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Supporting Information

Achieving Phthalide-Based Fluorescent Materials with Hybridized Local and Charge-Transfer Characteristics for Efficient deep Blue

OLEDs

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1. Experimental section

1.1 General information

All the reagents and solvents are used as received without further purification. ¹H NMR was recorded by Bruker AVANCE 500 spectrometer at 500 MHz, 126 MHz and 160 MHz with tetramethylsilane (TMS) as the internal standard. On a Flash EA 1112, CHNS-O elemental analysis instrument, elemental analysis was performed. An AXIMACFRTM plus apparatus produced MALDI-TOF-MS mass spectra. On a Perkin-Elmer thermal analysis equipment, thermal gravimetric analysis (TGA) was carried out between 30 and 900 °C. The NETZSCH (DSC-204) machine recorded differential scanning calorimetry (DSC) from 30 to 400 °C. Thermal evaporation in high vacuum was used to create organic films for optical measurements on clear quartz surfaces. Spectra in the UV-Vis range were captured using a Shimadzu UV-3100 spectrophotometer. With the use of an RF-5301PC spectrophotometer, steady state photoluminescence spectra were measured. The Edinburgh spectrometer LP920 was used to collect time-resolved photoluminescence spectra using a 365-nm laser flash as the excitation source. Using a FLS920 spectrometer and a 375-nm picosecond pulsed light-emitting diode excitation source (pulse width: 898.1 ps), the PL lifetime was determined. The integrating sphere was used to calculate the PLQY.

1.2 Electrochemical measurements

Cyclic voltammetry (CV) was measured by using BAS 100B/W electrochemical analyzer with standard one-compartment, three-electrode electrochemical cell. The working electrode was a glass-carbon disk electrode. The counter electrode was a Pt wire. The reference electrode was Ag/Ag^+ . Ferrocenium/ferrocene (Fc⁺ /Fc) redox couple was used as the internal standard and the formal potential of Fc⁺ /Fc was 4.8 eV below vacuum. All potentials relative to Ag/Ag^+ electrode obtained from CV measurement were eventually referenced against Fc⁺/Fc to calculate HOMO/LUMO levels. As a result, the Ag/Ag^+ electrode was just a pseudo reference. The HOMO/LUMO levels are calculated according to the following formalism:

$$HOMO = - (E_{ox} vs. Fc^{+}/Fc + 4.8) eV$$
 Equation S1

$$LUMO = - (E_{red} vs. Fc^+ / Fc + 4.8) eV$$
 Equation S2

where the Eox vs. Fc^+/Fc and E_{red} vs. Fc^+/Fc were oxidation and reduction onset potentials relative to Fc^+/Fc reference, respectively.

1.3 Device fabrications and measurements

ITO coated glasses with a sheet resistance of 20 Ω square⁻¹ were used as the substrate and cleaned by deionized water, isopropyl alcohol, acetone and toluene. Then the ITO glasses were irradiated in UV-zone for 30 min. The deposition system for organic and metal deposition has a base pressure lower than 5×10⁻⁶ mbar. The hole injecting layer HAT-CN was deposited at 0.1 Å s⁻¹. The deposition rate of all other organic layers was 1.0 Å s⁻¹. The electron injecting layer LiF was deposited at a rate of 0.1 Å s⁻¹ and then the capping Al metal layer was deposited at a rate of 4.0 Å s⁻¹. The EL characteristics were measured using a Keithley 2400 programmable electrometer and a PR-650 Spectro-scan spectrometer under ambient condition. The electroluminescent (EL) characteristics were measured using a Keithley 2400 programmable electrometer and a PR-650 Spectro-scan spectrometer under ambient condition at room temperature.

