Supporting Information

Intramolecular-Locking Modification Enables Efficient Asymmetric Donor-Acceptor-Donor' Type Ultraviolet Emitters for High-Performance OLEDs with Reduced Efficiency Roll-Off and High Color Purity

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Experimental Section

1. General information

The raw materials and reagents were used after purchase without further purification. ¹H and ¹³C nuclear magnetic resonance (NMR) spectra were performed on a Bruker AVAN CE NEO 400 spectrometer with tetramethyl silane (TMS) as the internal standard in chloroform-d (CDCl₃). High-resolution mass spectra (MS) of target materials were measured using a high-resolution quadrupole time of flight tandem mass spectrometer (TOF-MS) operating in MALDI-TOF mode. Ultraviolet-visible (UV-vis) absorption spectra in dilute solutions were measured by a HITACHI U-4100 spectrophotometer. The photoluminescence (PL) spectra were recorded on a F-4600 fluorescence spectrofluorometer. By using a FLS1000 transient fluorescence spectrometer, fluorescence lifetimes were measured. Photoluminescence quantum yields (PLQYs) of target compounds were tested by employing the integration sphere setup (Hamamatsu C11347-11) equipped with a xenon high-pressure lamp. Thermogravimetric analysis (TGA) curves of materials were performed using a Netzsch (209F1) thermogravimetric analyzer under a nitrogen atmosphere (50 mL min⁻¹) at a heating rate of 20 °C min⁻¹. Cyclic voltammetry (CV) was measured on a CHI660E electrochemical workstation in a conventional three-electrode system including a glass carbon working electrode, a platinum wire auxiliary electrode, and an Ag/Ag⁺ standard reference electrode, where tetrabutylammonium hexafluorophosphate (Bu4NPF6, 0.1 M) in anhydrous dichloromethane (DCM) acted as the supporting electrolyte and ferrocene served as the standard reference. The HOMO (E_{HOMO}) and LUMO (E_{LUMO}) energy levels can be calculated by the following formula:

 $E_{HOMO} = -(E_{ox} - E_{1/2}^{+} + 4.80) \text{ eV}$ (1)

$$E_{LUMO} = (E_{HOMO} + E_g) eV \qquad (2)$$

Here, E_{ox} is the oxidation onset potential. $E_{1/2}^+$ is half wave potentials of Fc/Fc⁺ acquired from the CV curve. E_g is the optical bandgap evaluated from the onset of absorption spectra.

2. Device fabrication and measurements

Patterned indium-tin-oxide (ITO) glasses underwent ultrasonic cleaning in detergents and deionized water, followed by drying at 120 °C for a duration of 30 minutes. Subsequently, the ITO-substrates were treated with oxygen plasma and then carefully transferred to the vacuum deposition system. The devices were crafted in a high-vacuum environment, maintaining a pressure below 2×10^{-4} Pa. Evaporation rates were precisely monitored using a frequency counter and calibrated with a Dektak 6 M profiler from Veeco. Organic materials, lithium fluoride (LiF), and aluminum (Al) were thermally evaporated through a shadow mask at controlled rates of 1-1.5, 0.2, and 5-10 Å s⁻¹ respectively. The emitting area of the devices, defined by the overlap between ITO and Al electrodes, measured $3 \times 3 \text{ mm}^2$. To assess device performance, we recorded the current density, luminance, and voltage characteristics using a Keithley 2450 source meter and an LS160 luminance meter. Additionally, electroluminescence (EL) spectra were captured with an optical analyzer, the FlAME-S-VIS-NIR photometer. Assuming the light emitted by the OLEDs follows a Lambertian distribution, we estimated the external quantum efficiencies (EQEs) based on the EL spectra, luminance, and current density measurements.

3. Theoretical calculations

All density functional theory (DFT) and time-dependent DFT (TDDFT) calculations for the target materials were conducted utilizing the Gaussian 09 software package. The optimized ground-state geometries, energy levels, and frontier molecular orbital (FMO) distributions were determined using the B3LYP/6-31G(d, p) basis set within the DFT framework. Furthermore, using TDDFT calculations with the same B3LYP/6-31G(d, p) method, the optimized excited-state geometries, natural transition orbitals (NTOs), singlet and triplet state energies, as well as oscillator strengths were calculated. Spin-orbit coupling (SOC) matrix elements were calculated by TD-DFT and the ORCA 4.1.1 package at B3LYP/G 6-31G(d, p). The graphics and visualization analyses were processed by the Visual Molecular Dynamics (VMD) program. The apparent contributions of charge transfer (CT) to each excited state were further assessed by calculating the charges of the donor and acceptor fragments using the Hirshfeld partition model, corrected for interfragment charge transfer (IFCT), with the aid of the Multiwfn program.

4. Synthesis and characterization of target materials



Scheme S1. Synthesis routes of target materials.

Synthesis of 2-(3-bromophenyl)-1-phenyl-1H-phenanthro[9,10-d]imidazole (M1)

A mixture of 9,10-phenanthraquinone (2.08 g, 10 mmol), acetic amide (3.85 g, 50 mmol), 3bromobenzaldehyde (1.06 mL, 10 mmol), aniline (3.70 mL, 40 mmol), and acetic acid (30 mL) were added to a 250 mL round flask and refluxed at 120 °C for 8 hours under N₂ atmosphere. Then the mixture was poured into water and extracted with dichloromethane for three times. The organic layer was collected and concentrated by rotary evaporator. The residue was purified by column chromatography on silica gel using DCM/petroleum ether (1/1, v/v) as the eluent to the final product M1 (3.51 g, yield: 78.1%). ¹H NMR (400 MHz, CDCl₃, δ , ppm): 8.87 (d, *J* = 8.0 Hz, 1H), 8.76 (d, *J* = 8.4 Hz, 1H), 8.70 (d, *J* = 8.2 Hz, 1H), 7.84 (t, *J* = 1.8 Hz, 1H), 7.75 (t, *J* = 7.5 Hz, 1H), 7.70 – 7.58 (m, 4H), 7.56 – 7.48 (m, 3H), 7.43 (t, *J* = 9.3 Hz, 2H), 7.31 – 7.23 (m, 1H), 7.19 (d, *J* = 8.3 Hz, 1H), 7.12 (t, *J* = 7.9 Hz, 1H).

