
Efficient selenium-integrated TADF OLEDs with reduced roll-off

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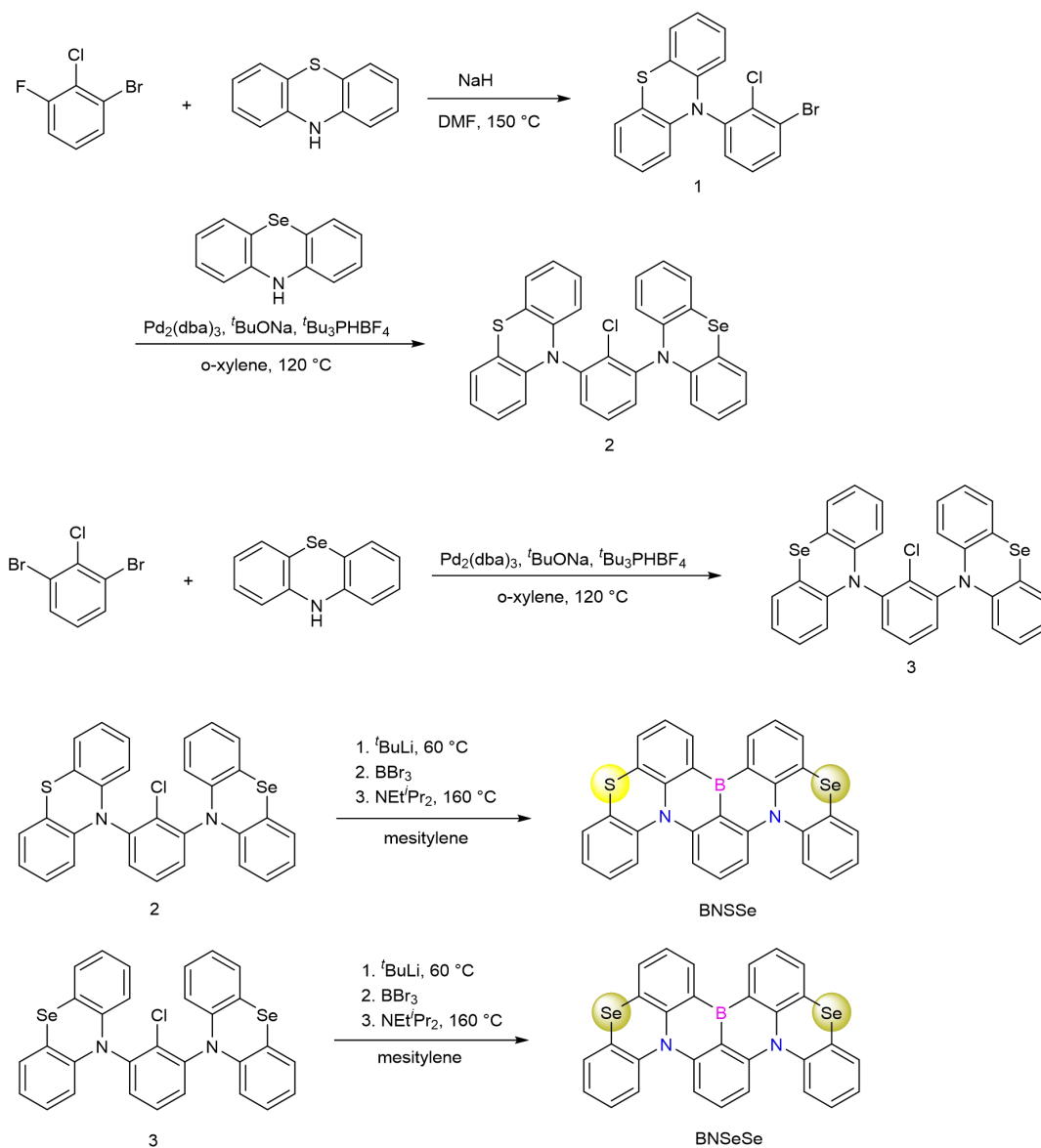
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Material synthesis and characterization

General procedure for material characterization

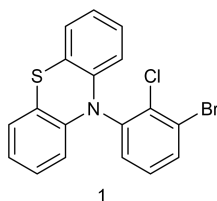
All raw materials and reagents for synthesizing the emitters were purchased from Aladdin, TCI, Bidepharm, J&K and used without additional purification. The reactions were carried out under the protection of the high-purity argon atmosphere. ^1H and ^{13}C NMR spectra were recorded with Bruker Advance 500 spectrometer and Bruker Advance 600 spectrometer. CDCl_3 was used as the solvent and tetramethylsilane (TMS) as internal standard. High-resolution mass spectra were performed using Thermo Scientific LTQ Orbitrap XL Gas Chromatography Mass spectrometer.

The synthesis routes are depicted in Supplementary Scheme 1.



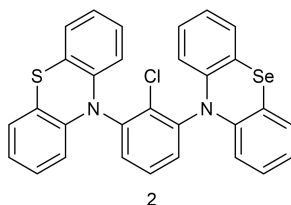
Supplementary Scheme 1 | Synthesis of BNSSe and BNSeSe.

Compound 1



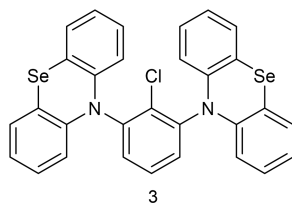
NaH (60% dispersion in mineral oil, 1.89 g, 47.5 mmol) was slowly added to a solution of phenothiazine (8.00 g, 40.1 mmol) in dimethyl formamide (80 mL) at 0 °C. After stirring for 30 min, 1-bromo-2-chloro-3-fluorobenzene (9.25 g, 44.2 mmol) was added in one portion and reaction mixture was refluxed at 170 °C under argon atmosphere for 20 h. After cooling to room temperature, the reaction mixture was poored into ice water, then extracted with dichloromethane and purified through column chromatography to give 1 (5.50 g, yield: 35%) as white solid.

