), 7.39 – 7.29 (m, 9H), 7.18 (dt, *J* = 8.5, 4.7 Hz, 12H), 7.09 (dd, *J* = 16.0, 7.4 Hz, 4H), 2.47 (s, 3H), 2.29 (s, 3H); **^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$), δ (ppm):** 197.63, 148.55, 147.61, 147.29, 146.65, 145.92, 141.15, 139.58, 139.44, 136.52, 134.36, 134.01, 132.51, 130.12, 129.44, 129.34, 129.23, 128.02, 127.81, 127.04, 126.86, 124.98, 124.61, 123.68, 123.57, 123.11, 122.97, 117.63, 110.23, 20.04, 18.74. **HRMS(m/z):** calcd for $C_{24}H_{24}BNO_2$, 793.3093. Found [M+1], 794.3156.

Synthesis of 4''-(diphenylamino)-4-(4'-(diphenylamino)-[1,1'-biphenyl]-4-carbonyl)-3,5-dimethyl-[1,1':4',1''-terphenyl]-2-carbonitrile (KCPhDPA):

A mixture of KC (200 mg, 0.426 mmol), TPA boronic acid (320.36 mg, 1.108 mmol), and $Pd(PPh_3)_4$, (492.34 mg, 0.426 mmol) was dissolved in Tetrahydrofuran (20ml) at 40 °C under nitrogen atmosphere. After this solution mixture became clear, was added a mixture of ethanol (5ml) and 2M aq. K_2CO_3 and the resulting mixture was heated to 70°C and refluxed for 24 hours under a nitrogen atmosphere. After completion of the reaction as indicated by TLC, stirring was stopped and the reaction mixture was allowed to cool to room temperature. The reaction mixture was then extracted from the DCM solution by water-DCM work-up and dried over sodium sulfate (Na_2SO_4). The product was purified by column chromatography. Green powder (Yield = 76%) **^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm):** 8.20 (d, *J* = 7.8 Hz, 4H), 8.02 (d, *J* = 8.0 Hz, 2H), 7.95 – 7.84 (m, 8H), 7.81 – 7.70 (m, 6H), 7.54 (d, *J* = 4.9 Hz, 2H), 7.52 (d, *J* = 4.9 Hz, 2H), 7.47 (tdd, *J* = 8.2, 3.2, 1.0 Hz, 4H), 7.40 (s, 1H), 7.35 (t, *J* = 7.4 Hz, 4H), 2.53 (s, 3H), 2.36 (s, 3H); **^{13}C{^{1}H} NMR: (100 MHz, $CDCl_3$), δ (ppm):** 197.63, 146.23, 145.87, 140.83, 140.66, 139.71, 139.57, 139.39, 138.43, 137.43, 137.32, 135.24, 130.24, 129.60, 129.47, 128.82, 128.59, 127.89, 127.51, 127.47, 127.45, 126.08, 126.03, 123.60, 123.50, 120.45, 120.37, 120.26, 120.07, 117.59, 110.42, 109.86, 109.76, 20.11, 18.82.

HRMS(m/z): calcd for $C_{24}H_{24}BNO_2$, 797.3406. Found [M+1], 798.3536.