Synthesis of 1-Phenyl-2-(3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-1H-pyrrolo[9,10-

d]imidazole (mPPI)

Intermediate M1 (3.34 g, 7.44 mmol), 1,3,2-dioxaborolane (2.83 g, 11.16 mmol), potassium acetate (1.15 g, 22.31 mmol), and [1,1'-bis(diphenylphosphino)ferrocene]dichloropalladium(II) (0.19 g, 0.26 mmol) were dissolved in 100 mL of 1,4-dioxane. The reaction was heated up to 100 °C and reacted for 13 hours under N₂ atmosphere. Then the mixture was poured into water and extracted with dichloromethane for three times. The organic layer was collected and concentrated by rotary evaporator. The residue was purified by column chromatography on silica gel using DCM/petroleum ether (2/1, v/v) as the eluent to the final product mPPI (3.04 g, yield: 82.4%). ¹H NMR (500 MHz, CDCl₃, δ , ppm): 8.90 (d, *J* = 8.0 Hz, 1H), 8.78 (d, *J* = 8.4 Hz, 1H), 8.71 (d, *J* = 8.3 Hz, 1H), 8.13 (s, 1H), 7.74 (d, *J* = 7.4 Hz, 2H), 7.68 – 7.62 (m, 1H), 7.61 – 7.53 (m, 4H), 7.53 – 7.47 (m, 3H), 7.30 – 7.24 (m, 1H), 7.24 – 7.19 (m, 2H).

Synthesis of 9-(4'-bromo-2',5'-difluoro-[1,1'-biphenyl]-3-yl)-9H-carbazole (M2)

3-(9H-carbazol-9-yl)phenylboronic acid (1.16 g, 4.05 mmol), 1,4-dibromo-2,5-difluorobenzene (1.00 g, 3.69 mmol), and the catalyst tetrakis(triphenylphosphine)palladium (0.13 g, 0.11 mmol) were dissolved in 30 mL of toluene and 10 mL of ethanol and 10 mL of potassium carbonate solution. The reaction was heated up to 90 °C and reacted for 12 hours under N₂ atmosphere. Then the mixture was poured into water and extracted with dichloromethane three times. The organic layer was collected and concentrated by rotary evaporator. The residue was purified by column chromatography on silica gel using DCM/PF (1/8, v/v) as the eluent to the final product M2 (0.40 g, yield:48.6%). ¹H NMR (400 MHz, CDCl₃, δ , ppm): 8.15 (dt, *J* = 7.8, 1.0 Hz, 2H), 7.75 (q, *J* = 1.9 Hz, 1H), 7.70 (t, *J* = 7.8 Hz, 1H), 7.65 – 7.56 (m, 2H), 7.49 – 7.38 (m, 5H), 7.34 – 7.24 (m, 3H).

Synthesis of 2-(3''-(9H-carbazol-9-yl)-2',5'-difluoro-[1,1':4',1''-terphenyl]-3-yl)-1-phenyl-1Hphenanthro[9,10-d]imidazole (mPImCZ2F)

mPPI (1.01 g, 2.03 mmol), M2 (0.80 g, 1.84 mmol) and tetraphenylphosphinepalladium (0.09 g, 0.07 mmol) were dissolved in 25 mL of toluene, 10 mL of ethanol, and 10 mL of potassium carbonate solution. The reaction was heated up to 105 °C and reacted for 36 hours under N₂ atmosphere. Then the mixture was poured into water and extracted with dichloromethane three times. The organic layer was collected and concentrated by rotary evaporator. The residue was purified by column chromatography on silica gel using DCM/petroleum ether (1/1, v/v) as the eluent to the final product mPImCZ2F (0.75 g, yield: 56.6%). ¹H NMR (400 MHz, CDCl₃, δ , ppm): 8.91 (d, *J* = 8.0 Hz, 1H), 8.81 – 8.74 (m, 1H), 8.71 (d, *J* = 8.3 Hz, 1H), 8.17 (dt, *J* = 7.7, 1.0 Hz, 2H), 7.82 (q, *J*

= 1.8 Hz, 1H), 7.78 – 7.61 (m, 10H), 7.60 – 7.55 (m, 3H), 7.54 – 7.48 (m, 3H), 7.47 – 7.40 (m, 3H), 7.34 – 7.26 (m, 4H), 7.21 (dd, J = 8.4, 1.4 Hz, 1H), 7.03 (dd, J = 10.9, 6.4 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃, δ , ppm) 156.95, 154.53, 150.20, 140.79, 138.79, 138.11, 137.47, 136.27, 134.24, 131.04, 130.38, 130.23, 130.02, 129.62, 129.60, 129.40, 129.32, 129.19, 128.67, 128.35, 128.30, 128.19, 128.11, 127.72, 127.69, 127.52, 127.49, 127.37, 127.20, 126.76, 126.34, 126.10, 125.74, 125.03, 124.16, 123.52, 123.16, 123.02, 122.82, 120.92, 120.41, 120.16, 117.93, 117.89, 117.62, 117.35, 117.31, 109.77. MALDI-TOF-MS(m/z):[M⁺H] calcd for C₅₁H₃₂F₂N₃ : 724.2564; Found: 724.2562.

Synthesis of 9-(4'-bromo-2',5'-difluoro-[1,1'-biphenyl]-2-yl)-9H-carbazole (oCZ2FBr)

1,4-dibromo-2,5-difluorobenzene (2.05 g, 7.52 mmol), (2-(9H-carbazol-9-yl)phenyl)boronic acid (1.20 g, 4.18 mmol), and tetrakis(triphenylphosphine)palladium (0.19 g, 0.17 mmol) were dissolved in 30 mL toluene, 10 mL ethanol, and 10 mL potassium carbonate solution. The reaction was heated up to 90 °C and reacted for 12 hours under N₂ atmosphere. Then the mixture was poured into water and extracted with dichloromethane three times. The organic layer was collected and concentrated by rotary evaporator. The residue was purified by column chromatography on silica gel using DCM/petroleum ether (1/8, v/v) as the eluent to the final product oCZ2FBr (0.88 g, yield: 48.5%). ¹H NMR (400 MHz, CDCl₃, δ , ppm): 8.05 (dd, *J* = 7.8, 1.2 Hz, 2H), 7.67 – 7.58 (m, 3H), 7.54 (dt, *J* = 7.2, 1.4 Hz, 1H), 7.32 (ddd, *J* = 8.2, 7.1, 1.2 Hz, 2H), 7.25 – 7.18 (m, 2H), 7.11 – 7.02 (m, 3H), 6.64 (dd, *J* = 8.6, 6.3 Hz, 1H).