1.4 Theoretical Calculations Method

In order to obtain molecular geometries, the ground-state (S_0) and lowest singlet excited state (S_1) geometries were optimized at the M06-2X/6-31G(d,p) level. The optimized result was in good agreement with the experiment's findings. The optimized S_0 state was used to determine the HOMO/LUMO distributions. On the basis of the optimized configuration of S_0 , the high excitation energy levels of the singlet and triplet states were computed using the TD-M062X/6-31G (d, p). Natural transition orbitals (NTOs) were assessed for the ten lowest excited levels, including singlet and triplet states under TD-M062X/6-31G (d, p), with the goal of examining the attributes of excited states. By diagonalizing the transition density matrix linked to each excitation, this method offered the most condensed representation of the electronic transitions in terms of an expansion into single particle orbitals.

1.5 Lippert-Mataga calculation

The properties of ground state (S_0) and the lowest singlet excited state (S_1) can be better

understood through solvatochromic experiment. One reliable way to explore the influence of solvent environment on the optical property of our sample was by using the Lippert-Mataga equation, a model that describes the interactions between the solvent and the dipole moment of solute:

$$hc(v_a - v_f) = hc(v_a^0 - v_f^0) - \frac{2(u_e - u_f)^2}{a^3}f(\varepsilon,n)$$
 Equation S3

where f was the orientational polarizability of solvents, μe was the dipole moment of excited state, μg was the dipole moment of ground state; a was the solvent cavity (Onsager) radius, derived from the Avogadro number (N), molecular weight (M), and density (d = 1.0 g cm⁻³); ε and n were the solvent dielectric and the solvent refractive index, respectively. f(ε ,n) and a can be calculated respectively as follows:

$$f(\varepsilon, n) = \frac{\varepsilon - 1}{2\varepsilon + 1} - \frac{n^2 - 1}{2n^2 + 1}$$
Equation S4
$$a = (3M/4N\pi d)^{1/3}$$
Equation S5

2. Supplementary Figures and Tables

2.1 Synthesis and characterization

The synthesis procedures of PPIB was according to our previous report.^[4]

Synthesis of **AnPT**:

9-Anthraceneboronic acid (1.11 g, 5 mmol), 5-Bromophthalide (1.07 g, 5 mmol), $Pd(PPh_3)_4$ (0.15 g, 0.15 mmol), K_2CO_3 (2.76 g, 20 mmol), distilled water (10 mL), and tetrahydrofuran (50 mL) were first mixed. The mixture was heated by 70 °C and refluxed under a nitrogen atmosphere for 24 h. After cooling to room temperature, the mixture was washed by water and extracted with dichloromethane consecutively. The product was purified by column chromatography on silica gel using a petroleum ether/dichloromethane mixture as the eluent to obtain pure product of **AnPT**. (1.36 g, yield: 88%) Mass spectrometry MALDI-TOF (m/z) [M⁺]: measured value 310.02, theoretical value 310.35.

Synthesis of BrAnPT:

AnPT (0.93 g, 3 mmol) was added into 100 mL chloroform. The mixture was stirring under lucifugal environment. And then *N*-Bromosuccinimide (0.64 g, 3.6 mmol) was

added into the mixture every 20 minutes for 6 times. The mixture was reacted at room temperature over night. The mixture was washed by NaCl aqueous solution and extracted with dichloromethane consecutively. After being collected and concentrated, the organic phase was then purified by recrystallization using petroleum ether as poor solvent to afford white solid. (1.13 g, yield: 97%) Mass spectrometry MALDI-TOF (m/z) [M⁺]: measured value 389.52, theoretical value 389.25.