3. NMR (^{1}H and ^{13}C) spectra of KCPhCz and KCPhDPA.

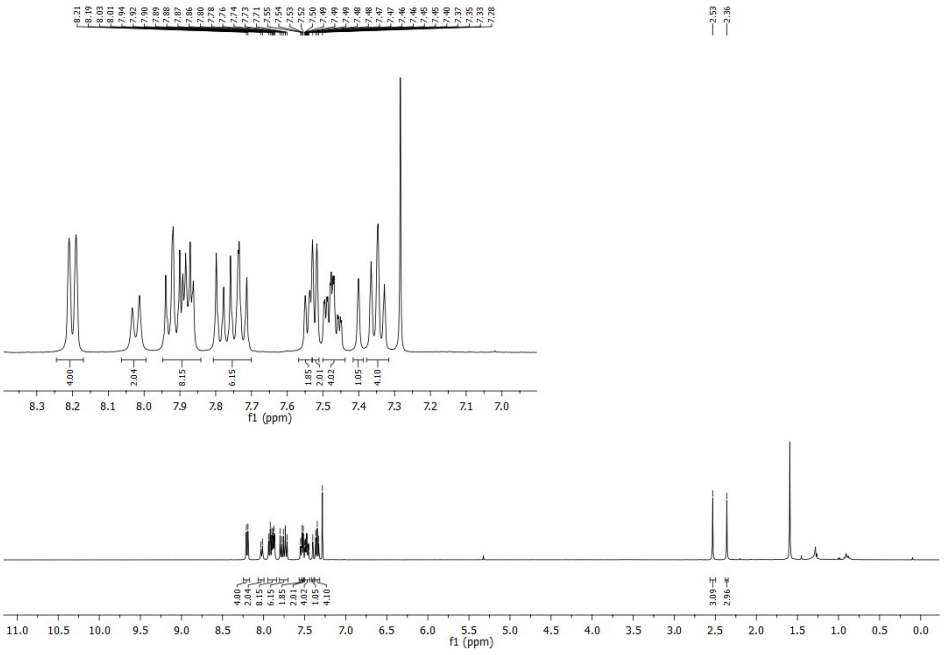


Figure S1. ^{1}H NMR spectrum of KCPhCz in $CDCl_3$.

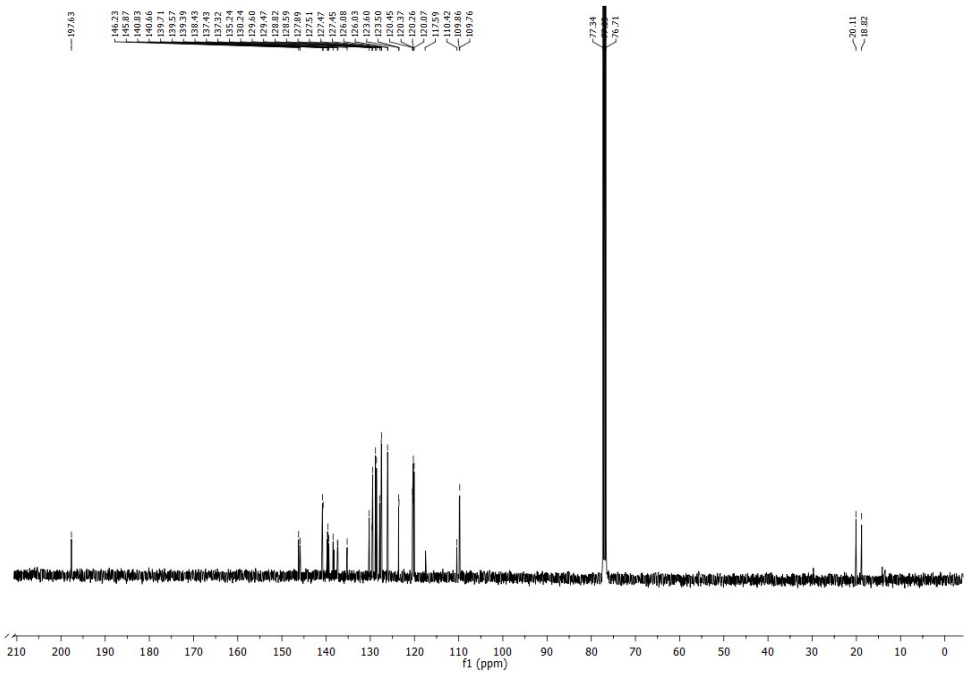


Figure S2. ^{13}C NMR spectrum of KCPhCz in $CDCl_3$.

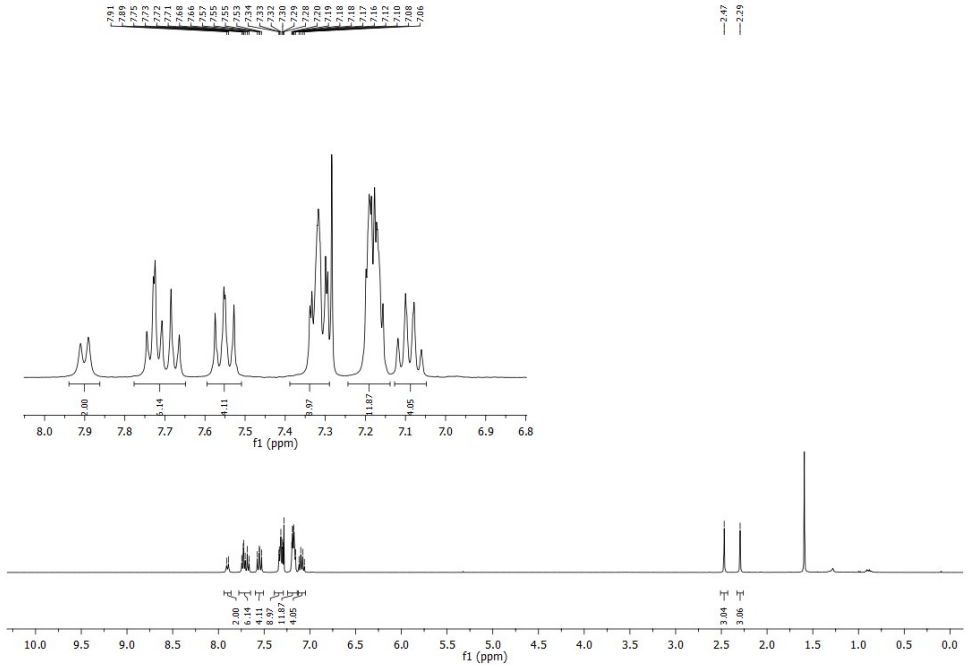


Figure S3. ^{1}H NMR spectrum of KCPhDPA in $CDCl_3$.

