Supporting Information

Multifunctional pyridine styrylphenanthroimidazoles: Electron transport materials for blue FOLEDs with low efficiency roll-off and host for PHOLEDs with low turn-on voltage

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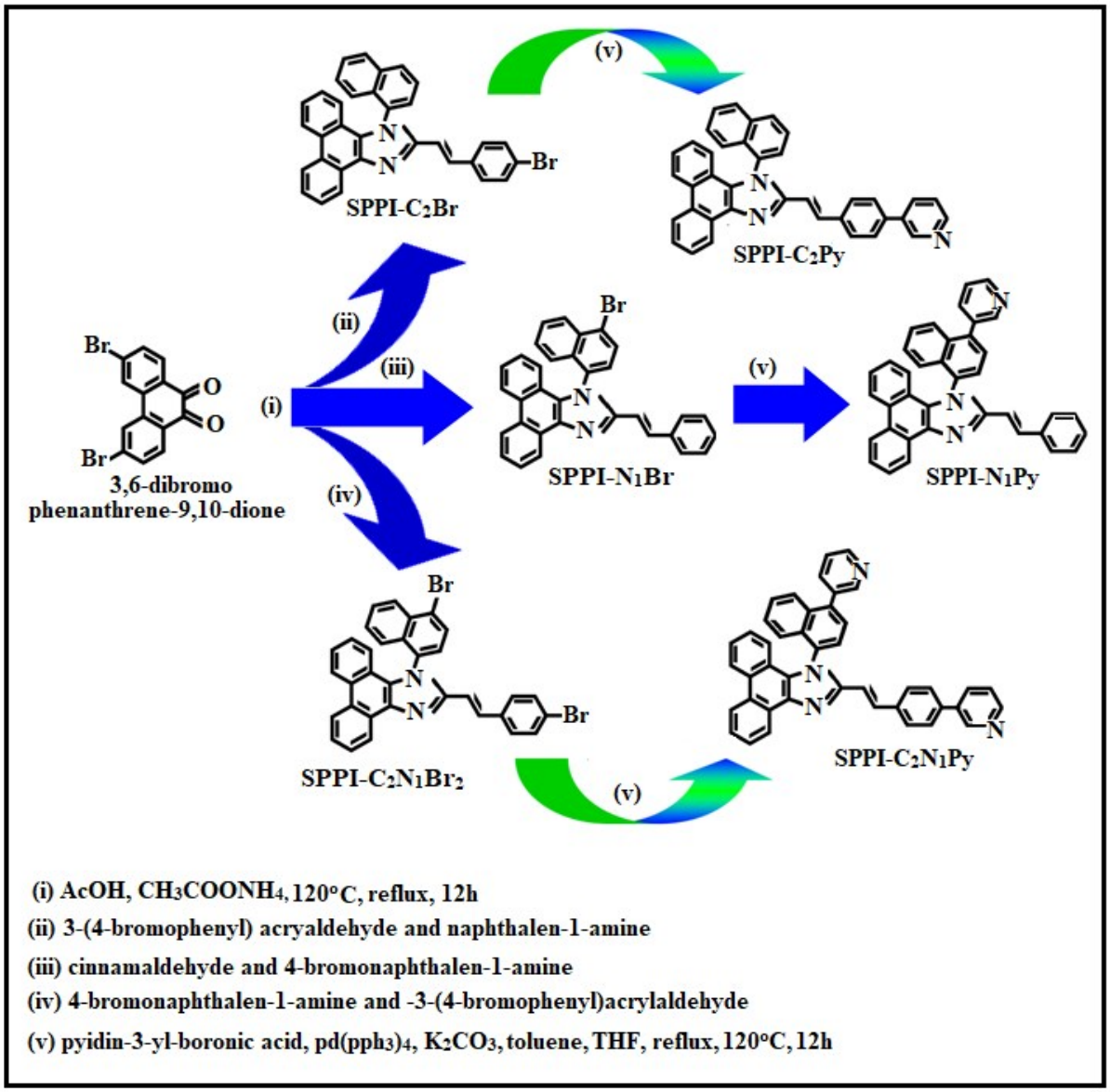


SI-2. Experimental Section

SI-2.1. Measurements

^{1}H and ^{13}C NMR measurements have been recorded on Bruker 400 MHz spectrometer and mass spectra were recorded on Agilent LCMS VL SD. The UV-Vis spectra were measured on Lambda 35 PerkinElmer (solution)/ Lambda 35 spectrophotometer (RSA-PE-20) (film). The emission spectra were measured with Perkin Elmer LS55 spectrometer and quantum yield was recorded with fluorescence spectrometer (Model-F7100 with integrating sphere). The decomposition temperature (T_d) and glass transition temperature (T_g) were measured with Perkin Elmer thermal analysis system (10 °C min^{-1}; N_2 flow rate - 100 ml min^{-1}) and NETZSCH (DSC-204) (10 °C min^{-1}; N_2 atmosphere), respectively. Fluorescence lifetime was estimated by time correlated single-photon counting (TCSPC) method on Horiba Fluorocube-01-NL lifetime system: nano LED is an excitation source with TBX-PS is detector; DAS6 software was employed to analyze the decay by reconvolution method. Oxidation potential of electron transport materials was measured from SP-200 electrochemical analyzer (Bilogic science instruments, France). Ferrocene was used as an internal standard with HOMO energy of -4.80 eV and 0.1 M tetrabutylammonium perchlorate in CH_2Cl_2 as supporting electrolyte.

SI-2.2. Synthesis of electron transport materials

The starting materials were obtained from Sigma-Aldrich and used without further purification. Synthetic route of these novel materials have been outlined in Scheme S1. The intermediates, 2-(4-bromostyryl)-1-(naphthalen-1-yl)-1H-phenanthro[9,10-d] imidazole (SPPI-C_2Br), 1-(1-bromonaphthalen-5-yl)-2-styryl-1H-phenanthro[9,10-d] imidazole (SPPI-N_1Br) and 2-(4-bromostyryl)-1-(1-bromonaphthalen-5-yl)-1H-phenanthro[9,10-d] imidazole (SPPI-$C_2N_1Br_2$) was obtained through one-pot reaction [1].

A mixture of 3,6-dibromophenanthrene-9,10-dione (8.2 mmol), 3-(4-bromophenyl) acrylaldehyde (12.3 mmol) and 1-naphthylamine (50.0 mmol) for SPPI-C_2Br [3,6-

dibromophenanthrene-9,10-dione (8.2 mmol), cinnamaldehyde (12.3 mmol) and 4-bromonaphthalen-1-amine (50.0 mmol) for SPPI-N_1Br / 3,6-dibromophenanthrene-9,10-dione (8.2 mmol), 3-(4-bromophenyl) acrylaldehyde (12.3 mmol) and 4-bromonaphthalen-1-amine (50 mmol) for SPPI-C_2N1Br and ammonium acetate (101.8 mmol) in glacial acetic acid (30 ml) was refluxed for 12 h (120 °C; N_2 stream). The reaction mixture was poured into ethanol and the separated solid SPPPI-C_2Br was washed with methanol and dried. The solid SPPPI-C_2Br was purified by column chromatography.