Compound 2



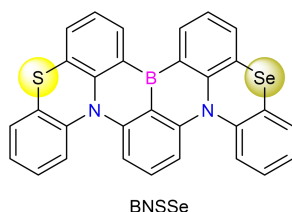
Compound 1 (5.11 g, 13.1 mmol), 10*H*-phenoselenazine (3.40 g, 13.8 mmol), sodium *tert*-butoxide (2.52 g, 26.2 mmol), tris(dibenzylideneacetone)dipalladium (0.241 g, 0.263 mmol) and tri-*tert*-butylphosphine tetrafluoroborate (0.952 g, 3.28 mmol) were dissolved in xylene (60 mL) under a argon atmosphere. After stirred at 120 °C for 16 h, the mixture was cooled to room temperature. The solvent was removed under vacuo and the residue was purified through column chromatography to give 2 (5.97 g, yield: 82%) as a white solid. ¹H NMR (500 MHz, Chloroform-*d*) δ 7.78 – 7.66 (m, 3H), 7.20 (dd, *J* = 7.5, 1.5 Hz, 2H), 7.00 (dd, *J* = 7.4, 1.6 Hz, 2H), 6.98 – 6.91 (m, 2H), 6.90 – 6.79 (m, 6H), 6.31 (dd, *J* = 8.2, 0.9 Hz, 2H), 6.09 (dd, *J* = 8.1, 1.1 Hz, 2H). ¹³C NMR (126 MHz, Chloroform-*d*) δ 142.67, 142.26, 142.21, 140.93, 138.69, 134.48, 133.96, 130.09, 129.71, 127.49, 127.14, 126.99, 123.60, 123.03, 120.10, 116.67, 116.10, 115.11.

Compound 3



2-bromo-1,3-dichlorobenzene (2.50 g, 9.25 mmol), 10*H*-phenoselenazine (4.78 g, 19.4 mmol), sodium *tert*-butoxide (3.55 g, 37.0 mmol), tris(dibenzylideneacetone)dipalladium (0.254 g, 0.277 mmol) and tri-*tert*-butylphosphine tetrafluoroborate (1.34 g, 4.62 mmol) were dissolved in xylene (50 mL) under a argon atmosphere. After stirred at 120 °C for 20 h, the mixture was cooled to room temperature. The solvent was removed under vacuo and the residue was purified through column chromatography to give **3** (4.33 g, yield: 78%) as a white solid. ¹H NMR (500 MHz, Chloroform-*d*) δ 7.73 (q, *J* = 5.2 Hz, 3H), 7.20 (dd, *J* = 7.5, 1.5 Hz, 4H), 6.94 (td, *J* = 8.4, 7.9, 1.6 Hz, 4H), 6.86 (td, *J* = 7.4, 1.1 Hz, 4H), 6.30 (dd, *J* = 8.2, 1.0 Hz, 4H). ¹³C NMR (126 MHz, Chloroform-*d*) δ 142.67, 142.15, 138.66, 134.27, 129.78, 129.68, 127.49, 123.57, 116.68, 116.02.