Synthesis of **PPT**:

PPIB (2.48 g, 5 mmol), 5-Bromophthalide (1.07 g, 5 mmol), Pd(PPh₃)₄ (0.15 g, 0.15 mmol), K₂CO₃ (2.76 g, 20 mmol), distilled water (10 mL), and tetrahydrofuran (50 mL) were first mixed. The mixture was heated by 70 °C and refluxed under a nitrogen atmosphere for 24 h. After cooling to room temperature, the mixture was washed by water and extracted with dichloromethane consecutively. The product was purified by column chromatography on silica gel using a petroleum ether/dichloromethane mixture as the eluent to obtain pure product of **PPT**. (2.06 g, yield: 82%) Mass spectrometry MALDI-TOF (m/z) [M+]: measured value 502.56, theoretical value 502.57. ¹H NMR (500 MHz, Methylene Chloride-*d*₂) δ 8.91 – 8.81 (m, 2H), 8.78 (d, *J* = 8.2 Hz, 1H), 7.98 (dd, *J* = 11.5, 7.0 Hz, 1H), 7.84 – 7.68 (m, 9H), 7.64 (dt, *J* = 7.9, 2.1 Hz, 4H), 7.58 (t, *J* = 7.6 Hz, 1H), 7.33 (t, *J* = 7.5 Hz, 1H), 7.25 (d, *J* = 8.5 Hz, 1H), 5.39 (d, *J* = 3.7 Hz, 2H). ¹³C NMR (126 MHz, CD₂Cl₂) δ 147.59, 146.21, 130.36, 130.06, 129.85, 129.13, 128.16, 127.39, 127.24, 126.42, 125.81, 125.09, 124.10, 123.24, 122.54, 120.97, 120.58, 102.46, 99.50, 84.36, 69.67.

Synthesis of **PPIPBr**:

PPIPBr was synthesized according to the same procedure as for **PPT** by using 1-Bromo-4-iodobenzene (1.13 g, 4 mmol) instead 5-Bromophthalide. White solid (1.54 g, yield: 72%). Mass spectrometry MALDI-TOF (m/z) [M+]: measured value 525.16, theoretical value 535.45.

Synthesis of **PAPT**:

PAPT was synthesized according to the same procedure as for **PPT** by using **BrAnPT** (1.56 g, 4 mmol) instead 5-Bromophthalide. Yellow solid (1.68 g, yield: 62%). Mass spectrometry MALDI-TOF (m/z) [M+]: measured value 678.37, theoretical value

678.79. ¹H NMR (500 MHz, Methylene Chloride- d_2) δ 8.88 (d, J = 8.5 Hz, 1H), 8.82 (d, J = 8.4 Hz, 1H), 8.17 (d, J = 7.5 Hz, 1H), 7.94 (s, 2H), 7.85 (d, J = 7.8 Hz, 1H), 7.80 – 7.68 (m, 10H), 7.67 (s, 1H), 7.64 – 7.59 (m, 3H), 7.49 (d, J = 7.8 Hz, 2H), 7.44 – 7.36 (m, 5H), 7.31 (d, J = 8.2 Hz, 1H), 5.51 (s, 2H). ¹³C NMR (126 MHz, CD₂Cl₂) δ 159.34, 151.69, 150.08, 146.93, 146.32, 129.22, 126.95, 126.24, 125.66, 125.35, 124.13, 121.03, 117.20, 112.76, 107.92, 103.29, 101.15, 95.48, 89.93, 87.26, 83.97, 69.81, 53.86.

Synthesis of PPIPB:

KOAc (2.94 g, 30 mmol), **PPIPBr** (1.34 g, 2.5 mmol), bis(pinacolato)diboron (5.06 g, 20 mmol), Pd(dppf)Cl₂ (0.25 g, 0.30 mmol) and dioxane (80 mL) were first mixed The mixture was heated by 90 °C and refluxed under a nitrogen atmosphere for 48 h After cooling to room temperature, the mixture was washed by water and extracted with dichloromethane consecutively The dichloromethane was removed by distillation The product was then further dried with MgSO4 and purified by column chromatography on silica gel using a petroleum ether/dichloromethane mixture as the eluent, and the pure product of **PPIPB** was finally obtained. White solid (1.17 g, yield: 82%). Mass spectrometry MALDI-TOF (m/z) [M⁺]: measured value 572.33, theoretical value 572.52.