Suzuki cross-coupling reaction was employed to synthesize the target ETMs namely, 2-(4-(pyridin-3-yl)styryl)-1-(naphthalen-1-yl)-1H-phenanthro[9,10-d]imidazole (SPPI-C_2Py), 1-(1-(pyridin-3-yl)naphthalen-4-yl)-2-styryl-1H-phenanthro[9,10-d]imidazole (SPPI-N_1Py) and 2-(4-(pyridin-3-yl)styryl)-1-(1-(pyridin-3-yl)naphthalen-4-yl)-1H-phenanthro[9,10-d] imidazole (SPPI-C_2N_1Py). A mixture of SPPI-C_2Br (SPPI-C_2Py) or SPPI-N_1Br (SPPI-N_1Py) or SPPI-$C_2N_1Br_2$ (SPPI-C_2N_1Py) (4.0 mmol), pyridin-3-yl-boronic acid (4.0 mmol), $Pd(PPh_3)_4$ (0.12 mmol) and K_2CO_3 (15 ml of 2.0 M aqueous solution) in toluene (30 ml) and ethanol (15.0 ml) was stirred at 100 °C for 12 h. The reaction mixture was extracted with dichloromethane and purified by column chromatography to afford white powder. The synthesised electron transport materials have been characterized by NMR spectroscopy, mass spectrometry and elemental analysis.

(i). 2-(4-bromostyryl)-1-(naphthalen-1-yl)-1H-phenanthro[9,10-d]imidazole (SPPI-C_2Br)

Yield: 66 %. ^{1}H NMR (400 MHz; $CDCl_3$) δ (ppm): 6.80 (d, 2H), 7.19 (d, 2H), 7.30- 7.36 (m, 5H), 7.38 (t, 3H), 7.42 (d, 2H), 7.79 (m, 4H), 8.10 (t, 2H), 8.43 (s, 1H). ^{13}C NMR (100 MHz; $CDCl_3$) δ (ppm): 109.0, 111.3, 113.0, 115.2, 117.8, 120.0, 122.1, 123.0, 124.0, 125.0, 126.0, 128.0, 130.0.

(ii). 1-(1-bromonaphthalen-5-yl)-2-styryl-1H-phenanthro[9,10-d]imidazole (SPPI-N_1Br)

Yield: 69 %.^{1}H NMR (400 MHz; $CDCl_3$) δ (ppm): 6.82 (d, 2H), 7.08 (d, 2H), 7.20-7.30 (m, 6H), 7.45-7.50 (m, 4H), 7.70 (t, 2H), 7.82-7.88 (m, 3H), 8.12-8.20 (m, 2H). ^{13}C NMR (100 MHz; $CDCl_3$) δ (ppm): 110.8, 111.1, 122.0, 114.0, 115.0, 118.0, 120.4, 122.0, 124.0, 127.0, 130.2, 131.0, 132.0.

(iii). 2-(4-bromostyryl)-1-(1-bromonaphthalen-5-yl)-1H-phenanthro[9,10-d]imidazole (SPPI-$C_2N_1Br_2$)

Yield: 52%.^{1}H NMR (400 MHz; $CDCl_3$) δ (ppm): 6.86 (d, 2H), 7.13 (d, 2H), 7.16-7.20 (m, 4H), 7.38-7.50 (m, 5H), 8.00-8.16 (m, 3H), 8.46 - 8.528 (m, 4H). ^{13}C NMR (100 MHz; $CDCl_3$) δ (ppm): 100.0, 105.0, 111.3, 115.0, 120.0, 122.0, 125.1, 128.0, 129.0, 130.0, 132.3, 134.0, 136.0, 139.0, 140.0.

(iv). 2-(4-(pyridin-3-yl)styryl)-1-(naphthalen-1-yl)-1H-phenanthro[9,10-d]imidazole (SPPI-C_2Py).

Yield: 69 %.^{1}H NMR (400 MHz; $CDCl_3$) δ (ppm): 6.86 (d, 2H), 7.13 (d, 2H), 7.16 - 7.20 (m, 5H), 7.38-7.45 (m, 4H), 7.56-7.63 (m, 4H), 7.82-7.88 (m, 4H), 8.53 - 8.66 (m, 4H). ^{13}C NMR (100 MHz; $CDCl_3$) δ (ppm): 112.8, 122.4, 124.1, 127.2, 127.4, 127.6, 127.8, 128.3, 130.7, 131.5, 132.2, 133.2, 133.4, 134.1, 134.6, 135.2, 135.6, 141.5, 148.0, 149.1. MS: m/z. 523.2 [M^+]; Calcd. 523.63. Anal. calcd (%) for $C_{38}H_{25}N_3$: C, 87.16; H, 4.81; N, 8.02. Found: C, 87.10; H, 4.79; N, 8.00.

(v). 1-(1-(pyridin-3-yl)naphthalen-4-yl)-2-styryl-1H-phenanthro[9,10-d]imidazole (SPPI-N_1Py)

Yield: 52%.^{1}H NMR (400 MHz; $CDCl_3$) δ (ppm): 6.99 (d, 2H), 7.10 (d, 2H), 7.14-7.21 (m, 3H), 7.30-7.44 (m, 5H), 7.4- 7.7 (m, 4H), 7.82-7.97 (t, 3H), 8.12 - 8.93 (m, 6H). ^{13}C NMR (100 MHz; $CDCl_3$) δ (ppm): 112.8, 122.4, 124.6, 125.6, 126.3, 126.4, 126.6, 128.0, 128.3, 131.2, 131.5, 132.2, 133.4, 133.6, 135.2, 136.1, 141.5, 148.0, 149.1. MS: m/z. 523.2 [M^+]; Calcd. 523.63. Anal. Calcd (%) for $C_{38}H_{25}N_3$: C, 87.16; H, 4.81; N, 8.02. Found: C, 87.15; H, 4.78; N, 8.04.

(vi). 2-(4-(pyridin-3-yl)styryl)-1-(1-(pyridin-3-yl)naphthalen-4-yl)-1H-phenanthro[9,10-d]imidazole (SPPI-C_2N_1Py)

Yield: 69 %. ^{1}H NMR (400 MHz; $CDCl_3$) δ (ppm): 6.85 (d, 2H), 7.10 (d, 2H), 7.15-7.25 (m, 4H), 7.30-7.44 (m, 4H), 7.7 (t, 3H), 7.82-7.88 (m, 3H), 7.97(m, 8H), 8.93 (d, 2H). ^{13}C NMR (100 MHz; $CDCl_3$) δ (ppm): 112.8, 122.4, 124.0, 125.6, 126, 126.6, 127.4, 127.6, 128.3, 131.2, 131.5, 132.2, 133.6, 134.1, 135.2, 135.6, 141.1, 148.0, 149.1. MS: m/z. 600.23. [M^+]; Calcd: 600.71. Anal. Calcd (%) for $C_{43}H_{28}N_4$: C, 85.98; H, 4.70; N, 9.33. Found: C, 85.82; H, 4.68; N, 9.26.

SI-2.3. Device fabrication and measurement

ITO glass (resistance 20 Ω/sq) was cleaned with acetone, deionized water and isopropanol and dried (120 ^{o}C) followed by UV treatment (20 min) and transferred into deposition system. The devices were fabricated by multiple source beam deposition method (vacuum pressure-4×10^{-5} mbar). Evaporation rate of 2-4 Å s^{-1} (organic materials) and 0.1 and 4 Å s^{-1} for LiF and metal electrodes were applied, respectively. The thickness of each deposition layer was monitored with quartz crystal thickness monitor. The EL measurement was recorded with USB-650-VIS-NIR spectrometer (Ocean Optics, Inc, USA). The current density-voltage-luminance (J-V-L) characteristics was performed using source meter (Keithley 2450) equipped with LS-110 light intensity meter. The external quantum efficiency was determined from luminance, current density and EL spectrum assuming Lambertian distribution.