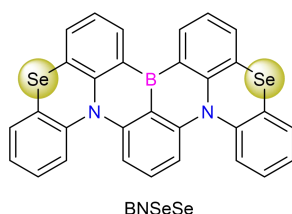
BNSSe



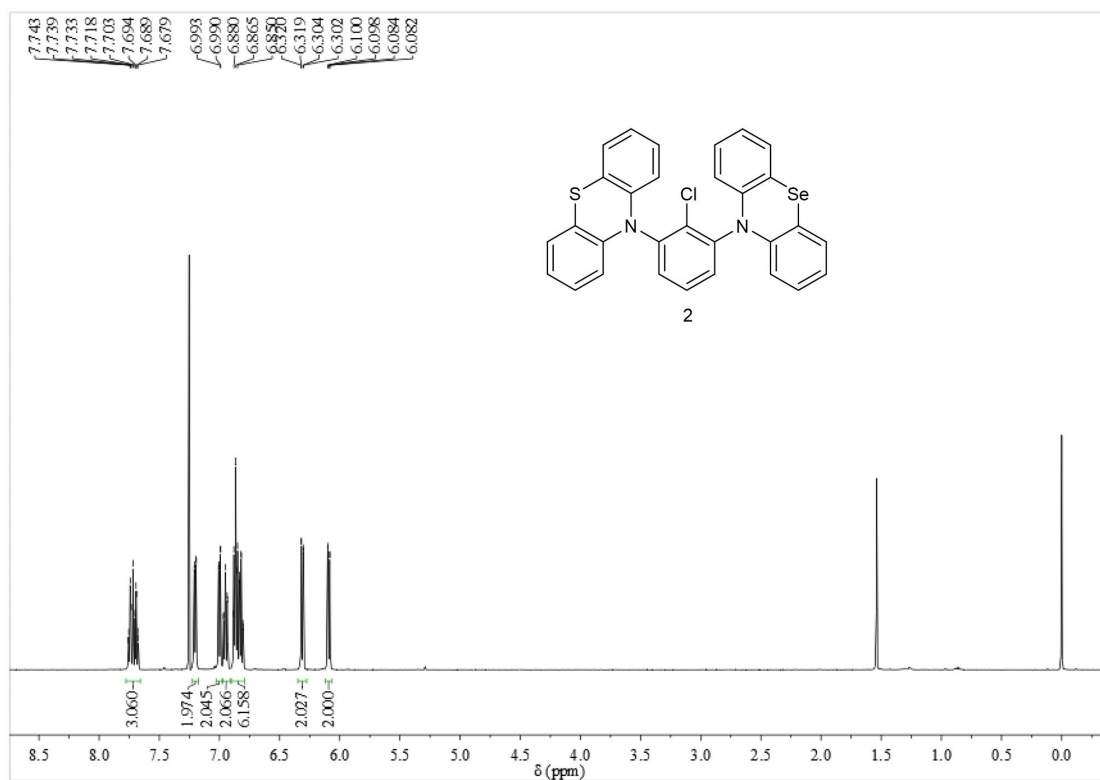
A solution of *tert*-butyllithium in pentane (13.9 mL, 1.3 M, 18.1 mmol) was added slowly to a solution of compound **2** (4.00 g, 7.22 mmol) in mesitylene (60 mL) at -40 °C under a argon atmosphere. After stirring at 60 °C for 5 h, pentane was removed in vacuo. After addition of boron tribromide (1.70 mL, 18.1 mmol) at 0 °C, the mixture was stirred at room temperature for 0.5 h. Then *N,N*-diisopropylethylamine (3.00 mL, 18.1 mmol) was added at 0 °C. After stirring at 160 °C for 14 h, the mixture was cooled to room temperature and the solvent was removed in vacuo. The residue was purified through column chromatography to give BNSSe (0.810 g, yield: 21%) as a orange-yellow solid. ¹H NMR (500 MHz, Chloroform-*d*) δ 8.35 – 8.27 (m, 2H), 7.71 (d, *J* = 7.2 Hz, 1H), 7.58 – 7.54 (m, 2H), 7.51 (d, *J* = 6.8 Hz, 2H), 7.40 (t, *J* = 8.1 Hz, 2H), 7.32 (q, *J* = 7.2 Hz, 2H), 7.28 (d, *J* = 9.1 Hz, 1H), 7.21 – 7.16 (m, 1H), 7.15 – 7.08 (m, 4H). ¹³C NMR (151 MHz,

Chloroform-*d*) δ 147.59, 147.34, 145.54, 144.27, 143.33, 142.65, 133.23, 132.80, 132.44, 131.65, 131.08, 129.75, 128.61, 128.37, 127.66, 127.25, 125.90, 125.55, 124.83, 124.73, 124.03, 123.88, 123.69, 122.26, 121.17, 112.56, 111.88. HRMS (ESI) m/z : $[M+H]^+$ calcd for $C_{30}H_{18}BN_2SSe^+$, 529.0444; found, 529.0448.