Synthesis of **PPPT**:

PPIPB (1.14 g, 2 mmol), 5-Bromophthalide (0.43 g, 2 mmol), Pd(PPh₃)₄ (0.06 g, 0.06 mmol), K₂CO₃ (2.76 g, 20 mmol), distilled water (10 mL), and tetrahydrofuran (50 mL) were first mixed. The mixture was heated by 70 °C and refluxed under a nitrogen atmosphere for 24 h. After cooling to room temperature, the mixture was washed by water and extracted with dichloromethane consecutively. The product was purified by column chromatography on silica gel using a petroleum ether/dichloromethane mixture as the eluent to obtain pure product of **PPPT**. White solid (1.00 g, yield: 86%). Mass spectrometry MALDI-TOF (m/z) [M+]: measured value 578.37, theoretical value 578.67. ¹H NMR (500 MHz, Methylene Chloride-*d*₂) δ 8.84 (m, 2H), 8.79 (d, *J* = 8.3 Hz, 1H), 8.00 (d, *J* = 8.0 Hz, 1H), 7.86 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.84 – 7.77 (m, 8H), 7.76 – 7.63 (m, 8H), 7.59 (t, *J* = 7.6 Hz, 1H), 7.34 (dd, *J* = 8.4, 6.9 Hz, 1H), 7.27 – 7.23

(m, 1H), 5.42 (s, 1H). ³C NMR (126 MHz, CD₂Cl₂) δ 130.37, 129.85, 129.13, 128.16, 127.99, 127.58, 126.66, 125.83, 124.10, 123.23, 120.97, 120.51, 116.74, 116.06, 77.63, 69.69.



Fig. S1 ¹H NMR spectra of **PPT** in deuterated CD₂Cl₂.





Fig. S2 ¹H NMR spectra of **PPPT** in deuterated CD_2Cl_2 .

Fig. S3 ¹H NMR spectra of **PAPT** in deuterated CD₂Cl₂.



Fig. S4 MALDI-TOF spectrum of PPT.



Fig. S5 MALDI-TOF spectrum of **PPPT**.



Fig. S6 MALDI-TOF spectrum of PAPT.

2.2 Crystal structures



Fig. S7 The single crystal structures of PPT.



2.3 Electrochemical properties

Fig. S8 (a) Cyclic voltammograms of **PT**, **PPT**, **PPPT** and **PAPT**. (b) LUMO levels of **PT** and common acceptors (detailed in Table S1).

| Number | Formula | LUMO/eV | Ref. |
|--------|---|---------|-----------|
| (1) | | -3.13 | [1] |
| (2) | $\langle I_{N}^{\circ} - \langle \rangle -$ | -2.83 | [2] |
| (3) | N= | -2.78 | [3] |
| (4) | | -2.73 | [4] |
| (5) | | -2.72 | [5] |
| (6) | | -2.71 | [6] |
| (7) | Ļ, | -2.66 | |
| (8) | ý, | -2.63 | This work |
| (9) | | -2.62 | [7] |
| (10) | | -2.42 | [8] |
| (11) | | -2.40 | [9] |
| (12) | | -2.38 | [10] |
| (13) | | -2.28 | [11] |

Table. S1 LUMO levels of **PT** and common acceptors.

2.4 Theoretical Calculations



Fig. S9 LUMO and HOMO distributions and energy levels of the molecular **PPT**, **PPPT** and **PAPT**.