SI-2.4. Computational details

The ground (S_0) (DFT) and excited (S_n*) (TD-DFT) state characteristics of SPPI -C_2Py, SPPI-N_1Py and SPPI-C_2N_1Py were analyzed by Gaussian 09 program [2] and Multiwfn [2]. The natural transition orbitals (HONTOs & LUNTOs) with hole-particle contribution were studied in detail.

SI-3: Natural Transition Orbitals

Figure S1. Distribution of natural transition orbital pairs with transition character of SPPI-C_2Py [*f*-oscillator strength and % weights of hole-particle].

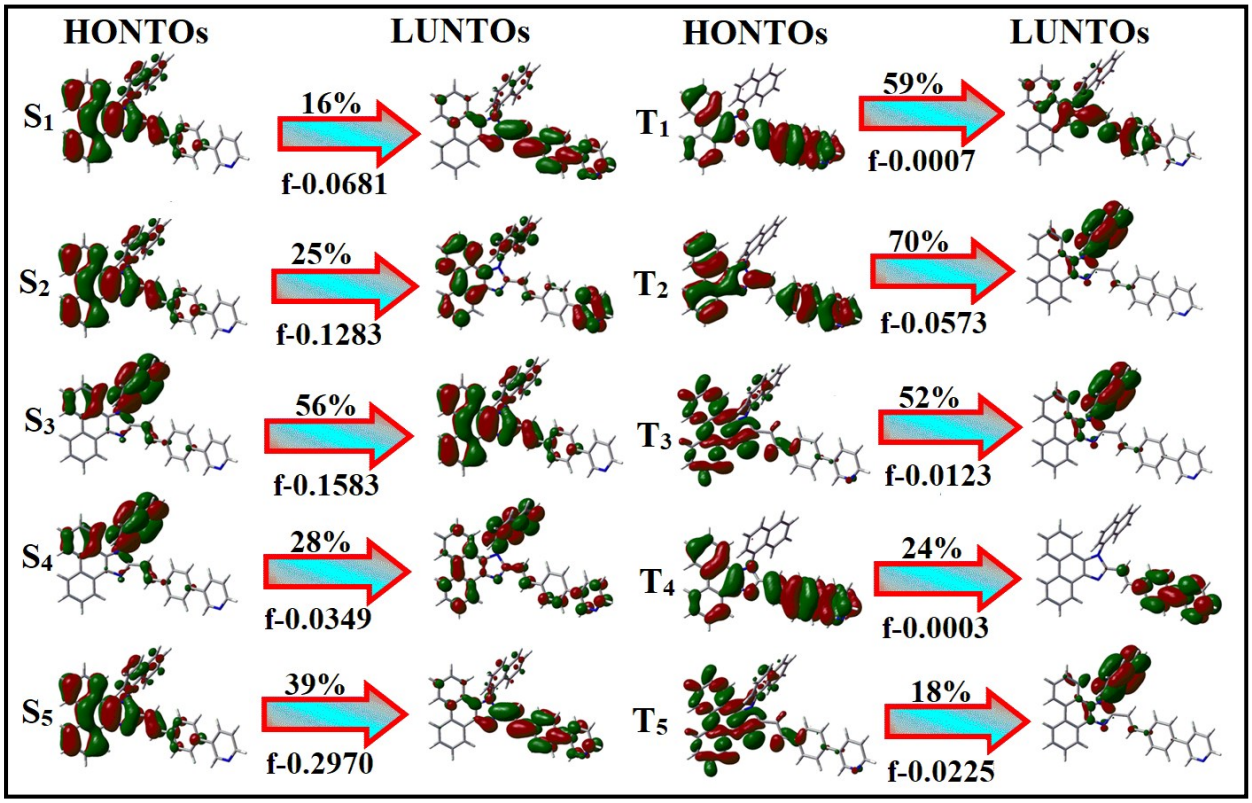


Figure S2. Distribution of natural transition orbital pairs with transition character of SPPI-N_1Py [*f*-oscillator strength and % weights of hole-particle].

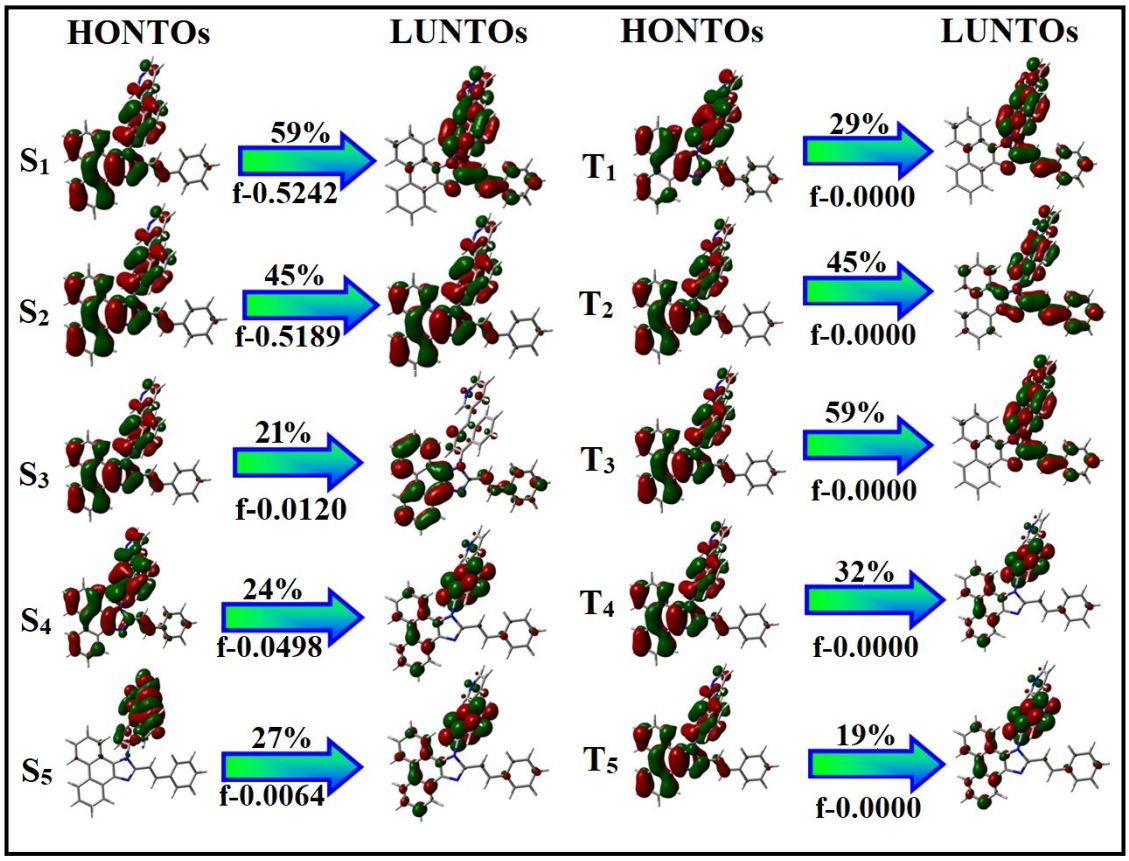
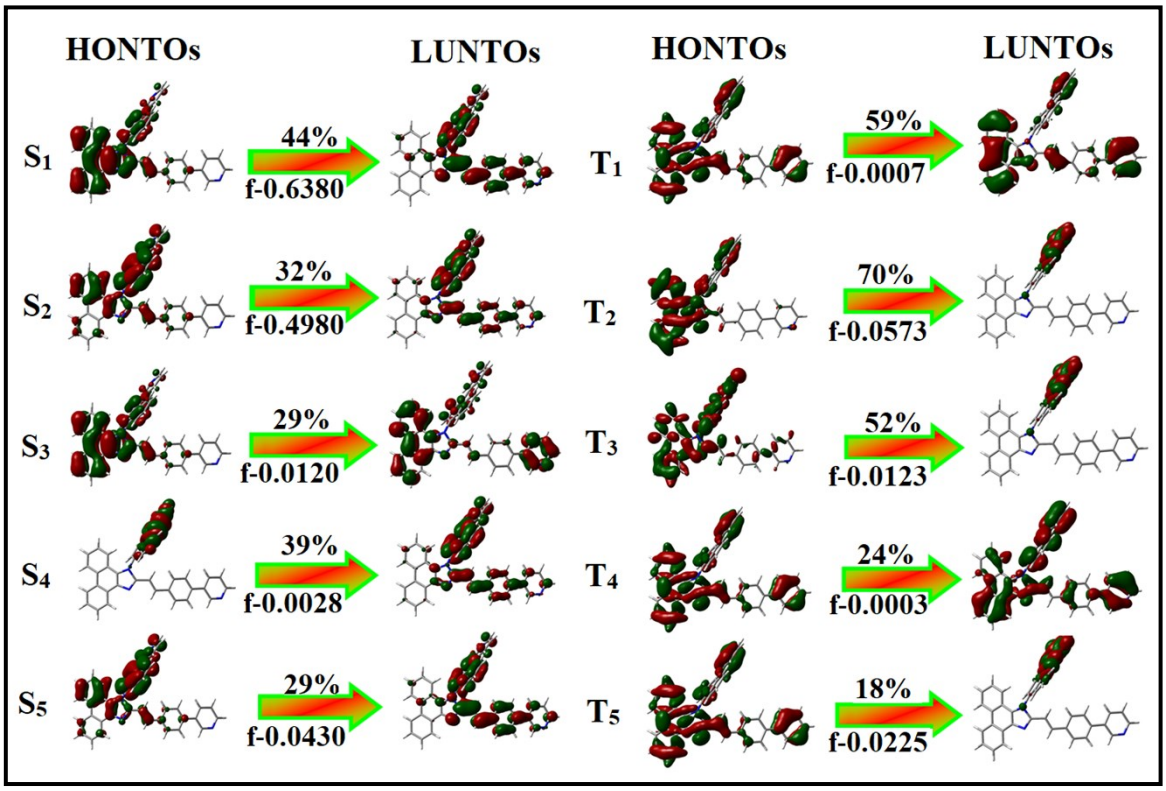