Synthesis of 2-(2''-(9H-carbazol-9-yl)-2',5'-difluoro-[1,1':4',1''-terphenyl]-3-yl)-1-phenyl-1Hphenanthro[9,10-d]imidazole (mPIoCZ2F)

mPPI (0.93 g, 1.88 mmol), oCZ2FBr (0.68 g, 1.57 mmol) and tetraphenylphosphinepalladium (0.06 g, 0.07 mmol) were dissolved in 25 mL of toluene, 4 mL of ethanol, and 4 mL of potassium carbonate solution. The reaction was heated up to 105 °C and reacted for 36 hous under N₂ atmosphere. Then the mixture was poured into water and extracted with dichloromethane three times. The organic layer was collected and concentrated by rotary evaporator. The residue was purified by column chromatography on silica gel using DCM as the eluent to the final product mPIoCZ2F (1.06 g, yield: 93,2%). ¹H NMR (400 MHz, CDCl₃, δ , ppm): 8.89 (s, 1H), 8.77 (d, *J* = 8.4 Hz, 1H), 8.70 (d, *J* = 8.3 Hz, 1H), 8.08 (d, *J* = 7.7 Hz, 2H), 7.75 (t, *J* = 7.5 Hz, 1H), 7.71 – 7.60 (m, 5H), 7.59 – 7.40 (m, 8H), 7.37 – 7.28 (m, 4H), 7.27 (s, 2H), 7.25 – 7.13 (m, 5H), 6.74 – 6.58 (m, 2H). ¹³C NMR (101 MHz, CDCl₃, δ , ppm) 156.66, 156.03, 154.21, 153.60, 150.10, 141.24, 138.64, 136.01, 134.22, 133.87,

132.29, 132.27, 130.27, 130.06, 129.96, 129.76, 129.47, 129.37, 129.11, 129.05, 128.79, 128.71, 128.48, 128.40, 128.31, 128.19, 127.37, 127.09, 126.69, 126.61, 126.52, 126.43, 126.32, 125.85, 125.73, 125.02, 124.14, 123.25, 123.13, 122.97, 122.85, 120.90, 120.17, 119.85, 117.41, 117.19, 117.15, 117.05, 117.01, 116.80, 116.76, 109.79. MALDI-TOF-MS(m/z): [M⁺H] calcd for C₅₁H₃₁F₂N₃: 723.2486; Found: 724.2567.

Synthesis of 9,9'-(4'-bromo-2',5'-difluoro-[1,1'-biphenyl]-3,5-diyl)bis(9H-carbazole) (mCP2FBr)

1,4-dibromo-2,5-difluorobenzene (1.87 g, 6.52 mmol), 9,9'-(5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3-phenylene)bis(9*H*-carbazole) (2.90 g, 5.43 mmol), and tetrakis(triphenylphosphine)palladium (0.25 g, 0.22 mmol) were dissolved in 30 mL toluene, 10 mL ethanol, and 10 mL potassium carbonate solution. The reaction was heated up to 90 °C and reacted for 12 hours under N₂ atmosphere. Then the mixture was poured into water and extracted with dichloromethane three times. The organic layer was collected and concentrated by rotary evaporator. The residue was purified by column chromatography on silica gel using DCM/petroleum ether (1/8, v/v) as the eluent to the final product mCP2FBr (1.00 g, yield: 30.7%). ¹H NMR (400 MHz, CDCl₃, δ , ppm): 8.17 (dt, *J* = 7.7, 1.0 Hz, 4H), 7.88 (dt, *J* = 12.8, 1.8 Hz, 3H), 7.60 (dt, *J* = 8.2, 0.9 Hz, 4H), 7.47 (ddt, *J* = 8.4, 7.1, 1.4 Hz, 5H), 7.43 – 7.36 (m, 1H), 7.34 (ddd, *J* = 8.0, 7.2, 1.0 Hz, 4H).

Synthesis of 2-(3",5"-di(9H-carbazol-9-yl)-2',5'-difluoro-[1,1':4',1"-terphenyl]-3-yl)-1-phenyl-1Hphenanthro[9,10-d]imidazole (mPImCP2F)

mPPI (0.79 g, 1.59 mmol), mCP2FBr (0.79 g, 1.33 mmol) and tetraphenylphosphinepalladium (0.06 g, 0.05 mmol) were dissolved in 25 mL of toluene, 3 mL of ethanol, and 3 mL of potassium carbonate solution. The reaction was heated up to 105 °C and reacted for 36 hours under N₂ atmosphere. Then the mixture was poured into water and extracted with dichloromethane three times. The organic layer was collected and concentrated by rotary evaporator. The residue was purified by column chromatography on silica gel using DCM/petroleum ether (1/1, v/v) as the eluent to the final product mPImCP2F (0.98 g, yield: 82.9%). ¹H NMR (400 MHz, CDCl₃, δ , ppm): 8.78 (d, *J* = 8.3 Hz, 1H), 8.72 (d, *J* = 8.2 Hz, 1H), 8.18 (dt, *J* = 7.8, 0.9 Hz, 4H), 7.94 (t, *J* = 1.6 Hz, 2H), 7.89 (t, *J* = 1.9 Hz, 1H), 7.76 (d, *J* = 6.0 Hz, 3H), 7.74 – 7.66 (m, 4H), 7.64 (dd, *J* = 8.4, 1.0 Hz, 5H), 7.61 – 7.57 (m, 3H), 7.57 – 7.26 (m, 12H), 7.21 (dd, *J* = 8.4, 1.3 Hz, 2H). ¹³C NMR (101 MHz, CDCl₃, δ , ppm) 140.52, 139.73, 137.78, 134.10, 130.44, 130.13, 129.61, 129.47, 129.15, 128.75, 128.39, 127.46, 126.40, 126.34, 125.99, 125.96, 125.15, 124.64, 124.19, 123.76, 123.15, 122.92, 120.94, 120.57, 118.21, 117.94, 117.51, 117.25, 109.72. MALDI-TOF-MS(m/z): [M⁺H] calcd for C₆₃H₃₈F₂N₄: 888.3065; Found: 889.3128.