| Hole | | Particle | Hole | | Particle |
|--|---|----------|-------|---|----------|
| :::::::::::::::::::::::::::::::::::::: | $\begin{array}{c} 99.66\% \\ \hline S_1 \rightarrow \ S_0 \end{array}$ | | ***** | $\begin{array}{c} \begin{array}{c} 94.75\% \\ \hline T_1 \rightarrow \ S_0 \end{array}$ | • |
| | $ \begin{array}{c} 86.77\% \\ \hline S_2 \rightarrow S_0 \end{array} $ | ***** | | $\begin{array}{c} \hline 56.68\% \\ \hline T_2 \rightarrow \ S_0 \end{array}$ | |
| | $\begin{array}{c} \underline{91.02\%}\\ \hline S_3 \rightarrow S_0 \end{array}$ | | 10-26 | | |
| | $\begin{array}{c} 90.23\%\\ \hline S_4 \rightarrow S_0 \end{array}$ | | | $\begin{array}{c} \hline 80.60\% \\ \hline T_4 \rightarrow \ S_0 \end{array}$ | |
| | $\begin{array}{c} 93.19\%\\\hline S_5 \rightarrow S_0 \end{array}$ | | | | |

Fig. S10 Natural transition orbital (NTO) analysis for PPT.



Fig. S11 Natural transition orbital (NTO) analysis for PPPT.



Fig. S12 Natural transition orbital (NTO) analysis for PAPT.



Fig. S13 Proportion of LE and CT of emitters.

2.5 Photophysical Properties



Fig. S14 (a) Absorption spectra of **PPT** in different solvents. (b) Absorption spectra of **PPPT** in different solvents. (c) Absorption spectra of **PAPT** in different solvents.

| | | | PPT | | РРРТ | | | | РАРТ | | |
|--|----------|--|---|-----------------------------------|-----------------------|--|--|---------------------------------------|----------------------|--|--|
| Solvents | f (ε, n) | $\lambda_{abs}\left(nm\right)$ | λ _{em} (nm) | v_a - v_f (cm ⁻¹) | $\lambda_{abs} (nm)$ | λ _{em} (nm) | v_a - v_f (cm ⁻¹) | $\lambda_{abs}\left(nm\right)$ | λ _{em} (nm) | v_a - v_f (cm ⁻¹) | |
| Hexane | ~ 0 | 364 | 423 | 3832 | 365 | 427 | 3978 | 393 | 436 | 2510 | |
| Toluene | 0.013 | 370 | 437 | 4144 | 366 | 437 | 4439 | 398 | 442 | 2501 | |
| Triethylamine | 0.0477 | 365 | 432 | 4144 | 365 | 432 | 4249 | 394 | 438 | 2550 | |
| Butylether | 0.0968 | 366 | 434 | 4281 | 365 | 433 | 4303 | 394 | 438 | 2550 | |
| Isopropylether | 0.1450 | 364 | 435 | 4484 | 364 | 436 | 4537 | 393 | 438 | 2614 | |
| Ethyl ether | 0.167 | 364 | 440 | 4745 | 364 | 435 | 4484 | 393 | 438 | 2614 | |
| Ethyl acetate | 0.200 | 365 | 446 | 4976 | 364 | 445 | 5001 | 394 | 440 | 2653 | |
| Tetrahydrofuran | 0.210 | 366 | 446 | 4951 | 365 | 447 | 5026 | 395 | 442 | 2692 | |
| Dichloromethane | 0.276 | 366 | 455 | 5344 | 365 | 458 | 5563 | 399 | 446 | 2641 | |
| Dimethylformami de | 0.276 | 366 | 471 | 6091 | 365 | 475 | 6345 | 398 | 446 | 2704 | |
| Acetone | 0.284 | 364 | 456 | 5686 | 362 | 463 | 6026 | 394 | 441 | 2705 | |
| Acetonitrile | 0.305 | 364 | 469 | 6151 | 362 | 474 | 6527 | 396 | 444 | 2730 | |
| (a) 10 ⁵ 10 ⁴ 10 ⁴ 10 ⁷ | | — Hexane — Ethyl ether — THF — DCM — IRF | (b) 10 ⁵ 10 ⁴ (sd) stur | | | — Hexane — Ethyl ethel — THF — DCM — IRF | r 10 ⁵ (c) (c) 10 ⁵ (c) 10 ⁶ (c) 10 ⁶ (c) 10 ⁷ (c) 10 ¹⁰ (c) 10 ¹⁰ (c) 10 ³ (c | | | Hexane Ethyl ether THF DCM IRF | |
| | 50 | РРТ И селото и селото и | පී 10 ² 10 ¹ | nalit, hult at us at a | 50 | PPPT Utration to an and a could plan a state | 10 ² 10 ¹ | da Nazaria da da Mila na Itila yan | 50 | | |

Table. S2 Detailed photophysical data of **PPT**, **PPPT** and **PAPT** in different solvents.