Figure S3. Distribution of natural transition orbital pairs with transition character of SPPI-C_2N_1Py [*f*-oscillator strength and % weights of hole-particle].



SI-4: Solvatochromism

Figure S4. Normalised absorption spectra of (a) SPPI-C_2Py; (b) SPPI-N_2Py; (c) SPPI-C_2N_1Py and (d) Potential energy surface (PES) scan of SPPI-C_2PY, SPPI-N_1Py and SPPI-C_2N_1Py.

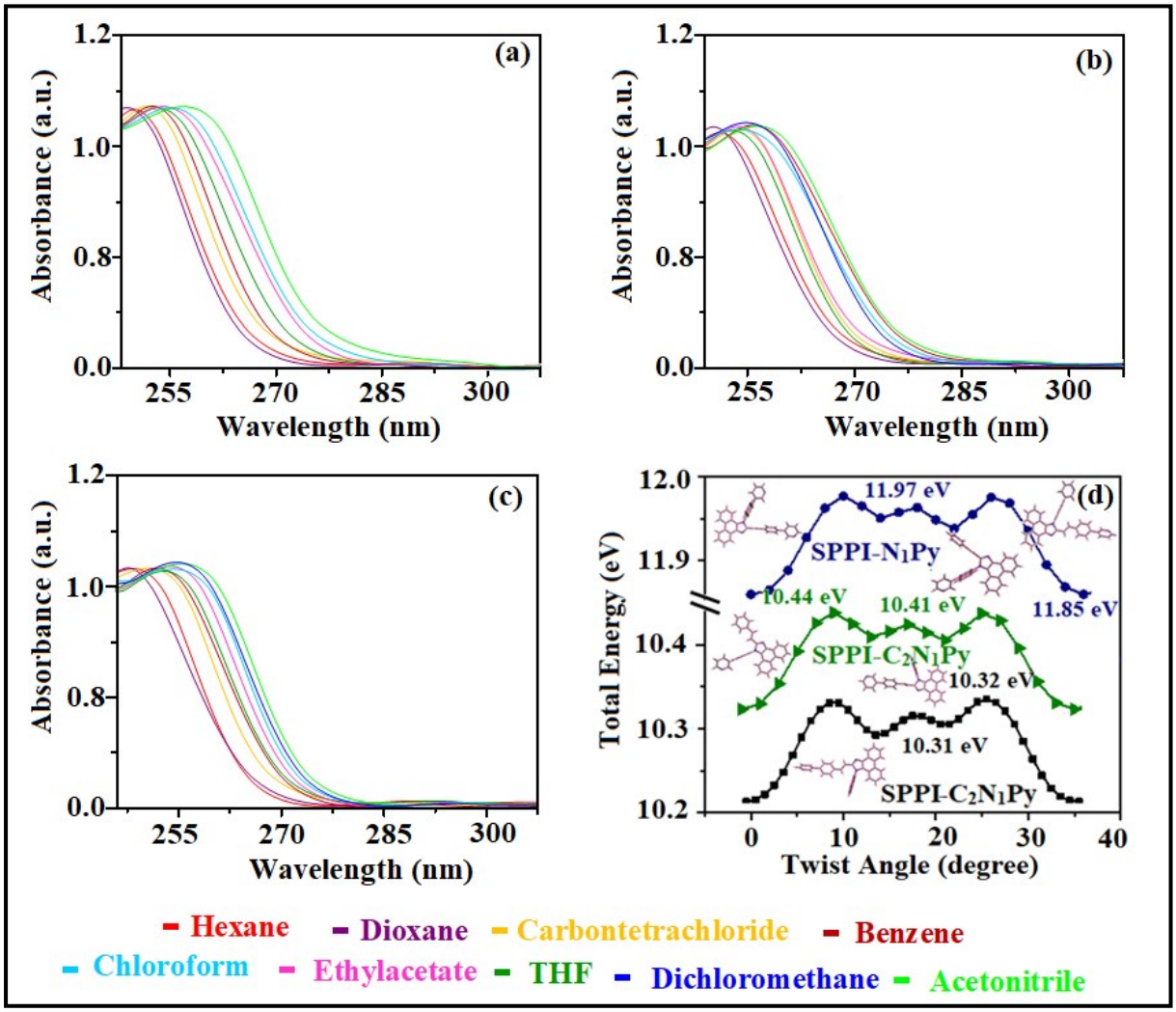


Figure S5. Normalised emission spectra of (a) SPPI-C_2Py; (b) SPPI-N_2Py; (c) SPPI-C_2N_1Py and (d) Decay curve of SPPI-C_2PY, SPPI-N_1Py and SPPI-C_2N_1Py.