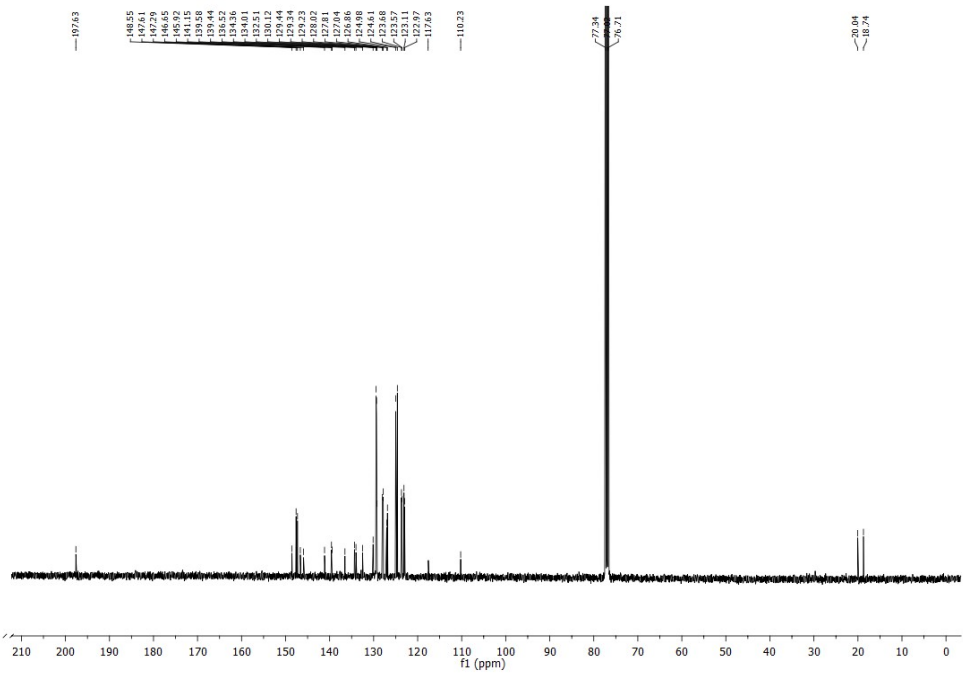


Figure S4. ^{13}C NMR spectrum of KCPhDPA in $CDCl_3$.

4. Mass spectra of KCPhCz and KCPhDPA.

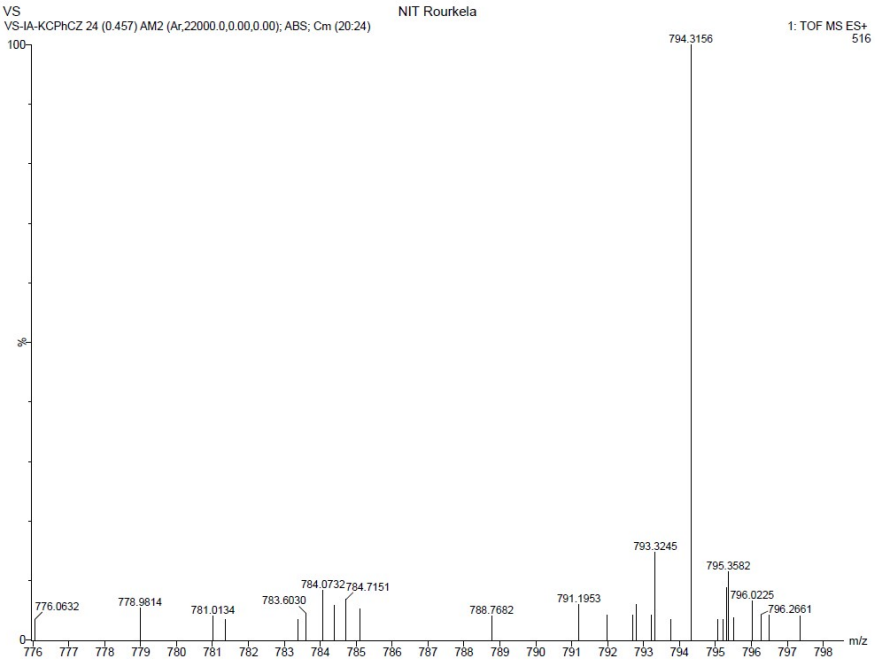


Figure S5. HRMS (TOF MS ES^+) spectrum of KCPhCz.