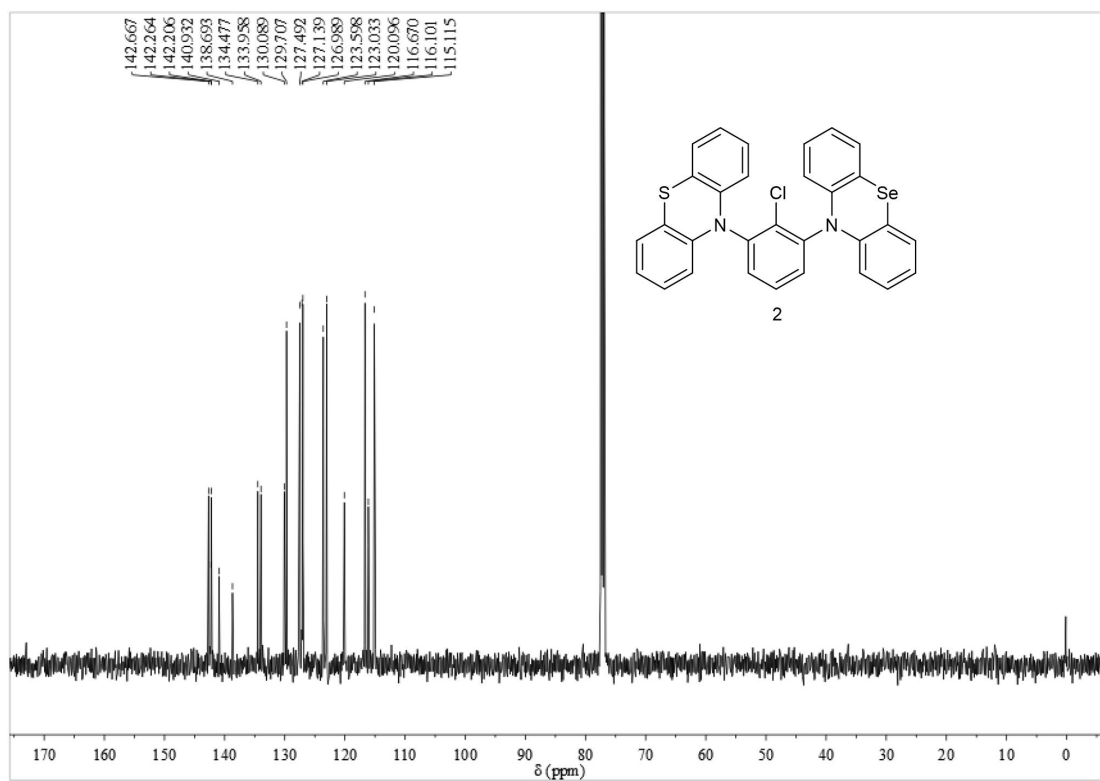
BNSeSe



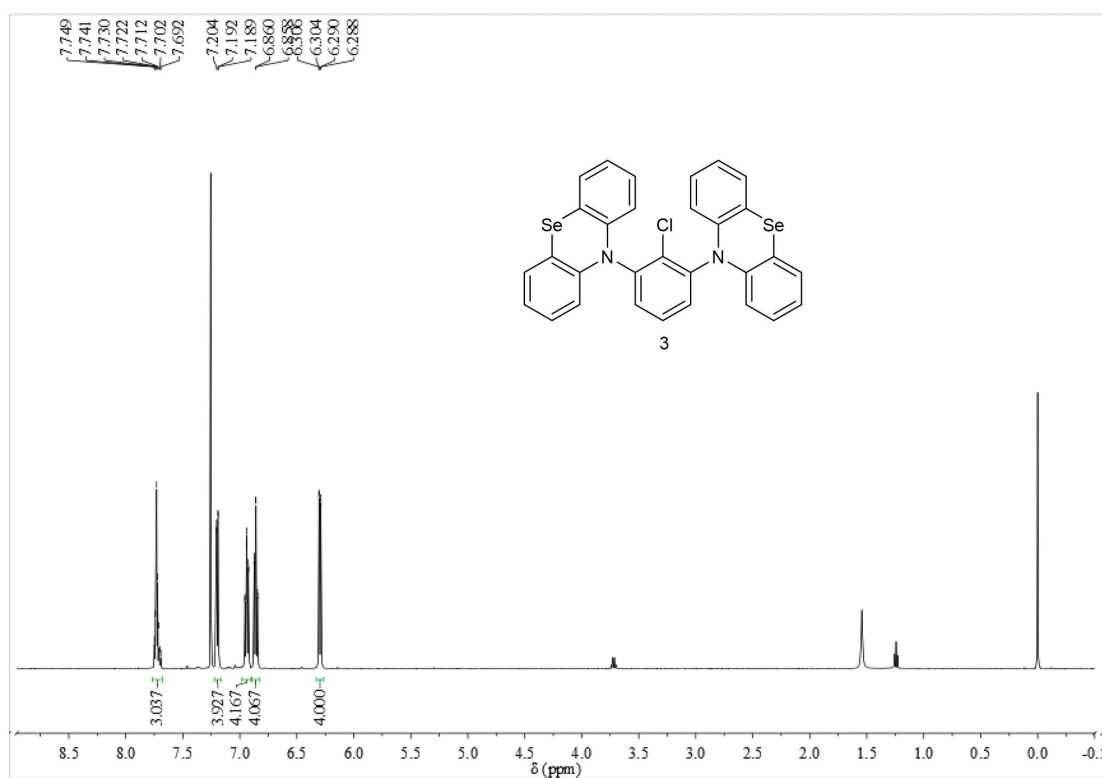
A solution of *tert*-butyllithium in pentane (12.2 mL, 1.3 M, 15.8 mmol) was added slowly to a solution of compound **3** (3.80 g, 6.32 mmol) in mesitylene (60 mL) at $-40\text{ }^{\circ}\text{C}$ under a argon atmosphere. After stirring at $60\text{ }^{\circ}\text{C}$ for 5 h, pentane was removed in vacuo. After addition of boron tribromide (1.50 mL, 15.9 mmol) at $0\text{ }^{\circ}\text{C}$, the mixture was stirred at room temperature for 0.5 h. Then *N,N*-diisopropylethylamine (5.20 mL, 31.5 mmol) was added at $0\text{ }^{\circ}\text{C}$. After stirring at $160\text{ }^{\circ}\text{C}$ for 14 h, the mixture was cooled to room temperature and the solvent was removed in vacuo. The residue was purified through column chromatography to give BNSeSe (1.08 g, 30%) as a orange-yellow solid. ^1H NMR (600 MHz, Chloroform-*d*) δ 8.34 (dd, $J = 7.4, 1.3\text{ Hz}$, 2H), 7.72 (dd, $J = 7.4, 1.4\text{ Hz}$, 2H), 7.59 – 7.55 (m, 2H), 7.52 – 7.48 (m, 1H), 7.38 (d, $J = 8.1\text{ Hz}$, 2H), 7.32 (t, $J = 7.4\text{ Hz}$, 2H), 7.17 (dt, $J = 7.3, 3.4\text{ Hz}$, 2H), 7.14 – 7.10 (m, 4H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 147.78, 145.62, 143.47, 133.45, 132.59, 131.88, 131.21, 127.81, 126.04, 124.82, 124.18, 124.04, 121.31, 112.73. HRMS (ESI) m/z : $[M+H]^+$ calcd for $C_{30}H_{18}BN_2Se_2^+$, 576.9888; found, 576.9890.