Synthesis of 9,9'-(2',5'-difluoro-[1,1':4',1''-terphenyl]-3,3''-diyl)bis(9H-carbazole) (DmCZ2F)

3-(9*H*-carbazol-9-yl) phenylboronic acid (0.86 g, 2.99 mmol), 1,4-dibromo-2,5-difluorobenzene (0.74 g, 2.71 mmol), and tetrakis(triphenylphosphine)palladium (0.09 g, 0.08 mmol) were dissolved in 20 mL toluene, 10 mL ethanol, and 10 mL potassium carbonate solution. The reaction was heated up to 100 °C and reacted for 18 hours under N₂ atmosphere. Then the mixture was poured into water and extracted with dichloromethane three times. The organic layer was collected and concentrated by rotary evaporator. The residue was purified by column chromatography on silica gel using DCM/petroleum ether (1/6, v/v) as the eluent to the final product DmCZ2F (1.18 g, yield:73%). ¹H NMR (400 MHz, CDCl₃, δ , ppm): 8.16 (dt, *J* = 7.9, 1.1 Hz, 2H), 7.83 (q, *J* = 1.8, 1.4 Hz, 1H), 7.76 – 7.60 (m, 3H), 7.54 – 7.26 (m, 7H). ¹³C NMR (101 MHz, CDCl₃, δ , ppm) 157.02, 154.56, 140.74, 138.14, 136.15, 130.25, 128.83, 128.73, 128.60, 127.69, 127.49, 126.82, 126.08, 123.52, 120.39, 120.15, 117.87, 117.75, 117.68, 117.57, 109.75. MALDI-TOF-MS(m/z): [M⁺H] calcd for C₄₂H₂₇F₂N₂: 597.2142; Found: 597.2140.

Synthesis of 9,9',9'',9'''-(2',5'-difluoro-[1,1':4',1''-terphenyl]-3,3'',5,5''-tetrayl)tetrakis(9H-carbazole) (DmCP2F)

1,4-dibromo-2,5-difluorobenzene (1.87 g, 6.52 mmol), 9,9'-(5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2yl)-1,3-phenylene)bis(9*H*-carbazole) (2.90 g, 5.43 mmol), and tetrakis(triphenylphosphine)palladium (0.25 g, 0.22 mmol) were dissolved in 30 mL toluene, 10 mL ethanol, and 10 mL potassium carbonate solution. The reaction was heated up to 90 °C and reacted for 12 hours under N₂ atmosphere. Then the mixture was poured into water and extracted with dichloromethane three times. The organic layer was collected and concentrated by rotary evaporator. The residue was purified by column chromatography on silica gel using DCM/petroleum ether (1/6, v/v) as the eluent to the final product DmCP2F (0.38 g, yield: 11.3%). ¹H NMR (400 MHz, CDCl₃, δ , ppm): 8.09 (dd, *J* = 7.8, 1.1 Hz, 4H), 7.85 (dd, *J* = 16.4, 1.9 Hz, 3H), 7.56 (d, *J* = 8.3 Hz, 4H), 7.40 (ddd, *J* = 8.3, 7.1, 1.3 Hz, 5H), 7.31 – 7.22 (m, 4H). ¹³C NMR (101 MHz, CDCl₃, δ , ppm) 156.07, 153.61, 139.40, 138.76, 136.38, 127.54, 127.42, 127.30, 125.27, 124.86, 123.75, 122.70, 119.54, 119.50, 117.00, 116.88, 116.81, 116.70, 108.61. MALDI-TOF-MS(m/z): [M⁺H] calcd for C₆₆H₄₀F₂N₄: 926.3211; Found: 927.3291. 5.



Figure S1. The molecular geometries in the ground state, NTO calculations of the lowest singlet and triplet states for the donors phenyl-phenanthro[9,10-d]imidazole (PPI) and phenylcarbazole.



Figure S2. Calculated reduced density gradient isosurfaces (below) and scattering diagrams (above) based on optimized S₀ geometries of mPImCZ2F, mPIoCZ2F, and mPImCP2F.



Figure S3. The existence of multiple C-H···F noncovalent interactions in mPImCZ2F, mPIoCZ2F, and mPImCP2F.



Figure S4. Molecular geometries in the ground state, FMO distributions and calculated energy levels of DmCZ2F and DmCP2F. For DmCZ2F and DmCP2F molecules, the LUMOs were localized on the central triphenylene units. Their HOMO and HOMO-1 with similar energy levels and distributions which are delocalized on the two D' units, resulting in energetically degenerate HOMO and HOMO-1 orbitals.

	mPImCZ2F										
	Sin	glets		Triplets							
	Hole		Particle		Hole		Particle				
$S_0 \rightarrow S_1$	State State State	99.35%		$S_0 \rightarrow T_1$	South and and and an	79.01%	A State Stat				
$S_0 \rightarrow S_2$		99.52%		$S_0 \rightarrow T_2$	Sala and a sala a s	60.40%					
$S_0 \rightarrow S_3$	State and a state of the state	91.35%	San	$S_0 \rightarrow T_3$	Ser Calego	50.41%					
$S_0 \rightarrow S_4$	A A A A A A A A A A A A A A A A A A A	88.57%	A A A A A A A A A A A A A A A A A A A	$S_0 \rightarrow T_4$		78.19%					
$S_0 \rightarrow S_5$		99.95%		$S_0 \rightarrow T_5$	ૢૺ૾૽ૺૹ૱	76.04%					
$S_0 \rightarrow S_6$	Service Supervised	88.71%		$S_0 \rightarrow T_6$	Solution and the second	88.04%	A CARGE ST				
$S_0 \rightarrow S_7$	State	61.78%	and the second sec	$S_0 \rightarrow T_7$		89.36%	1998 - 1998 - 1998 - 1998 - 1998 - 1998 - 1998 - 1998 - 1998 - 1998 - 1998 - 1998 - 1998 - 1998 - 1998 - 1998 -				
$S_0 \rightarrow S_8$	Sector Sector	97.92%		$S_0 \rightarrow T_8$	Maria States	81.83%	and the second s				
$S_0 \rightarrow S_9$		86.69%		$S_0 \rightarrow T_9$	Ser Seres	38.38%	State State				
$S_0 \rightarrow S_{10}$	State and a state of the	62.95%	and the second sec	$S_0 \rightarrow T_{10}$		38.06%	See a				

Figure S5. The NTOs analysis of singlet and triplet excited states from the first to the tenth for mPImCZ2F.