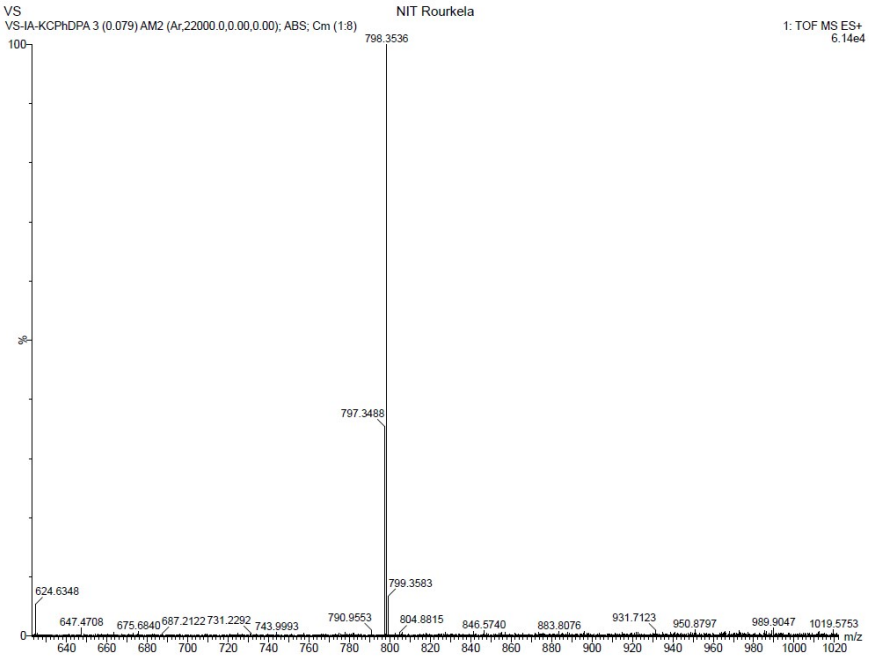


Figure S6. HRMS (TOF MS ES$^+$) spectrum of KCPhDPA.

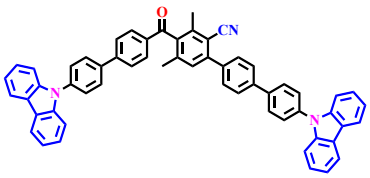
5. DFT Calculations.

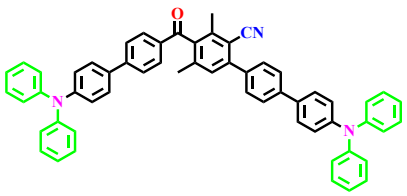
Table S1. Key DFT and TD-DFT parameter for the KCPhCz and KCPhDPA emitters.

Material	HOMO (eV)	HOMO-1 (eV)	LUMO (eV)	LUMO+1 (eV)	Band gap ($\Delta E_{H\text{-}L}$) (eV)	Dihederal angle (θ_1, θ_2, θ_3)	ΔE_{ST} (eV)
KCPhCz	-5.3462	-5.5108	-2.1859	-1.6550	3.1603	51.94 °, 72.63 °, 53.50 °	0.31
KCPhDPA	-4.9487	-5.1593	-1.9404	-1.4245	3.0008	35.27 °, 72.18 °,	0.38

						38.74 °	

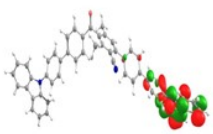
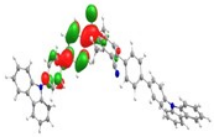
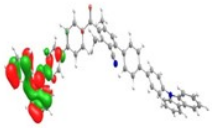
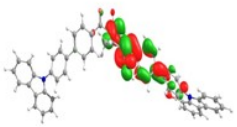
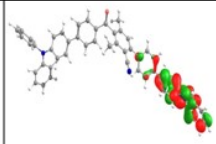
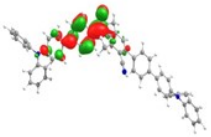
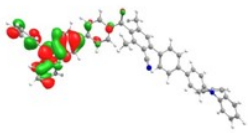
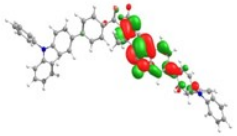
Table S2. The computed vertical transitions Energy, Absorption, oscillator strength (*f*) and transition configurations of KCPhCz and KCPhDPA.