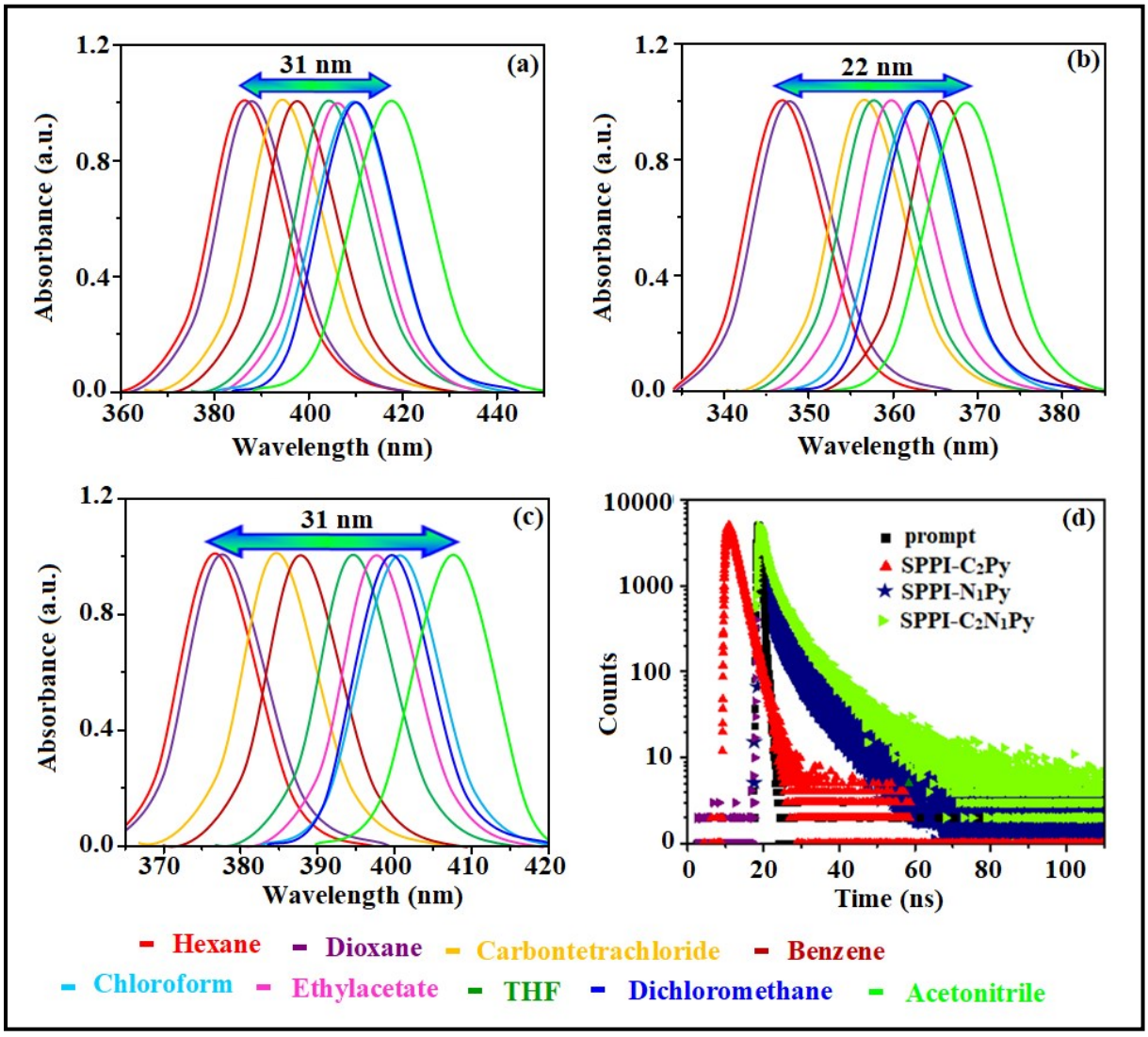


Figure S6. (a) Energy level diagram of hole only device (ITO/MoO_3 (6nm)/TAPC (50 nm)/MADN: 3 wt% BUBD-1 (50 nm)/MoO_3 (6 nm)/Al(100 nm)) and (b) electron only device (Al/LiF (1 nm)/ MADN: 3 wt% BUBD-1 (50 nm)/ SPPI-C_2Py or SPPI-N_1Py or SPPI-C_2N_1Py or BPhen (20 nm)/LiF (1 nm)/ Al(100 nm)); (c) Current density -Voltage (J-V) characteristics of hole-only and electron-only devices and (d) Comparison of device operational stability for devices.