			mPIo	oCZ2F					
	Sing	glets		Triplets					
	Hole		Particle		Hole		Particle		
$S_0 \rightarrow S_1$. Solo	99.44%		$S_0 \rightarrow T_1$		72.92%			
$S_0 \rightarrow S_2$	*	99.57%		$S_0 \rightarrow T_2$	S OF A	62.62%			
$S_0 \rightarrow S_3$		88.34%		$S_0 \rightarrow T_3$		80.12%			
$S_0 \rightarrow S_4$		87.26%		$S_0 \rightarrow T_4$	·ionece	61.31%			
$S_0 \rightarrow S_5$		99.01%		$S_0 \rightarrow T_5$	*	92.32%			
$S_0 \rightarrow S_6$	- Bare	99.36%		$S_0 \rightarrow T_6$	all a	89.90%	a series		
$S_0 \rightarrow S_7$		95.32%		$S_0 \rightarrow T_7$. de	83.97%			
$S_0 \rightarrow S_8$		82.06%		$S_0 \rightarrow T_8$		76.44%			
$S_0 \rightarrow S_9$	-	57.47%	-	$S_0 \rightarrow T_9$		38.83%			
$S_0 \rightarrow S_{10}$. Con	64.82%		$S_0 \rightarrow T_{10}$		29.88%			

Figure S6. The NTOs analysis of singlet and triplet excited states from the first to the tenth for mPIoCZ2F.

			mPIr	nCP2F					
	Sin	glets		Triplets					
	Hole		Particle		Hole		Particle		
$S_0 \rightarrow S_1$		99.29%		$S_0 \rightarrow T_1$		77.19%			
$S_0 \rightarrow S_2$	A Charles	98.98%		$S_0 \rightarrow T_2$	- painter	63.55%	pla		
$S_0 \rightarrow S_3$	* *****	99.83%	9545	$S_0 \rightarrow T_3$		50.39%	At Alt		
$S_0 \rightarrow S_4$		93.06%	-	$S_0 \rightarrow T_4$		90.66%			
$S_0 \rightarrow S_5$	***	86.44%		$S_0 \rightarrow T_5$	Section of the sectio	53.47%	.		
$S_0 \rightarrow S_6$		99.95%		$S_0 \rightarrow T_6$	and the second s	51.47%	an a		
$S_0 \rightarrow S_7$		99.97%		$S_0 \rightarrow T_7$	A date	73.96%	Harry States		
$S_0 \rightarrow S_8$		95.98%		$S_0 \rightarrow T_8$		91.30%			
$S_0 \rightarrow S_9$		73.92%	- Bales	$S_0 \rightarrow T_9$	*******	90.08%			
$S_0 \rightarrow S_{10}$		86.69%	and the second s	$S_0 \rightarrow T_{10}$	and the second second	91.51%			

Figure S7. The NTOs analysis of singlet and triplet excited states from the first to the tenth for mPImCP2F.

Excited States	S energy level [eV]	CTs [%]	S Oscillator Strength	Transition configuration of S	T energy level [eV]	CTs [%]	Transition configuration of T
1	3.362	72.60	0.0280	H→L (98.1%)	2.679	17.82	H→L+1 (56.0%) H→L (11.9%)
2	3.408	75.62	0.0115	H-1→L (96.6%)	2.950	18.40	H-4 \rightarrow L (39.4%) H \rightarrow L+7 (10.6%) H \rightarrow L (10.4%) H-3 \rightarrow L+2 (6.0%)
3	3.679	30.43	0.6003	H→L+1 (79.4%) H→L+2 (8.5%)	3.117	30.50	$\begin{array}{l} \text{H-1} & \rightarrow \text{L} \ (15.7\%) \\ \text{H-4} & \rightarrow \text{L} \ (11.9\%) \\ \text{H} & \rightarrow \text{L}^+7 \ (10.4\%) \\ \text{H} & \rightarrow \text{L} \ (9.8\%) \\ \text{H-3} & \rightarrow \text{L}^+2 \ (8.4\%) \\ \text{H} & \rightarrow \text{L}^+1 \ (5.8\%) \end{array}$
4	3.796	40.56	0.0668	$H \rightarrow L+2 (76.1\%)$ $H \rightarrow L+1 (10.8\%)$ $H-3 \rightarrow L+1 (7.0\%)$	3.179	14.21	$H-2 \rightarrow L+3 (72.7\%)$ $H-1 \rightarrow L+10$ (13.3%)
5	3.845	7.48	0.0001	-	3.278	54.30	H-1→L (54.2%) H-4→L (11.8%) H→L+1 (8.1%)
6	3.972	40.30	0.1360	-	3.340	53.51	$H \rightarrow L (44.2\%)$ $H \rightarrow L+1 (16.2\%)$ $H \rightarrow L+2 (15.3\%)$
7	4.015	42.38	0.0442	-	3.366	69.96	H-1→L+3 (82.4%)
8	4.028	23.61	0.0014	-	3.369	64.57	$\begin{array}{c} H \rightarrow L + 2 \ (43.7\%) \\ H \rightarrow L \ (11.6\%) \\ H \rightarrow L + 5 \ (8.6\%) \\ H \rightarrow L + 4 \ (7.7\%) \end{array}$
9	4.031	64.49	0.0513	-	3.551	64.67	$\begin{array}{l} \text{H-1} \rightarrow \text{L+6 (11.7\%)} \\ \text{H} \rightarrow \text{L+7 (10.7\%)} \\ \text{H-3} \rightarrow \text{L+1 (9.9\%)} \\ \text{H-3} \rightarrow \text{L+2 (9.3\%)} \\ \text{H-1} \rightarrow \text{L (5.9\%)} \\ \text{H-11} \rightarrow \text{L+6 (5.5\%)} \\ \text{H} \rightarrow \text{L (5.2\%)} \end{array}$
10	4.066	34.31	0.0086	-	3.617	70.94	$\begin{array}{l} \text{H-1} \rightarrow \text{L+6 (21.3\%)} \\ \text{H} \rightarrow \text{L+7 (14.2\%)} \\ \text{H-3} \rightarrow \text{L+2 (8.5\%)} \\ \text{H-3} \rightarrow \text{L+1 (6.9\%)} \\ \text{H-11} \rightarrow \text{L+6 (6.7\%)} \end{array}$

Table S1. Energy levels and proportion of CT component for singlet and triplet states, oscillator strengths of singlet states, and transition configuration of singlet and triplet states for mPImCZ2F in a vacuum.