Sr. No.	Emitter	λ_{max}(nm)	Energy levels	Energy (ev)	*f*	Transition Configuration (%)
1	**KCPhCz** 	418	S_1	2.9637	0.2090	H-1 → L (50.51) H → L (48.61)
		417	S_2	2.9733	0.0941	H → L (50.81)
		370	S_3	3.3419	0.2899	H → L+1 (68.83) H → L+2 (10.95)
		367	S_4	3.3774	0.0001	H-3 → L (70.31)
		364	S_5	3.4005	0.0000	H-2 → L (70.60)
		357	S_6	3.4722	0.0126	H-11 → L (24.98) H-8 → L (35.81) H-7 → L (35.92) H-7 → L (36.28)
		341	S_7	3.6308	0.0157	H → L+2 (70.30)
		329	S_8	3.7650	0.0736	H-8 → L (58.10)
		327	S_9	3.7946	0.0000	H-2 → L+1 (69.25) H-2 → L+2 (10.98)
		320	S_{10}	3.8701	0.1017	H-2 → L+2 (66.60)
		466	T_1	2.6554	-	H-5 → L (34.72) H-1 → L (56.25)
		435	T_2	2.8500	-	H-4 → L (16.08) H-4 → L+1 (34.50) H-4 → L+2 (13.47)
		414	T_3	2.9933	-	H-4 → L+1 (18.26) H → L (42.25)
		412	T_4	3.0061	-	H → L (46.62) H-12 → L (21.37) H-9 → L (26.56) H-8 → L (26.42) H-6 → L (26.02) H-4 → L (14.48)
		392	T_5	3.1638	-	H-3 → L+3 (57.93) H-1 → L+11 (24.38) H-3 → L (19.49)
		390	T_6	3.1737	-	H-5 → L (48.77) H-17 → L (19.08)
		390	T_7	3.1775	-	H-2 → L+6 (60.03)
		386	T_8	3.2140	-	H-12 → L (17.36) H-12 → L+1 (12.31) H-8 → L+2 (13.06)

						H → L+4 (11.63) H→ L+9 (11.76)
		369	T_9	3.3537	-	H → L+6 (65.93) H-6 → L+12 (13.18) H-4→ L+6 (10.68)
		367	T_{10}	3.3742	-	H-1 → L+3 (66.02) H-1→ L+4 (10.48)
2	**KCPhDPA** 	443	S_1	2.7946	0.0633	H → L (69.86)
		429	S_2	2.8885	0.6044	H-1 → L (69.59)
		390	S_3	3.1777	0.4078	H → L+1 (69.39)
		356	S_4	3.4805	0.0337	H-1 → L+1 (70.16)
		354	S_5	3.4978	0.0093	H-13 → L (22.04) H-8 → L (14.26) H-7 → L (35.91) H-6 → L (26.86) H-4 → L (26.63)
		335	S_6	3.6974	0.3103	H → L+2 (67.98) H → L+4 (11.75)
		322	S_7	3.8453	0.0330	H-2 → L (59.41) H-13 → L (24.62) H-7 → L (19.60) H-6 → L (10.63) H-4 → L (26.63)
		322	S_8	3.8516	0.0117	H → L+6 (69.01)
		321	S_9	3.8655	0.0138	H-1 → L+3 (68.03)
		309	S_{10}	4.0095	0.0908	H-1 → L+2 (65.47)
		512	T_1	2.4187	-	H-3 → L (21.95) H-1 → L (62.30) H-1 → L+4 (15.24)
		467	T_2	2.6528	-	H-2 → L+1 (20.25) H → L (32.88) H → L+2 (44.18) H → L+3 (24.90) H → L+4 (14.23)
		438	T_3	2.8266	-	H → L (61.33)
		412	T_4	3.0070	-	H → L (11.41) H-13 → L (22.16) H-8 → L (13.83) H-7 → L (34.10) H-6 → L (26.02) H-4 → L (24.55) H-3 → L (13.13)
		393	T_5	3.1572	-	H-13 → L (17.90) H-13 → L+1 (11.48) H-7 → L (14.25) H-7 → L+1 (10.47)

						H-6 → L+2 (13.90) H-2 → L+1 (35.50) H → L+9 (16.41)
		390	T_6	3.1813	-	H → L+8 (58.35) H-11 → L+14 (11.23) H-4 → L+6 (10.25) H → L+6 (15.53)
		386	T_7	3.2136	-	H-1 → L+5 (57.16) H-9 → L+12 (10.78)
		382	T_8	3.2400	-	H-3 → L (43.90) H-7 → L (24.09) H-5 → L+7 (10.32)
		367	T_9	3.3806	-	H-1 → L+1 (43.32) H-1 → L (28.94)
		364	T_{10}	3.4072	-	H → L+1 (45.34) H → L+9 (15.66) H-6 → L+1 (11.06) H → L+15 (10.34)

Table S3. Ground state frontier molecular orbitals (FMO's) of KCPhCz and KCPhDPA.