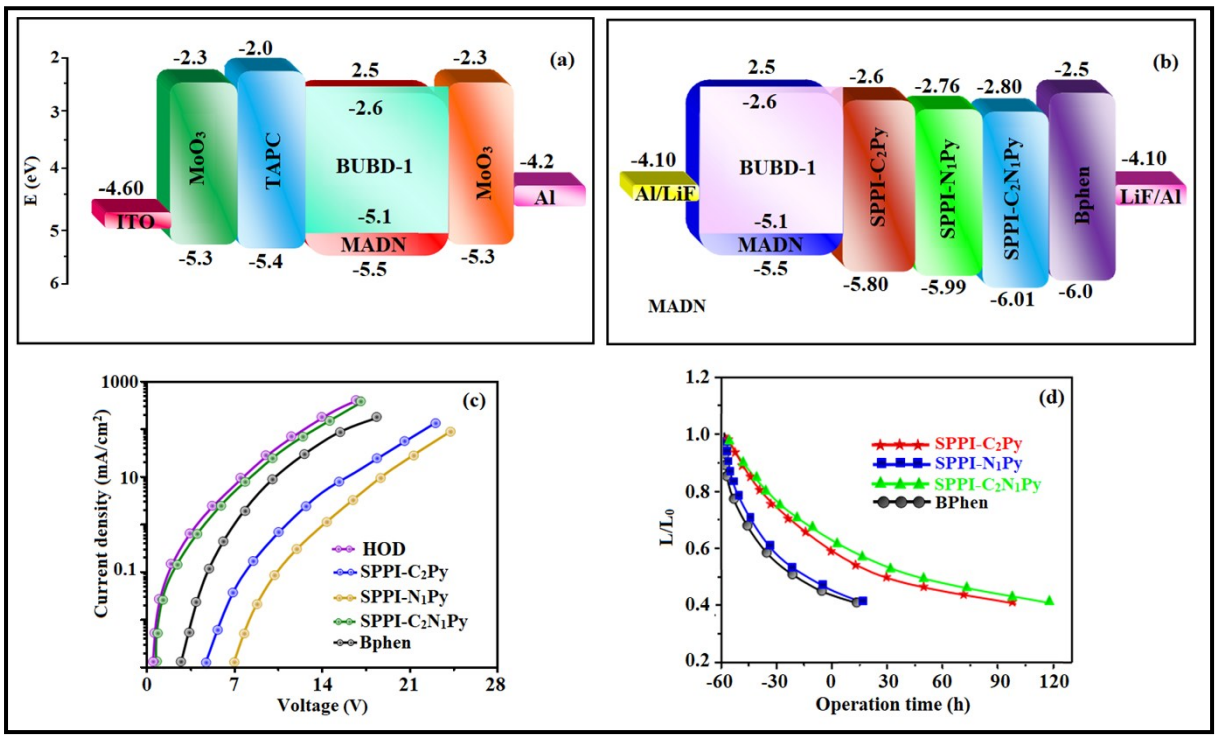
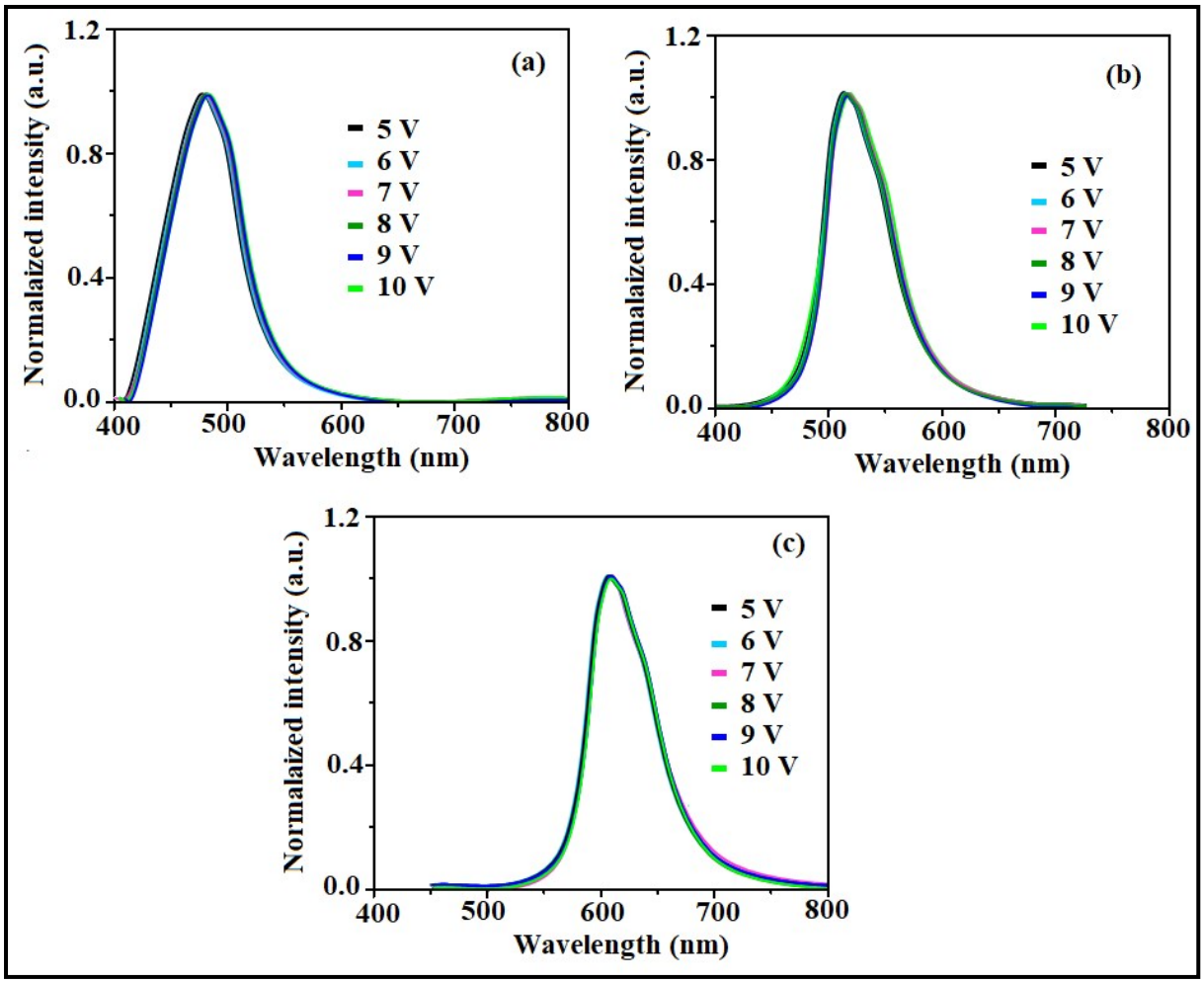


Figure S7. EL spectra of (a) blue; (b) red and (c) yellow PHOLEDs at different voltages.



SI–5: Tables

Table S1. Computed excitation energy (eV), excitation coefficient, Δr intex (Å), oscillator strength (f) and dipolemoment (μ) for singlet and triplet states of SPPI-C_2Py.

States	Excitation energy	Excitation coefficient	Δr intex	Oscillator strength	μ	NTO Transitions
S1	3.22	0.4286	8.5845	0.6813	1.40	$96 \xrightarrow{64\%} 97$
S2	3.57	0.4042	7.4312	0.1283	0.45	$96 \xrightarrow{25\%} 100$
S3	3.64	0.4119	3.4340	0.1583	0.56	$95 \xrightarrow{56\%} 96$
S4	3.70	0.4224	4.8019	0.0349	0.30	$95 \xrightarrow{28\%} 100$
S5	3.85	0.4010	7.5693	0.2970	0.25	$96 \xrightarrow{39\%} 99$
T1	1.34	0.7826	3.2051	0.0007	0.40	$95 \xrightarrow{59\%} 97$
T2	1.45	0.8526	5.2762	0.0573	0.25	$94 \xrightarrow{70\%} 96$
T3	1.79	0.8352	4.7198	0.0123	0.25	$84 \xrightarrow{52\%} 96$
T4	2.05	0.7002	5.8626	0.0003	0.49	$95 \xrightarrow{24\%} 100$
T5	2.10	0.6735	5.1118	0.0225	0.44	$95 \xrightarrow{18\%} 96$

Table S2. Computed excitation energy (eV), excitation coefficient, Δr intex (Å), oscillator strength (f) and dipole moment (μ) for singlet and triplet states of SPPI-N_1Py.

States	Excitation energy	Excitation coefficient	Δr intex	Oscillator strength	μ	NTO Transitions
S1	3.32	0.4391	4.9251	0.5242	0.40	$96 \xrightarrow{59\%} 97$
S2	3.35	0.4150	4.0085	0.5189	0.25	$96 \xrightarrow{45\%} 98$
S3	3.62	0.4160	2.7423	0.0120	0.25	$96 \xrightarrow{21\%} 99$
S4	3.64	0.4133	3.9192	0.0498	0.49	$95 \xrightarrow{24\%} 100$
S5	3.77	0.4212	4.6690	0.0064	0.44	$92 \xrightarrow{27\%} 100$
T1	1.25	0.3891	3.6508	0.0000	0.40	$95 \xrightarrow{29\%} 97$
T2	1.55	0.3422	5.2126	0.0000	0.25	$96 \xrightarrow{45\%} 98$
T3	1.77	0.3525	3.9134	0.0000	0.25	$96 \xrightarrow{59\%} 97$
T4	2.21	0.3107	5.5096	0.0000	0.49	$95 \xrightarrow{32\%} 100$
T5	2.22	0.2858	5.3152	0.0000	0.44	$96 \xrightarrow{19\%} 100$

Table S3. Computed excitation energy (eV), excitation coefficient, Δr intex (Å), oscillator strength (f)) and dipole moment (μ) for singlet and triplet states of SPPI-C_2N_1Py.