Excited States	S energy level [eV]	CTs [%]	S Oscillator Strength	Transition configuration of S	T energy level [eV]	CTs [%]	Transition configuration of T
1	3.326	72.86	0.0231	H→L (98.3%)	2.725	17.12	H→L+1 (48.4%) H→L (12.4%) H-4→L (7.5%) H-2→L+3 (7.3%)
2	3.504	70.13	0.0051	H-1→L (97.8%)	2.925	17.85	H-4 \rightarrow L (39.9%) H \rightarrow L (11.0%) H \rightarrow L+5 (8.3%) H-2 \rightarrow L+3 (7.6%)
3	3.720	30.84	0.3656	H→L+1 (66.3%) H→L+3 (20.1%)	3.155	14.58	H-3→L+2 (67.6%) H-1→L+10 (7.3%) H-3→L (5.5%)
4	3.804	33.76	0.0732	$\begin{array}{c} H \rightarrow L+3 \ (62.7\%) \\ H \rightarrow L+1 \ (23.0\%) \\ H-2 \rightarrow L+1 \\ (6.9\%) \end{array}$	3.200	37.35	$\begin{array}{c} H \rightarrow L \ (22.9\%) \\ H-4 \rightarrow L \ (22.3\%) \\ H-2 \rightarrow L+3 \ (10.0\%) \\ H \rightarrow L+1 \ (8.4\%) \\ H \rightarrow L+5 \ (5.1\%) \end{array}$
5	3.857	24.07	0.0016		3.301	65.67	$H-1 \rightarrow L (44.0\%)$ $H-1 \rightarrow L+2$ (39.7%)
6	3.959	13.74	0.0004		3.330	56.25	$\begin{array}{l} H \to L \ (33.0\%) \\ H \to L + 3 \ (25.0\%) \\ H \to L + 1 \ (24.2\%) \\ H - 2 \to L + 3 \ (6.9\%) \end{array}$
7	3.982	25.20	0.0024		3.367	66.08	$\begin{array}{l} H \to L{+}3 \; (51.0\%) \\ H \to L \; (10.6\%) \\ H \to L{+}6 \; (10.2\%) \end{array}$
8	4.042	67.30	0.0404		3.489	63.44	$H-1 \rightarrow L+2$ (42.3%) $H-1 \rightarrow L$ (23.3%) $H-12 \rightarrow L+4$ (5.6%)
9	4.103	70.22	0.4459		3.578	70.50	$ \begin{array}{c} \hline H-2 \rightarrow L+3 \\ (17.0\%) \\ H \rightarrow L+5 \ (16.7\%) \\ H-2 \rightarrow L+1 \ (9.4\%) \\ H-1 \rightarrow L \ (7.8\%) \\ H \rightarrow L+6 \ (7.2\%) \end{array} $
10	4.166	56.85	0.0287		3.648	64.11	$\begin{array}{c} \text{H-1} \to \text{L} \ (9.0\%) \\ \text{H-12} \to \text{L+4} \\ (7.4\%) \\ \text{H-1} \to \text{L+4} \ (6.0\%) \end{array}$

Table S2. Energy levels and proportion of CT component for singlet and triplet states, oscillator strengths of singlet states, and transition configuration of singlet and triplet states for mPIoCZ2F in a vacuum.

Excited States	S energy level [eV]	CTs [%]	S Oscillator Strength	Transition configuration of S	T energy level [eV]	CTs [%]	Transition configuration of T
1	3.322	71.59	0.0313	$\mathrm{H} \rightarrow \mathrm{L} \ (97.4\%)$	2.684	17.70	$H \rightarrow L+1 (51.7\%)$ $H \rightarrow L (13.2\%)$ $H-6 \rightarrow L (5.8\%)$
2	3.329	69.20	0.0371	H-1 → L (92.6%)	2.915	17.75	$H-6 \rightarrow L (47.8\%)$ $H-2 \rightarrow L (7.9\%)$ $H \rightarrow L+8 (7.7\%)$
3	3.381	76.99	0.0006	H-2 → L (93.9%)	3.092	33.11	$\begin{array}{l} H \rightarrow L{+}8 \; (15.9\%) \\ H \rightarrow L \; (15.2\%) \\ H{-}2 \rightarrow L \; (11.7\%) \\ H{-}5 \rightarrow L{+}2 \; (9.9\%) \end{array}$
4	3.669	35.90	0.6398	$H \rightarrow L+1 (88.0\%)$	3.166	59.38	$H-1 \rightarrow L (73.6\%)$ $H-2 \rightarrow L (7.5\%)$
5	3.752	48.16	0.0152		3.175	14.22	$\begin{array}{l} \text{H-4} \rightarrow \text{L+4} \ (49.3\%) \\ \text{H-3} \rightarrow \text{L+6} \ (13.4\%) \\ \text{H-3} \rightarrow \text{L+5} \ (8.9\%) \\ \text{H-2} \rightarrow \text{L+11} \ (7.6\%) \end{array}$
6	3.764	91.70	0.0000		3.176	14.25	$\begin{array}{l} \text{H-3} \rightarrow \text{L+6} \ (28.6\%) \\ \text{H-4} \rightarrow \text{L+4} \ (20.1\%) \\ \text{H-3} \rightarrow \text{L+5} \ (19.0\%) \\ \text{H-1} \rightarrow \text{L+12} \ (7.0\%) \\ \text{H-1} \rightarrow \text{L} \ (5.5\%) \end{array}$
7	3.784	92.48	0.0001		3.267	44.89	$H-2 \rightarrow L (42.1\%)$ $H-6 \rightarrow L (21.3\%)$
8	3.931	68.95	0.1256		3.296	60.38	$H \rightarrow L (57.2\%)$ $H \rightarrow L+1 (24.0\%)$
9	3.963	59.94	0.1448		3.358	36.15	$H \rightarrow L+2 (59.7\%)$ $H \rightarrow L+7 (22.0\%)$
10	4.012	58.36	0.2034		3.373	29.37	$H-2 \rightarrow L+4 (66.1\%)$ $H-1 \rightarrow L+4 (12.6\%)$

Table S3. Energy levels and proportion of CT component for singlet and triplet states, oscillator strengths of singlet states, and transition configuration of singlet and triplet states for mPImCP2F in a vacuum.



Figure S8. The probable high-lying reverse intersystem crossing (hRISC) channels for mPImCZ2F, mPIoCZ2F, and mPImCP2F facilitate the utilization of triplet excitons in the EL process.



Figure S9. Absorption (a) and PL (b) spectra of DmCZ2F, DmCP2F mPImCZ2F, mPIoCZ2F, and mPImCP2F in dilute toluene solution (10 μ M) at room temperature. And the PL spectrum of PPI unit.

Table S4. The photophysical and electrochemical properties of DmCZ2F and DmCP2F.