Molecules	HOMO	LUMO	HOMO-1	LUMO+1
KCPhCZ				
KCPhDPA				

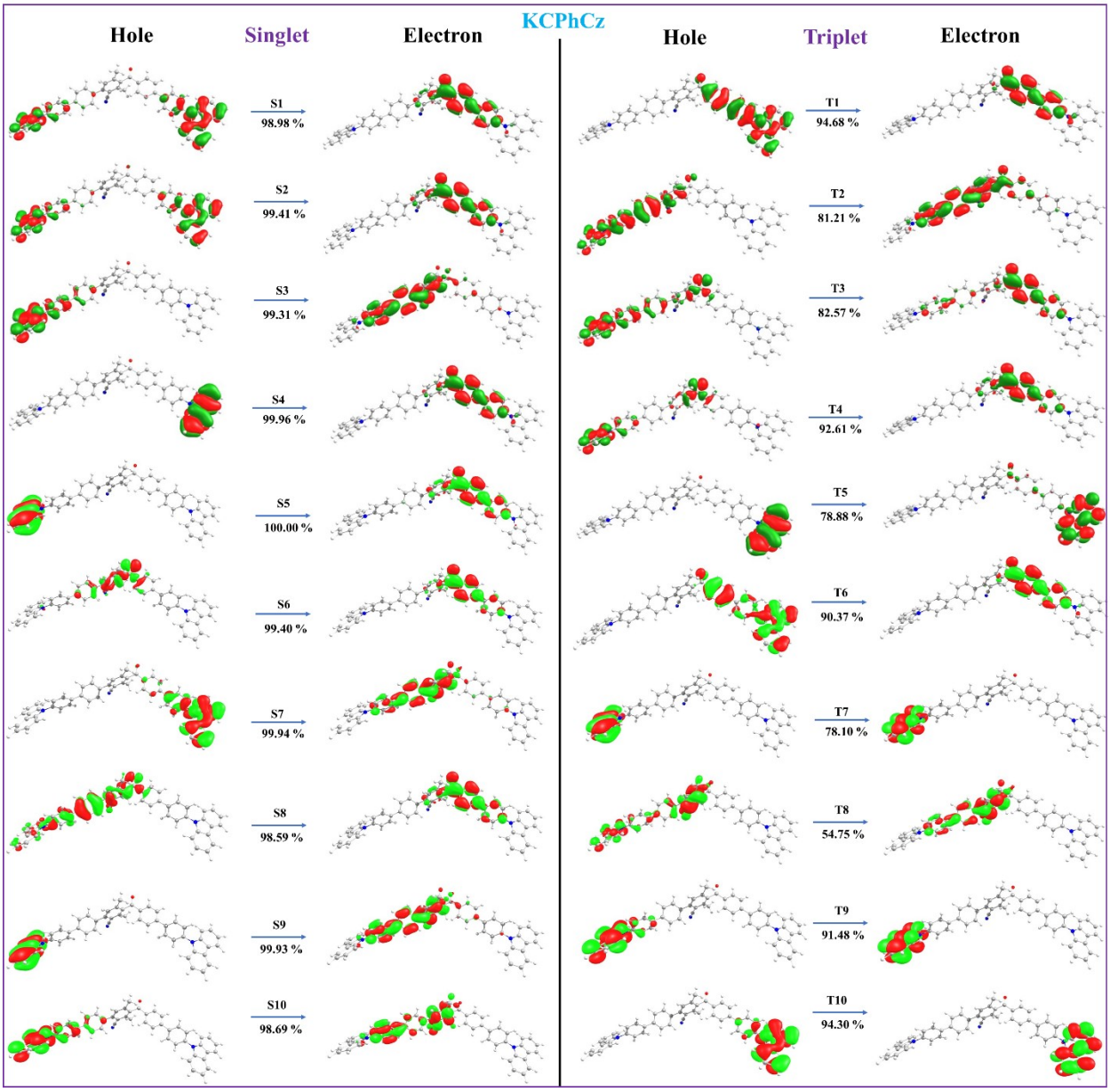


Figure S7. Natural transition orbitals of KCPhCz.