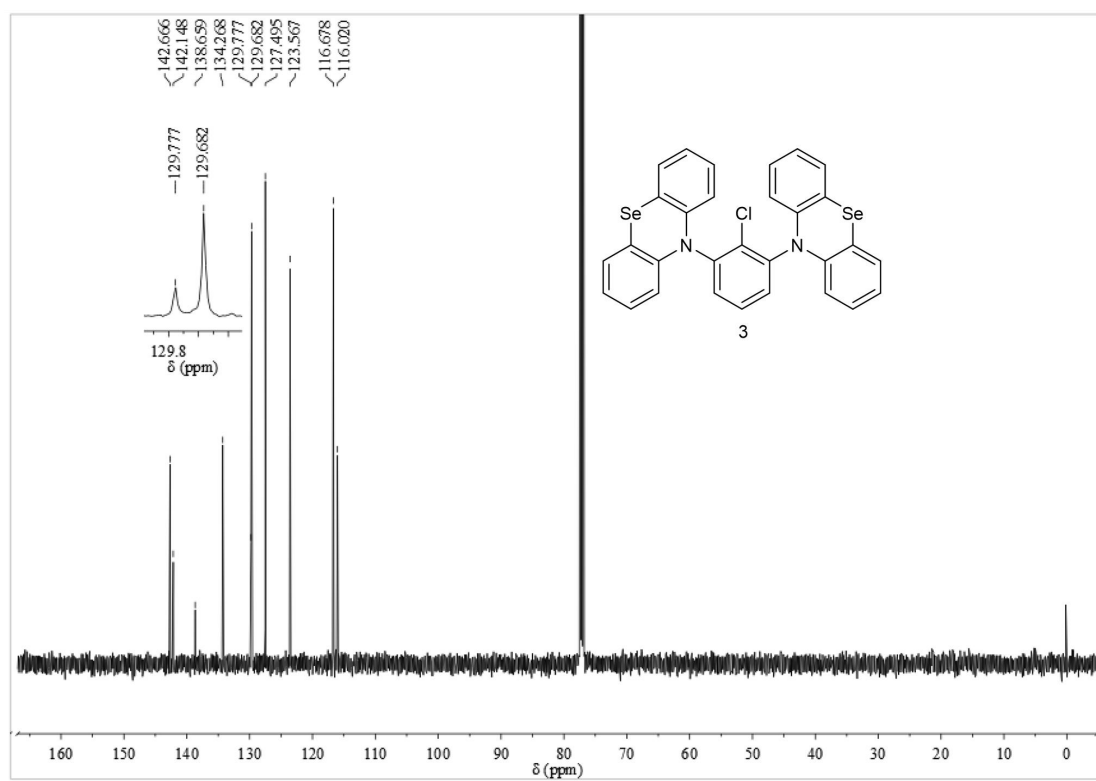
Supplementary Figure 1 | ¹H NMR spectrum of 2 in CDCl₃ at room temperature.



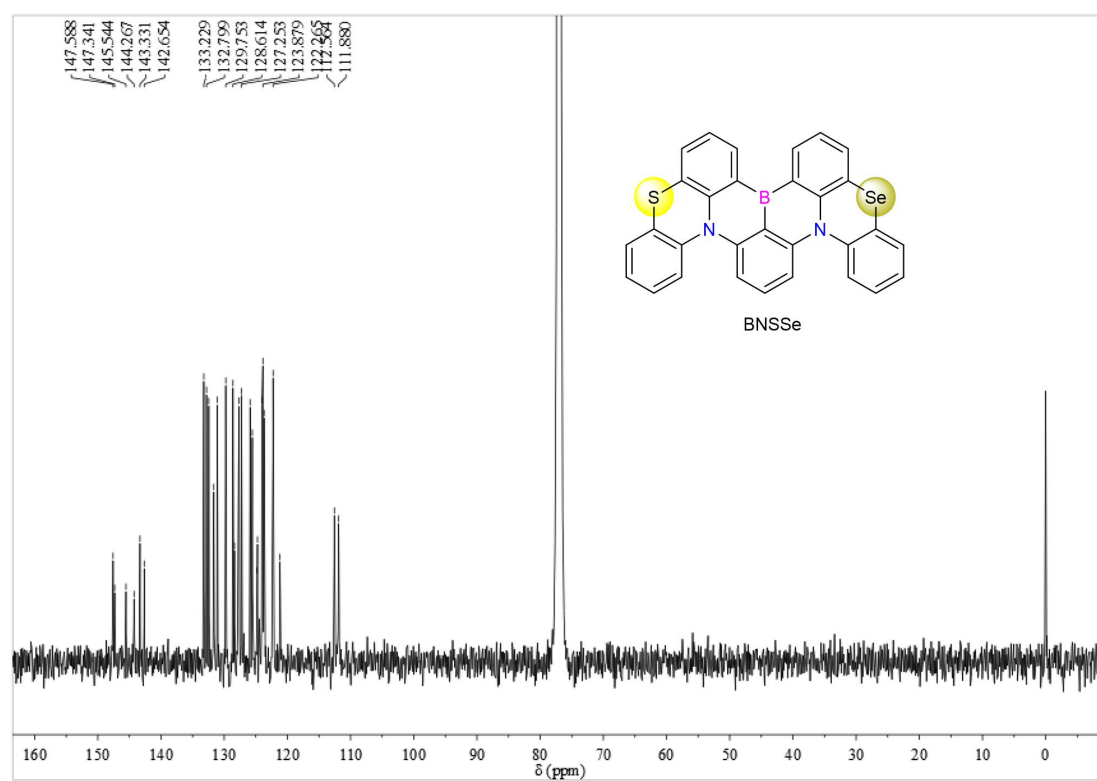
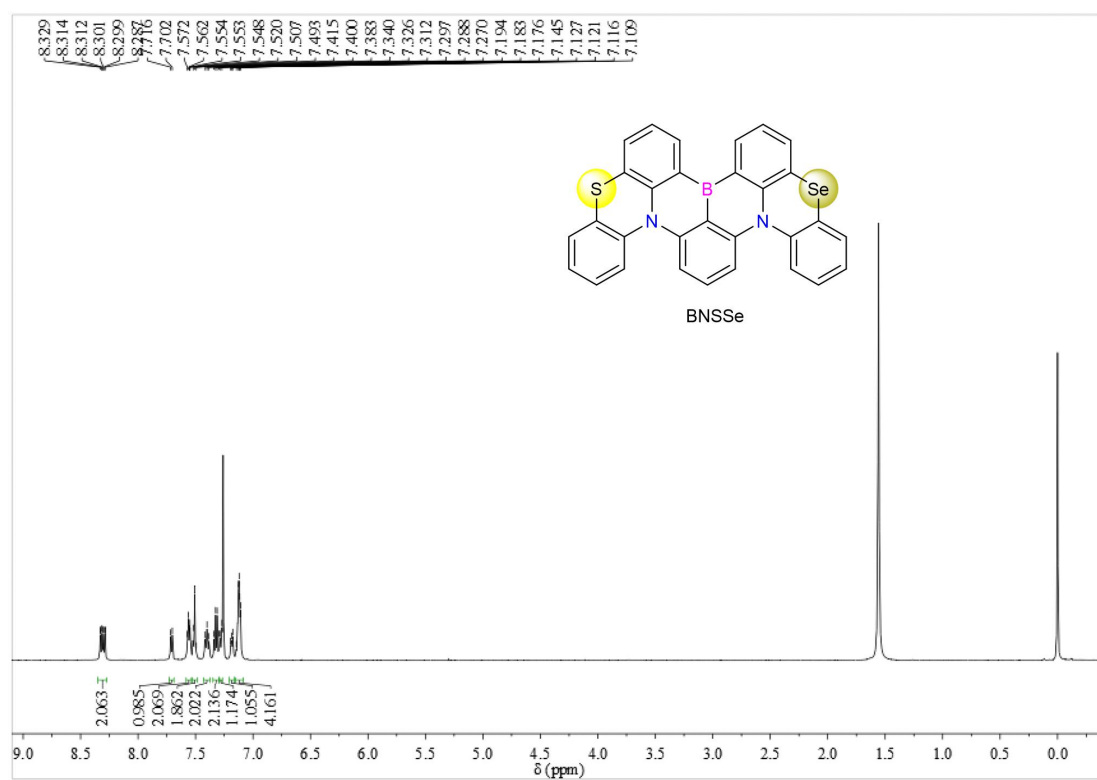
Supplementary Figure 2 | ¹³C NMR spectrum of 2 in CDCl₃ at room temperature.