Fig. S15 (a) PL decay of **PPT** in different solvents. (b) PL decay of **PPPT** in different solvents. (c) PL decay of **PAPT** in different solvents.

Time (ns)

Time (ns)

Time (ns)



Fig. S16 Low-temperature fluorescence and phosphorescence spectra at 77 K of (a) **PPT** and (b) **PPPT** were measured in THF.



Fig. S17 Low-temperature fluorescence spectrum of **PAPT**, low-temperature phosphorescence spectra of **PAPT**, **PAPT** & **PtOEP** and **PtOEP** in THF.

| | | РРТ | | РРРТ | | | | РАРТ | | |
|-----------------|---------------------------|-----------|--|---------------------------|-----------|--|---------------------------|-----------|--|--|
| Solvents | $\Phi_{F}\left(\%\right)$ | Time (ns) | $k_{\rm r} (imes 10^8 { m s}^{-1})$ | $\Phi_{F}\left(\%\right)$ | Time (ns) | $k_{\rm r} (imes 10^8 { m s}^{-1})$ | $\Phi_{F}\left(\%\right)$ | Time (ns) | $k_{\rm r}$ (× 10 ⁸ s ⁻¹) | |
| Hexane | 72.54 | 1.44 | 5.04 | 75.79 | 1.20 | 6.32 | 61.83 | 2.21 | 2.80 | |
| Ethyl ether | 82.06 | 1.77 | 4.64 | 82.33 | 1.46 | 5.64 | 67.75 | 2.32 | 2.92 | |
| Tetrahydrofuran | 82.27 | 1.86 | 4.42 | 82.01 | 1.54 | 5.33 | 65.52 | 2.09 | 3.13 | |
| Dichloromethane | 86.82 | 2.07 | 4.19 | 85.77 | 1.78 | 4.82 | 66.12 | 2.24 | 2.95 | |

Table. S3 The PLQYs, life times and k_r s of **PPT**, **PPPT** and **PAPT** in different solvents.

2.6 Electroluminescence properties



Fig. S18 Device structure and energy level diagrams of functional layers.



Fig. S19 (a) Non-doped device of **PPT** electroluminescence spectrum at different voltage. (b) Non-doped device of **PPPT** electroluminescence spectrum at different voltage. (c) Non-doped device of **PAPT** electroluminescence spectrum at different voltage.



Fig. S20 (a) Doped device of **PPT** electroluminescence spectrum at different voltage.(b) Doped device of **PPPT** electroluminescence spectrum at different voltage. (c) Doped device of **PAPT** electroluminescence spectrum at different voltage.



Fig. S21 (a) Current density-voltage-luminance (J–V–L) characteristics of non-doped devices of **PPT**, **PPPT** and **PAPT**. (b) Current density-voltage-luminance (J–V–L) characteristics of doped devices of **PPT**, **PPPT** and **PAPT**. (c) Current density-luminance curves of non-doped devices of **PPT**, **PPPT** and **PAPT**. (d) Current density-luminance curves of doped devices of **PPT**, **PPPT** and **PAPT**.