Compound	λ _{PL} ^{a)} [nm]	Ф _{РL} ^{b)} [%]	λ _{peak} ^{c)} [nm]	Φ _{PL} ^{c)} [%]	E _g ^{d)} [eV]	HOMO/LUMO ^{e)} [eV]	E _{S1} /E _{T1} /ΔE _{S1T1} ^{f)} [eV]
DmCZ2F	425	78	403/382	28/46	3.57	-5.39/-1.82	3.20/2.52/0.68
DmCP2F	436	66	411/401	22/17	3.56	-5.38/-1.82	3.17/2.71/0.46

^{a)} Measured in THF solution at 300 K. ^{b)} Measured in non-doped and doped films at 300 K. ^{c)} Measured in non-doped and doped films at 300 K. ^{d)} Calculated from the absorption onset. ^{e)} HOMO energy level obtained from CV measurement. LUMO energy level calculated by $E_{LUMO} = E_{HOMO} + E_g$. ^{f)} Estimated by the peaks of low-temperature fluorescence and phosphorescence spectra at 77 K, $\Delta E_{S1T1} = E_{S1} - E_{T1}$.



Figure S10. The transient PL decay spectra of mPImCZ2F, mPIoCZ2F, and mPImCP2F in THF solvent.



Figure S11. The transient PL decay spectra of mPImCZ2F (a) and mPImCP2F (b) in the doped and neat films.

Compound	Φ _{PL} ^{a)} [%]	Φ _{PF} ^{b)} [%]	Φ _{DF} ^{c)} [%]	τ _{PF} ^{d)} [ns]	τ _{DF} ^{e)} [ns]	$k_{\rm r}^{\rm f)}$ [10 ⁷ s ⁻¹]	$k_{\rm nr}^{\rm g)}$ [10 ⁷ s ⁻¹]	$k_{\rm ISC}^{\rm h)}$ [10 ⁸ s ⁻¹]	$k_{\rm RISC}^{i}$ ⁱ⁾ [10 ⁷ s ⁻¹]
mPImCZ2F	34/70	9/34	25/36	1.95/3.88	7.79/7.41	4.73/8.84	9.18/3.79	3.74/1.32	4.73/2.76
mPIoCZ2F	53/48	24/32	29/16	2.18/1.30	7.63/6.01	11.14/24.92	9.88/27.00	2.49/2.50	2.86/2.47
mPImCP2F	35/54	9/19	26/35	2.15/1.93	8.35/6.86	4.07/9.98	7.56/8.50	3.49/3.33	4.79/4.09

^{a)} Photoluminescence quantum yield (Φ_{PL}) of neat and doped films. ^{b)} Prompt fluorescent quantum yields of films ($\Phi_{PF} = \Phi_{\tau_{PF}A_{PF}}/(\tau_{PF}A_{PF} + \tau_{DF}A_{DF})$). ^{c)} Delayed fluorescent quantum yield of films ($\Phi_{DF} = \Phi_{PL}\tau_{DF}A_{DF}/(\tau_{PF}A_{PF} + \tau_{DF}A_{DF})$). ^{d)} Prompt fluorescence lifetime. ^{e)} Delayed fluorescence lifetime. ^{f)} Rate of radiative transition ($k_r = \Phi_{PF}/\tau_{PF}$). ^{g)} Rate of non-radiative transition ($k_{nr} = k_r/\Phi_{PL} - k_r$). ^{h)} Rate of intersystem crossing ($k_{ISC} = k_r/\Phi_{PF} - k_r - k_{nr}$). ⁱ⁾ Rate of reverse intersystem crossing ($k_{RISC} = (k_{PF}k_{DF}\Phi_{DF})/(k_{ISC}\Phi_{PF})$).



Figure S12. Solvation effects on PL spectra of mPImCZ2F (a), mPIoCZ2F (b), and mPImCP2F (c) in dilute solutions (10 uM).



Figure S13. Thermogravimetric analysis curves of (a) mPImCZ2F, (b) mPIoCZ2F, (c) mPImCP2F.



Figure S14. CV curves of mPImCZ2F, DmCZ2F, mPIoCZ2F, mPImCP2F and DmCP2F.



Figure S15. Current density-voltage curves of electron-only and hole-only devices (EODs and HODs) for mPImCZ2F (a), mPIoCZ2F (b), and mPImCP2F (c), respectively. The structure of EODs: ITO/1,3,5-tris(1phenyl-1H-benzimidazol-2-yl)-benzene (TPBi) (10 nm)/mPImCZ2F, mPIoCZ2F, or mPImCP2F (80 nm)/TPBi (10 nm)/LiF (1 nm)/Al (100 nm). The structure of HODs: ITO/N,N'-bis(1-naphthalenyl)-N,N'-bisphenyl-(1,1'biphenyl)-4,4'-diamine (NPB) (10 nm)/mPImCZ2F (80 nm)/NPB (10 nm)/Al (100 nm). ITO/hexaazatriphenylenehexacarbonitrile (HATCN) (10 nm)/mPIoCZ2F or mPImCP2F (80 nm)/HATCN (10 nm)/Al (100 nm).



Figure S16. Current density–voltage curves of EODs and HODs for DmCZ2F (a) and DmCP2F (b). Carrier mobility-electric field characteristics for DmCZ2F (c) and DmCP2F (d). The structure of EODs: ITO/TPBi (10 nm)/DmCZ2F or DmCP2F (80 nm)/TPBi (10 nm)/LiF (1 nm)/Al (100 nm). The structure of HODs: ITO/NPB (10 nm)/DmCZ2F (80 nm)/NPB (10 nm)/Al (100 nm). ITO/HATCN (10 nm)/DmCP2F (80 nm)/HATCN (10 nm)/Al (100 nm).

Detailed analysis of dependence of hole/electron mobilities on the electric field

Hole and electron mobilities can be evaluated by a space-charge-limited current (SCLC) method, described by the Mott–Gurney equation, provides a means for analysis (1):

$$\frac{9}{J=8}\varepsilon_0\varepsilon_r\mu\frac{E^2}{L}$$
(1)

In this context, *J* denotes the current density, ε_0 signifies the vacuum permittivity with a value of 8.85×10^{-14} C V⁻¹ cm⁻¹, ε_r represents for the relative dielectric constant, assumed to be 3.0 for the organic semiconductor, μ stands the carrier mobility, E indicates the electric field intensity, and L refers to the thickness of the emitters. Considering the influence of energetic disorder on carrier mobility, the electric field-dependent mobility can be formulated using the Poole–Frenkel equation:

$$\mu = \mu_0 e^{-\gamma \sqrt{E}} \tag{2}$$

Here, μ_0 represents the zero-field mobility and γ denotes the Poole–Frenkel factor. Consequently, the SCLC that depends on the electric field can be formulated as follows:

$$J = \frac{9}{8} \varepsilon_{\gamma} \varepsilon_{0} \mu_{0} \exp \left(0.891 \gamma \sqrt{\frac{V}{L}} \right) \frac{V^{2}}{L^{3}}$$
(3)