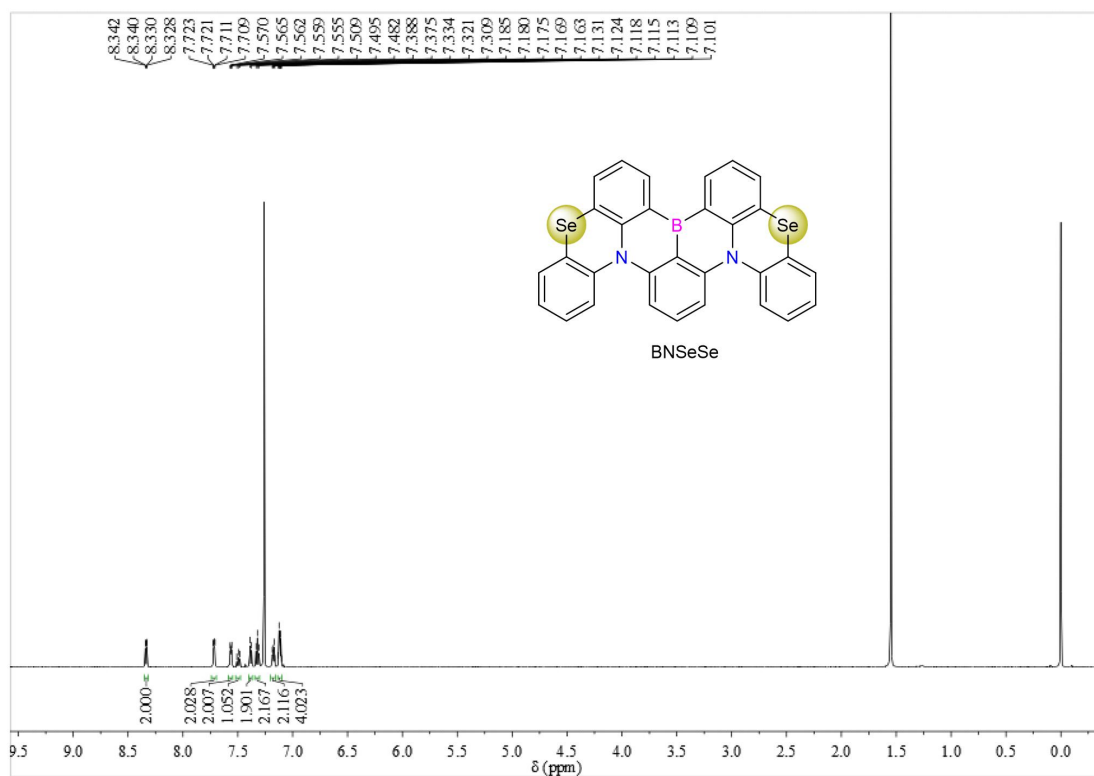


Supplementary Figure 3 | ¹H NMR spectrum of 3 in CDCl₃ at room temperature.