States	Excitation energy	Excitation coefficient	Δr intex	Oscillator strength	μ	NTO Transitions
S1	3.244	0.4122	7.3862	0.6383	2.05	$^{44\%}$ 110 → 100
S2	3.33	0.4478	5.2105	0.4980	0.58	$^{32\%}$ 109 → 98
S3	3.59	0.3666	7.1865	0.0120	0.56	$^{29\%}$ 110 → 100
S4	3.60	0.4221	5.4879	0.0028	0.99	$^{39\%}$ 106 → 99
S5	3.63	0.3793	5.4318	0.0430	0.50	$^{29\%}$ 109 → 98
T1	1.25	0.3638	4.3975	0.0007	0.42	$^{59\%}$ 95 → 97
T2	1.48	0.2913	6.4795	0.0573	0.17	$^{70\%}$ 94 → 96
T3	1.72	0.3144	7.5338	0.0123	0.38	$^{52\%}$ 84 → 96
T4	2.07	0.2314	5.5455	0.0003	0.93	$^{24\%}$ 95 → 100
T5	2.22	0.3332	4.7561	0.0225	0.52	$^{18\%}$ 95 → 96

Table S4. Photophysical properties of SPPI-C_2Py in different solvents.

Solvents	ε	n	f(ε,n)	λ_{ab} (nm)	ν_{ab} (cm^{-1})	λ_{em} (nm)	ν_{em} (cm^{-1})	ν_{ss} (cm^{-1})
Hexane	1.88	1.37	0.0004	250	40000	387	25839.79	14160.20
Dioxane	2.22	1.42	0.0214	249	40160.64	388	25773.19	14387.45
Carbontetrachloride	2.238	1.46	0.0110	252	39682.54	395	25316.45	14366.08
Benzene	2.284	1.42	0.0266	253	39525.69	398	25125.63	14400.06
Chloroform	4.81	2.22	0.1482	256	39062.5	410	24390.24	14672.25
Ethyl acetate	6.09	1.41	0.1865	255	39215.69	407	24570.02	14645.66
THF	7.52	1.40	0.2096	254	39370.08	405	24691.35	14678.72
Dichloromethane	9.08	1.42	0.2183	256	39062.5	410	24390.24	14672.25
Acetonitrile	37.5	1.34	0.3053	258	38759.69	418	23923.44	14836.24

Table S5. Photophysical properties of SPPI-N_1Py in different solvents.

Solvents	ε	n	f(ε,n)	λ_{ab} (nm)	ν_{ab} (cm^{-1})	λ_{em} (nm)	ν_{em} (cm^{-1})	ν_{ss} (cm^{-1})
Hexane	1.88	1.37	0.0004	251	39840.64	347	28818.44	11022.19
Dioxane	2.22	1.42	0.0214	250	40000	348	28735.63	11264.36
Carbontetrachloride	2.23	1.46	0.0110	254	39370.08	357	28011.20	11358.87
Benzene	2.28	1.42	0.0266	256	39062.5	366	27322.40	11740.09
Chloroform	4.81	1.44	0.1482	255	39215.69	363	27548.21	11667.48
Ethyl acetate	6.09	1.41	0.1865	254	39370.08	360	27777.78	11592.30
THF	7.52	1.40	0.2096	253	39525.69	358	27932.96	11592.73
Dichloromethane	9.08	1.42	0.2183	255	39215.69	363	27548.21	11667.48
Acetonitrile	37.5	1.34	0.3053	257	38910.50	369	27100.27	11810.23

Table S6. Photophysical properties of SPPI-C_2N_1Py in different solvents.

Solvents	ε	n	f(ε,n)	λ_{ab} (nm)	ν_{ab} (cm^{-1})	λ_{em} (nm)	ν_{em} (cm^{-1})	ν_{ss} (cm^{-1})
Hexane	1.88	1.37	0.0004	248	40322.58	377	26525.19	13797.38
Dioxane	2.22	1.42	0.0214	247	40485.83	378	26455.03	14030.80
Carbontetrachloride	2.23	1.46	0.0110	250	40000	385	25974.02	14025.97
Benzene	2.28	1.42	0.0266	251	39840.64	388	25773.19	14067.44
Chloroform	4.81	1.44	0.1482	254	39370.08	401	24937.65	14432.42
Ethyl acetate	6.09	1.41	0.1865	253	39525.69	398	25125.63	14400.06
THF	7.52	1.40	0.2096	252	39682.54	395	25316.45	14366.08
Dichloromethane	9.08	1.42	0.2183	254	39370.08	400	25000	14370.08
Acetonitrile	37.5	1.34	0.3053	256	39062.5	408	24509.80	14552.69

Table S7. Summary of blue efficiencies with reported efficiencies.

Emitter	V_{on}(V)	L(cd/m^2)	EL(nm)	η_c(cd/A)	η_p(lm/W)	CIE(x,y)	ref
SPI-C_2Py	**2.8**	**20236**	**482**	**14.28**	**9.32**	**(0.15,0.31)**	**This work**
SPI-N_1Py	**3.0**	**15589**	**482**	**9.63**	**4.74**	**(0.15,0.31)**	**This work**
SPI- C_2N_1Py	**2.6**	**19108**	**482**	**16.93**	**11.23**	**(0.15,0.31)**	**This work**
Cz-DPVI	3.4	13629	419	4.9	4.3	(0.15,0.08)	3
PPI	3.8	3307	412	0.71	0.40	(0.161,0.065)	4
mTPA-PPI	3.2	4065	404	0.84	0.48	(0.161,0.049)	4
L-BPPI(50nm)	8.5	70	440	0.01	-	(0.16,0.11)	5
L-BPPI(40nm)	6.5	295	440	0.13	-	(0.16,0.11)	5
L-BPPI(30nm)	5.0	420	440	0.40	-	(0.16,0.10)	5
L-BPPI(20nm)	4.5	391	440	0.68	-	(0.16,0.10)	5
Z-BPPI(50nm)	6.5	105	440	0.07	-	(0.17,0.12)	5
Z-BPPI(40nm)	5.0	502	440	0.34	-	(0.16,0.12)	5
Z-BPPI(30nm)	4.5	267	440	0.45	-	(0.16,0.12)	5
Z-BPPI(20nm)	5.0	100	440	0.31	-	(0.16,0.11)	5
MADN(BUBD)	7.8	-	440	2.1	-	(0.15,0.10)	6
CPPPI	-	3322	420	0.65	0.48	(0.165,0.050)	7
PPICPPPI	-	4329	428	1.53	0.86	(0.166,0.056)	7
PhBPI	2.8	-	450	1.87	1.85	-	8
bilayer-TPBI	3.2	-	468	2.03	1.00	(0.15,0.15)	9
TPA-BPI	2.8	-	448	1.83	1.58	(0.15,0.09)	10
DPVBi	7.5	-	457	0.03	-	(0.15, 0.13)	11
DPVICz	4.2	-	470	0.92	-	(0.15, 0.22)	11
DPVTCz	3.8	-	470	1.94	-	(0.14, 0.22)	11
3,6-DPVTCz	5.0	-	449	0.11	-	(0.15, 0.11)	11
PEDOt-PSS:3(100nm)	4.0	2800	460	0.61	0.14	(0.15,0.14)	12
PEDOt-PSS:3(50nm)	3	10600	407	1.68	1.10	(0.16,0.13)	12
PEDOt-PSS:4(40nm)	2.5	21200	392	1.90	1.55	(0.16,0.14)	12
BBTPI	2.7	-	-	5.48	4.77	0.15, 0.10	13
BiPI-1	2.8	-	-	4.62	4.55	0.15, 0.08	14
3-CzPOPPI	2.9	-	-	2.71	2.73	0.15, 0.06	15
TTP-TPI	3.1	-	-	2.10	1.88	0.16, 0.05	16
DPT-TPI	2.9	-	-	3.13	3.22	0.16, 0.07	16
PMSO	3.2	-	-	4.64	4.0	0.152, 0.077	17
PPI-2TPA	3.0	-	-	4.40	4.60	0.150, 0.063	18
PPI-2NPA	3.0	-	-	3.98	3.88	0.151, 0.066	18
TPIBNCz	3.2	-	-	3.29	2.80	0.157, 0.074	19
PPi-Pid + CBP	3.15	-	-	4.13	-	0.151, 0.076	20

Table S8. Summary of blue PHOLEDs efficiencies with reported efficiencies.