| device | V _{on} ^a (V) | EQE _{max} ^b (%) | λ _{EL} ° (nm) | L_{max}^{d} (cd m ⁻²) | CIE (x, y) | Ref. |
|----------------|-------------------------------------|--|---------------------------|-------------------------------------|------------------|-----------|
| PPT | 3.3 | 9.0 | 436 | 6548 | (0.154, 0.073) | This work |
| PPPT | 3.4 | 8.3 | 432 | 9857 | (0.154, 0.100) | This work |
| PAPT | 3.1 | 10.2 | 444 | 13784 | (0.151, 0.085) | This work |
| 2BuCz-CNCz | 3.6 | 5.24 | 408 | 2625 | (0.157, 0.050) | [12] |
| POPCN-2CP | 3.5 | 7.5 | 404 | 4290 | (0.159, 0.035) | [13] |
| 2Na-CzCN | 3.7 | 5.92 | 398 | 4759 | (0.15, 0.06) | [14] |
| CSiTPI | 3.2 | 7.1 | 404 | 2445 | (0.16, 0.06) | [15] |
| PPI-3-SBF | 3.0 | 8.41 | 428 | 16365 | (0.16, 0.07) | [16] |
| IPD-MP-DPA | 2.9 | 4.4 | 428 | 4158 | (0.154,0.078) | [17] |
| 2M-ph-pCzAnBzt | 3.4 | 10.44 | 450 | 3085 | (0.151, 0.057) | [18] |
| TPA-PI-SBF | 3.1 | 6.76 | 448 | 4901 | (0.152, 0.059) | [19] |
| 2MCz-CNMCz | 3.0 | 7.76 | 404 | 4757 | (0.158, 0.039) | [20] |
| 9-PCZCFOXZ | 3.2 | 7.2 | 417 | 5740 | (0.1537, 0.0757) | [21] |
| SP | 3.0 | 11.3 | 436 | 13488 | (0.158, 0.068) | [22] |
| TPA-DFCP | 3.54 | 8.3 | 436 | 2482 | (0.153, 0.077) | [23] |
| PIAnTPh | 3.3 | 8.09 | 440 | 13653 | (0.15, 0.06) | [24] |
| PyIAnTPh | 3.1 | 8.44 | 440 | 20980 | (0.15, 0.07) | |
| TTT-TPA-tBu | 4.0 | 10.25 | 438 | - | (0.15, 0.08) | [25] |
| MCNPIBI | 3.8 | 2.8 | 441 | 6569 | (0.15, 0.08) | [26] |
| DPCN | 4.4 | 3.3 | 424 | 884 | (0.158, 0.062) | [27] |
| PhIF-2 | 3.4 | 2.7 | 434 | 1020 | (0.16, 0.09) | [28] |
| PPI-NPA-CN | 6.5 | 3.05 | 437 | 1269 | (0.16, 0.08) | [29] |
| PT-1 | 3.2 | 6.72 | 414 | 3567 | (0.151, 0.072) | [30] |
| PT-2 | 3.2 | 5.32 | 414 | 4731 | (0.151, 0.082) | |
| DSiPPI | 3.8 | 7.08 | - | 479 | (0.167, 0.078) | [31] |
| TPAFPI | 2.9 | 10.1 | 429/455 | 34835 | (0.15, 0.06) | [32] |
| CZFPI | 3.0 | 8.8 | 424/454 | 28875 | (0.15, 0.07) | |

Table. S4 Recent representative high-efficiency deep-blue OLEDs based on HLCT materials.

| CZFPY | 3.0 | 7.6 | 426/455 | 37328 | (0.15, 0.07) | |
|--------|-----|-------|---------|-------|----------------|------|
| PIPTPh | 3.0 | 11.83 | 436 | 18637 | (0.15, 0.07) | [33] |
| PITPh | 3.3 | 6.10 | 424 | 5634 | (0.16, 0.06) | |
| PPIS | 2.9 | 6.68 | - | 11584 | (0.156, 0.090) | [34] |
| PPISCN | 2.8 | 5.56 | - | - | (0.157, 0.073) | |

^{a)} V_{on} : turn-on voltage; ^{b)} EQEmax: maximum external quantum efficiency; ^{c)} λ_{EL} : EL emission peak; ^{d)} L_{max} : maximum luminance.

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