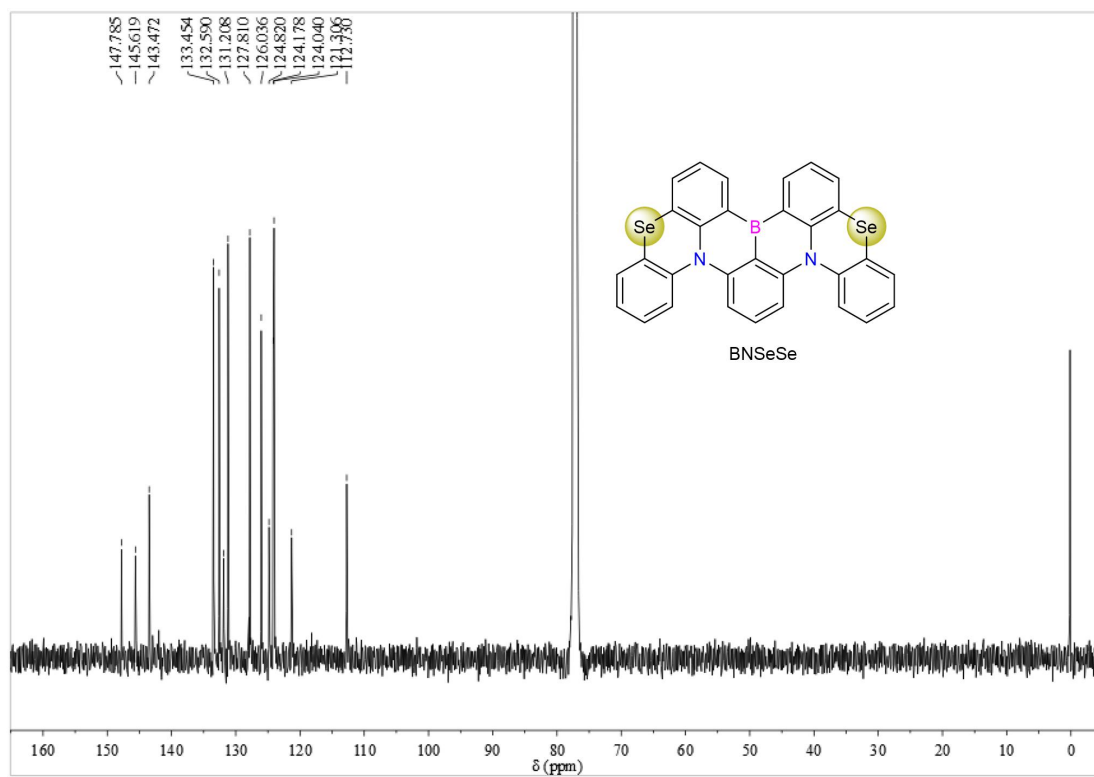


Supplementary Figure 4 | ¹³C NMR spectrum of 3 in CDCl₃ at room temperature.



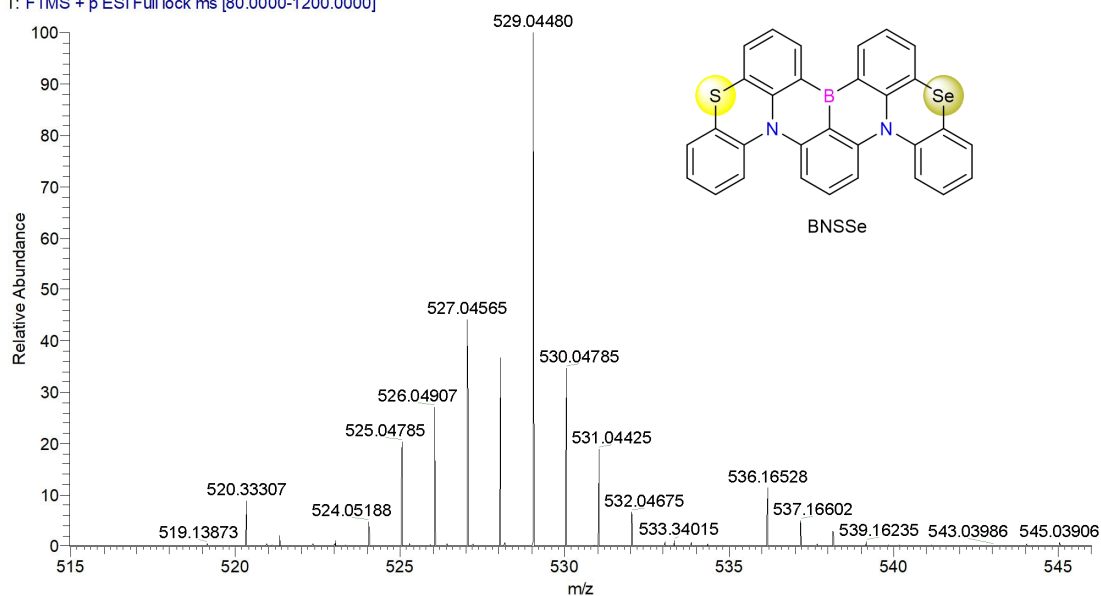


Supplementary Figure 7 | ¹H NMR spectrum of BNSeSe in CDCl₃ at room temperature.



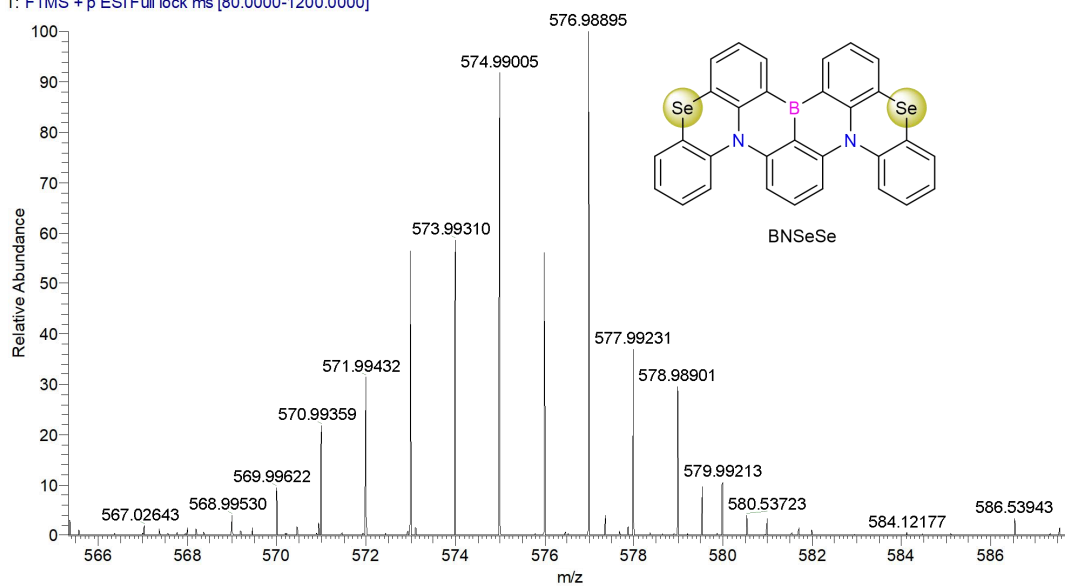
Supplementary Figure 8 | ¹³C NMR spectrum of BNSeSe in CDCl₃ at room temperature.