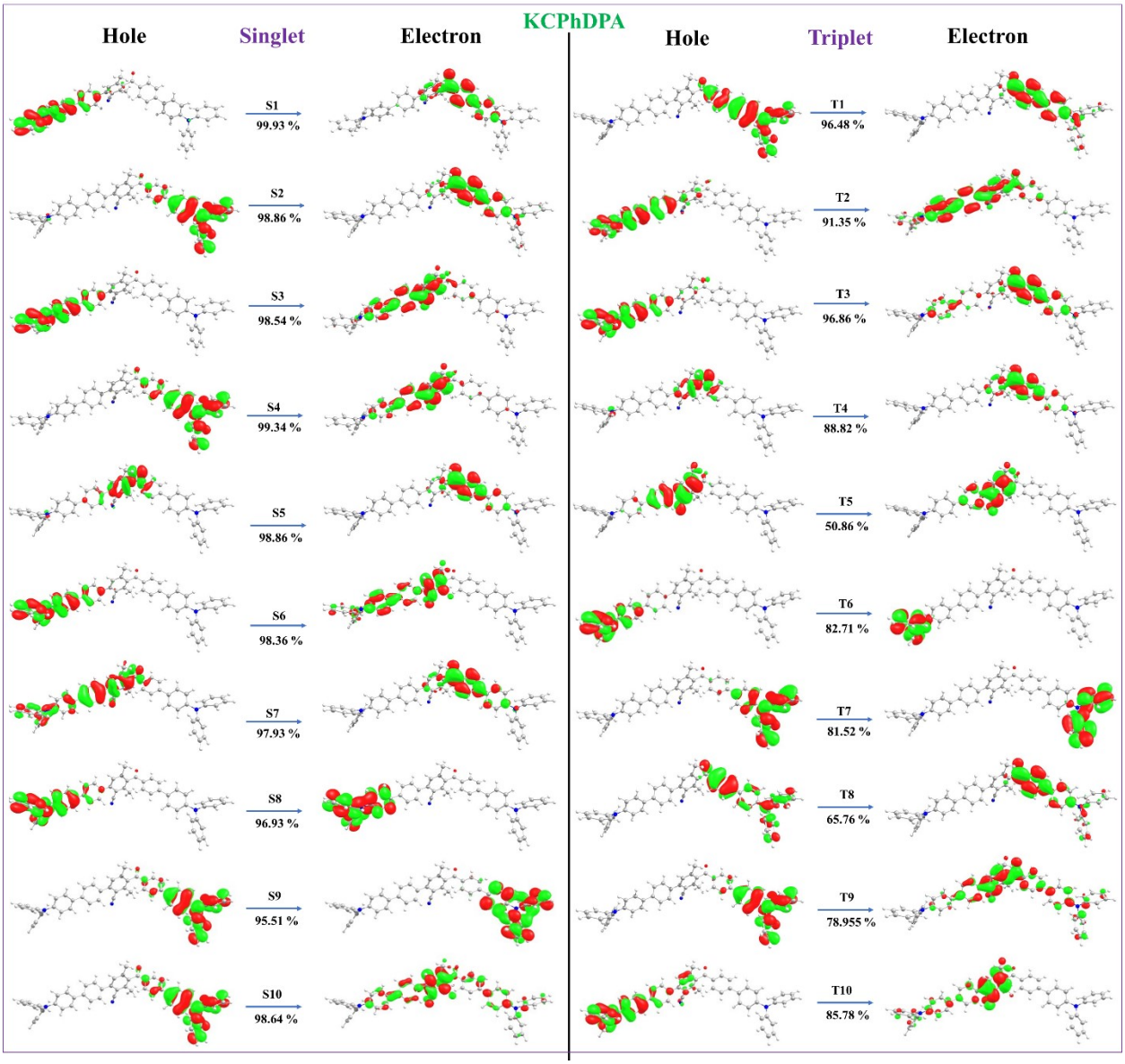


Figure S8. Natural transition orbitals of KCPhDPA.