According to the above method, the hole/electron mobilities dependent on the electric field can be obtained. As shown in Figure 4, and Table S6, under an electric field of 5×10^5 V cm⁻¹, the electron mobilities of mPImCZ2F, mPIoCZ2F, and mPImCP2F reach 2.31×10^{-5} , 1.49×10^{-5} , and 2.21×10^{-5} cm² V⁻¹ s⁻¹, respectively. The hole mobilities for these molecules are 1.95×10^{-7} , 4.29×10^{-6} , 1.32×10^{-6} cm² V⁻¹ s⁻¹, Both the electron mobilities and hole mobilities of these three molecules are higher than those of symmetric molecules DmCZ2F and DmCP2F.

Table S6. The electron and hole mobilities of mPImCZ2F, mPIoCZ2F, mPImCP2F, DmCZ2F, and DmCP2F under an electric field of 5×10^5 V cm⁻¹.

Mobility	mPImCZ2F	mPIoCZ2F	mPImCP2F	DmCZ2F	DmCP2F
Electron mobility (cm ² V ⁻¹ s ⁻¹)	$2.31 imes 10^{-5}$	1.49×10^{-5}	2.21×10^{-5}	$5.48 imes 10^{-7}$	$2.54 imes 10^{-8}$
Hole mobility (cm ² V ⁻¹ s ⁻¹)	$1.95 imes 10^{-7}$	$4.29 imes 10^{-6}$	1.32×10^{-6}	1.26×10^{-9}	$2.27 imes 10^{-10}$



Figure S17. (a) Chemical structure of organic materials used in the OLEDs. (b) Energy level alignment of the materials used in the OLEDs.



Figure S18. Power efficiency-luminance-current efficiency characteristics of the devices N1-5.



Figure S19. (a) EQE–luminance characteristics of the devices N1-5. (b) EL spectra of devices N4 and N5 at 5 V.

Table S6. Summary of representative EL performance of non-doped OLEDs with an EL peak wavelength \leq 410 nm.

Compounds	Year	EL peak (nm)	EQE _{max} (%)	Ref.
mPIoCZ2F	2024	393	6.62	this work
POPCN-CP	2022	404	5.30	[1]
POPCN-2CP	2022	404	7.50	[1]
mTPA-PPI	2015	404	3.33	[2]
DCZ2F	2023	404	5.62	[3]
CTPPI	2022	403	8.10	[4]
2MCz-CNMCz	2022	404	7.76	[5]
2BuCz-CNCz	2021	408	5.24	[6]
VDMP-36PhCz	2023	402	6.27	[7]
mP2MPC	2022	395	6.09	[8]
2DBF-CZCN	2024	390	3.00	[9]
4DBF-CZCN	2024	388	2.86	[9]
DCz-oPy	2022	400	2.70	[10]
DCz-mPy	2022	397	2.60	[10]
DCz-pPy	2022	397	3.60	[10]
o-DCz-Pm	2023	397	3.40	[11]
DCz-mPy-PhCz	2024	395	4.07	[12]
DCz-mPy-Na	2024	388	4.00	[12]
3,6-CNCzC3	2024	407	6.69	[13]



Figure S20. EL spectra of the device D3 at different voltages (Insert: CIE coordinates at 5 V).



Figure S21. Power efficiency–luminance–current efficiency characteristics of the doped devices D1-3.



Figure S22. Luminance–current density characteristics and their linear fits ($R^2 > 0.997$) for doped devices D1-3.

Compounds	EQE _{max} (%)	EQE ₁₀₀₀ (%)	EL peak (nm)	FWHM (nm)	CIE (x, y)	Ref.
mPIoCZ2F(D)	8.71	7.95	391	40	(0.167, 0.025)	this work
mPImCZ2F(D)	8.13	7.43	389	42	(0.167, 0.028)	this work
mPImCP2F(D)	6.58	6.41	392	43	(0.168, 0.028)	this work
3,6-mPPICNC3	7.67	7.65	412	44	(0.160, 0.032)	[14]
3,6-mPPICNC3(D)	7.85	7.48	391	41	(0.161, 0.025)	[14]
POPCN-CP	5.30	2.3	404	51	(0.160, 0.034)	[1]
POPCN-2CP	7.50	6.1	404	52	(0.159, 0.035)	[1]
POPCN-2CP(D)	8.20	5.7	404	50	(0.161, 0.034)	[1]
TPBCzC1	4.34	-	422	-	(0.160, 0.035)	[15]
DCZ2F	5.62	4.23	404	47	(0.163, 0.038)	[3]
CTPPI	8.10	4.2	403	-	(0.160, 0.040)	[4]
TBOSi (D)	9.15	-	414	-	(0.165, 0.034)	[16]
TBOSiCz (D)	8.91	-	414	-	(0.163, 0.031)	[16]
FIP-CZ (D)	10.40	7.3	427	49	(0.158, 0.039)	[17]
TPBCzC1	4.34	-	438	-	(0.159, 0.037)	[18]
2MCz-CNMCz	7.76	5.61	404	-	(0.158, 0.039)	[5]
ICZ-TAZ (D)	4.02	-	406	46	(0.162, 0.037)	[19]
2BuCz-CNCz (D)	10.79	6.80	396	-	(0.161, 0.031)	[6]
VDMP-36PhCz (D)	7.55	5.37	404	50	(0.159, 0.039)	[7]
SPA-DBS (D)	1.02	-	428	55	(0.16, 0.04)	[20]
TFPy4 (D)	5.10	-	404	54	(0.16, 0.02)	[21]
2Na-CzCN (D)	6.15	5.73	392	36	(0.16, 0.04)	[22]
mP2MPC	6.09	5.56	395	51	(0.163, 0.028)	[8]
3,6-CNCzC3	6.69	5.95	407	45	(0.161, 0.028)	[13]
BO-bph	11.3	-	394	48	(0.166, 0.021)	[23]
BTP-Nap	11.9	-	404,421	45	(0.161, 0.022)	[23]
CDFDB(D)	12	-	398	55	(0.16, 0.04)	[24]

Table S7. Summary of reported doped (D) and non-doped OLEDs with the CIEy smaller than 0.040 in recent years.

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