Emitter	V_{on} (V)	L (cd/m^2)	EL (nm)	EQE (%)	η_c (cd/A)	η_p (lm/W)	CIE (x,y)	ref
B1	2.6	8961	**478**	18.56	34.32	32.09	**(0.15,0.37)**	**This work**
B2	3.0	8032	**478**	16.32	30.65	28.32	**(0.15,0.37)**	**This work**
B3	2.5	10238	**478**	22.43	43.23	40.54	**(0.15,0.37)**	**This work**
1	7	1390	474	1.9	3.9	1.4	(0.17, 0.38)	21
2	7	1440	472	3.8	7.1	2.7	(0.17, 0.36)	21
3	7	1080	472	4.3	10.1	4.0	(0.24, 0.43)	21
4	9	470	472	5.2	8.9	3.1	(0.24, 0.41)	21
5	6.5	2290	477	4.6	10.1	3.6	(0.16, 0.38)	21
6	7	1560	478	3.2	7.7	2.7	(0.18, 0.43)	21
5	7	5455	477	8.7	19.1	6.6	(0.18, 0.39)	21
1	6	1960	472	2.8	4.4	2.0	(0.16, 0.29)	21
1	5.5	1640	472	3.3	6.3	3.3	(0.16, 0.33)	21
1	6	1800	472	2.5	5.2	2.4	(0.17, 0.36)	21
1	6.5	1410	474	1.4	3.2	1.3	(0.19, 0.39)	21
1	7	1430	478	0.7	1.7	0.6	(0.21, 0.41)	21
5	8	530	478	1.9	2.1	0.8	(0.17, 0.25)	21
5	7	920	474	4.7	7.0	3.4	(0.16, 0.35)	21
5	5.5	2850	478	5.5	11.8	5.6	(0.17, 0.38)	21
5	5	4600	478	6.8	14.9	7.7	(0.17, 0.40)	21
5	5	4370	478	6.8	15.1	7.7	(0.17, 0.41)	21
5	5	4600	478	10.4	23.7	12.6	(0.18, 0.40)	21

Table S9. Summary of red PHOLEDs efficiencies with reported efficiencies.

Emitter	V_{on}(V)	L(cd/m^2)	EL(nm)	EQE(%)	η_c(cd/A)	η_p(lm/W)	CIE(x,y)	ref
R1	**2.6**	**40876**	**564**	**15.67**	**17.78**	**16.34**	**(0.62,0.36)**	**This work**
R2	**2.6**	**32013**	**564**	**13.32**	**16.31**	**14.89**	**(0.62,0.36)**	**This work**
R3	**2.6**	**44879**	**564**	**18.56**	**25.7**	**22.68**	**(0.62,0.36)**	**This work**
TPP	-	42	655			-	(0.70, 0.28)	22
TPC	-	100	660		-	0.061	(0.67, 0.29)	23
TPDPP	-	150	635		-	0.035	(0.69, 0.29)	24
ACY	-	6400	-		-	1.3	(0.68, 0.32)	25
CQY	-	1000	-		-	0.28	(0.70, 0.30)	25
BDPMB	-	2880	640		1.34	-	(0.67, 0.33)	26
NPAMLMe	-	8000	650		1.5	0.9	(0.66, 0.32)	27
ACEN3	-	2705	630		0.31	0.27	(0.65, 0.34)	28
ACEN4	-	1528	630		0.28	0.12	(0.64, 0.32)	28
BZTA2		9138	626		2.0	1.6	(0.63, 0.35)	29
BZTA1	-	8087	640		0.91	0.58	(0.63, 0.35)	29
INDMLMe	-	1750	650		-	-	(0.63, 0.36)	30
pAAA	-	-	616		0.6	-	(0.63, 0.36)	31

Table S10. Summary of yellow PHOLEDs efficiencies with reported devices.

Emitter	V_{on} (V)	L (cd/m^2)	EQE (%)	CE (cd/A)	PE (lm/W)	CIE(x,y)	ref
SPPI-C_2py	**2.7**	**94231**	**21.67**	**65.32**	**36.34**	**(0.49,0.50)**	**This work**
SPPI-N_1py	**2.7**	**92645**	**20.56**	**62.67**	**34.88**	**(0.49, 0.50)**	**This work**
SPPI- C_2N_1py	**27**	**99863**	**25.89**	**70.53**	**40.86**	**(0.49, 0.50)**	**This work**
Y-1	3.1	11360	-	10.54	-	-	32
Y-2	5.2	9311	-	6.5	-	-	32
Y-3	3.2	14270	-	11.84	-	-	32
PO-01 : TCTA	8.8	70	10.9	34.0	12.2	(0.49, 0.50)	33
PO-01 : CBP	9.6	295	18.3	53.9	17.7	(0.51, 0.49)	33
PO-01 : TPBI	6.7	420	17.2	50.3	23.7	(0.51, 0.49)	33
PO-01 : DBFTrz	7.7	391	18.0	54.5	22.4	(0.51, 0.49)	33
PO-01 : CTA:DBFTrz	7.0	105	18.5	56.0	25.2	(0.50, 0.49)	33
PO-01 : CBP:TPBI	6.9	502	16.5	47.8	21.7	(0.50, 0.48)	33
PO-01 : CBP:DBFTrz	7.9	267	19.0	58.4	23.3	(0.50, 0.49)	33
5a	5.93	2862	5.28	17.63	9.38	(0.49, 0.51)	34
5b	8.29	23857	7.17	13.01	3.74	(0.49, 0.51)	34
5c	-	51960	3.61	13.01	0.48	(0.49, 0.51)	34
C1	2.8		4.5	13.3		(0.50 0.49)	35
C2	2.9		6.9	21.2		(0.47, 0.51)	35
D1	2.9		2.8	8.07		(0.41, 0.46)	35
D2	2.9		8.7	28.0		(0.44, 0.54)	35
III	3.4	40700	15.1	45.2	40.1	(0.50,0.49)	36
(F-BT)2Ir(acac)	-		14.6	45.6	55.1	-	37
pPhBICP	2.2	31 950	19.3	57.2	59.8	(0.51, 0.49)	38
mPhBICP	3.1	34 350	16.9	49.6	46.4	(0.51, 0.49)	38
pPhBINCP	3.0	33 200	19.3	57.3	55.3	(0.50, 0.48)	38
MPhBINCP	2.8	32 700	17.5	52.9	54.7	(0.49, 0.49)	38

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