6. Photophysical study.

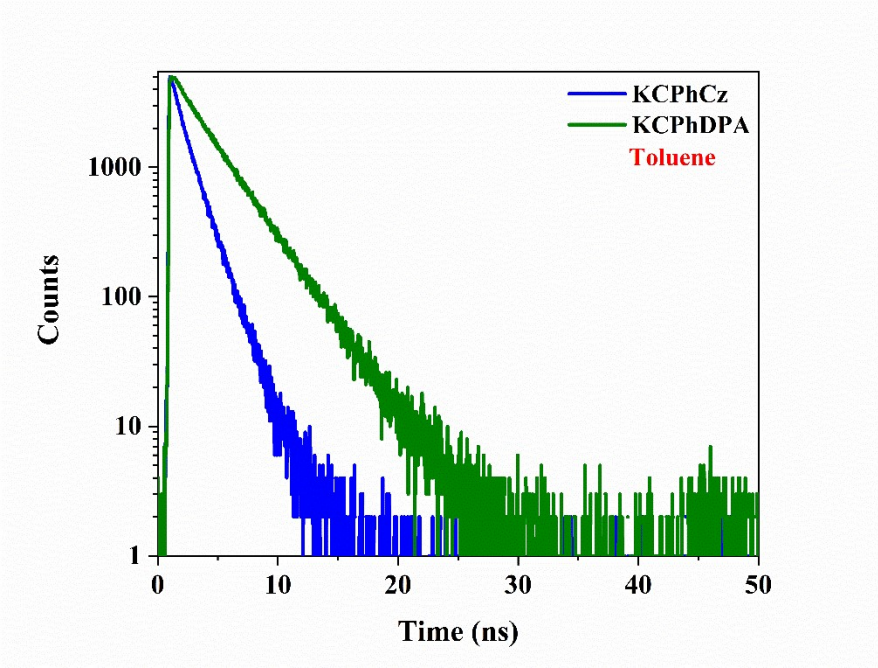


Figure S9. Time-resolved fluorescence decay of KCPhCz and KCPhDPA in toluene.

7. Electroluminescence Study.

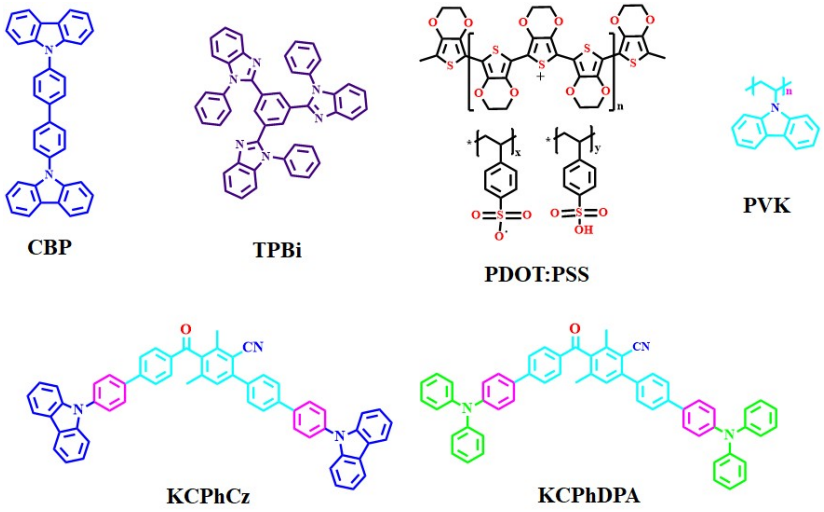


Figure S10. Chemical structures of the materials used in different devices.

Table S4. HOMO/LUMO energy values of the materials used in the devices.

Material	HOMO (eV)	LUMO (eV)
PDOT: PSS	5.0	3.3

PVK	5.8	2.2
CBP	6.0	2.9
KCPhCz	5.8	2.8
KCPhDPA	5.8	2.8
TPBi	6.2	2.78

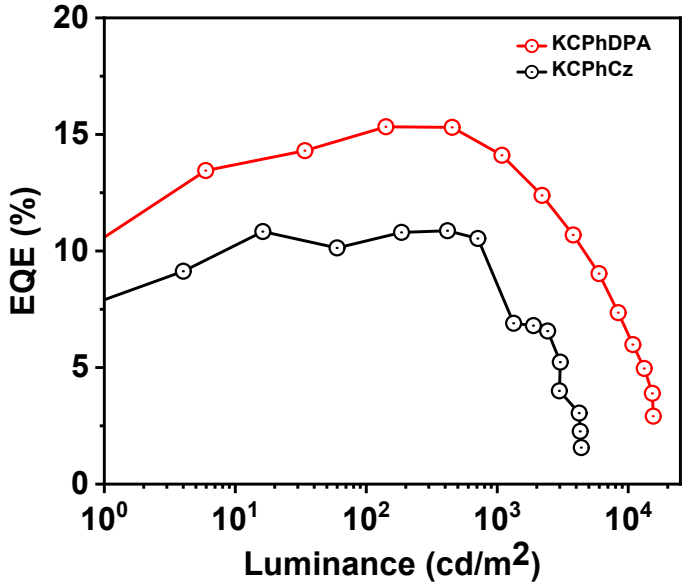


Figure S11. External quantum efficiency-Luminance curves for best optimized concentration of KCPhDPA and KCPhCz.

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