3-5 #14 RT: 0.09 AV: 1 NL: 5.76E6
T: FTMS + p ESI Full lock ms [80.0000-1200.0000]



Supplementary Figure 9 | HRMS spectrum of BNSSe.

3-4 #14 RT: 0.09 AV: 1 NL: 1.38E6
T: FTMS + p ESI Full lock ms [80.0000-1200.0000]

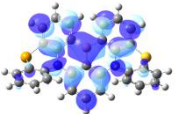
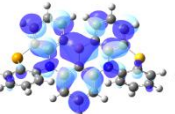
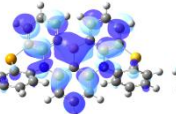
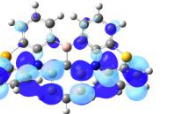
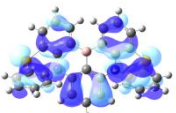
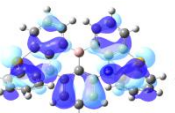
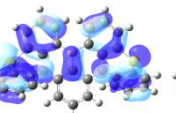
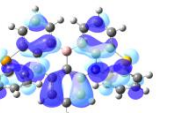
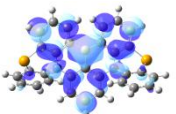
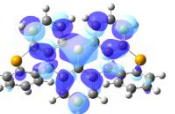
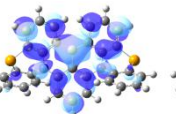
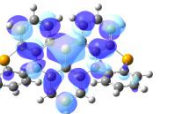


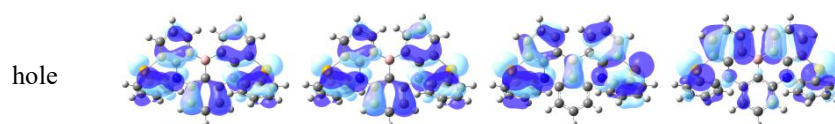
Supplementary Figure 10 | HRMS spectrum of BNSeSe.

Theoretical calculations

Quantum chemical calculations were performed by the Gaussian 09 program package, density functional theory (DFT) using the B3LYP/6-31G(d,p) was performed for achieved optimized molecular geometries. Based on the optimized geometric configurations, the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) were obtained logically. Time-dependent DFT (TD-DFT) calculations were performed at the B3LYP/6-31G(d,p) level to obtain the vertical transitions and NTOs (natural transition orbitals) of the singlet and triplet states based on the corresponding S_0 geometries. The SDD pseudopotential was used for Se atoms. SCS-CC2 and ADC(2) calculations were performed using the MRCC Program with cc-pVDZ basis set.^{1,2} The SOC (spin-orbit coupling) calculations were further evaluated using PySOC program. The optical simulation of OLED devices was performed using SETFOS 5.1 (Fluxim) program. The input parameters include refractive index value, extinction coefficient, thickness of each layer values (all measured by ellipsometry), as well as photoluminescence spectrum of the emitting layer.

Supplementary Table 1 | Calculated natural transition orbitals (NTOs) and dominant transition of BNSSe and BNSeSe for S_1 , T_1 , T_2 and T_3 states.

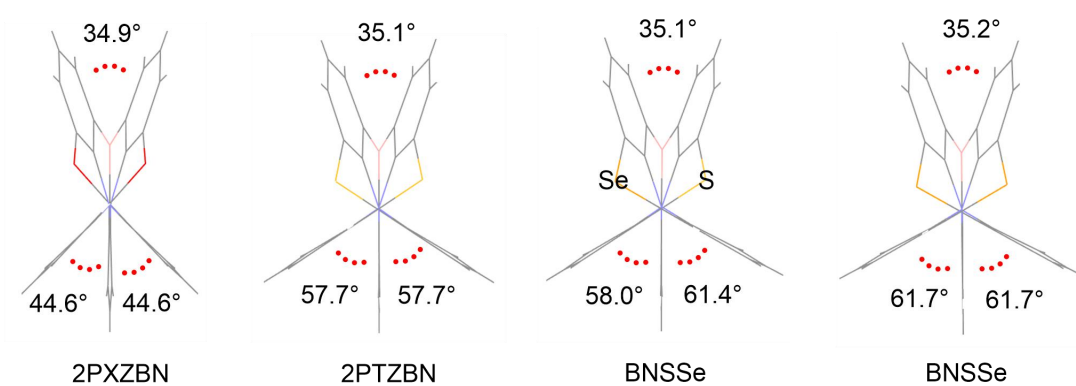
		S_1	T_1	T_2	T_3
BNSSe	particle				
	percentage	0.9851	0.9642	0.8836	0.7277
	hole				
BNSeSe	particle				
	percentage	0.9855	0.9615	0.8989	0.6761



*Blue arrows from holes to particles refer to corresponding dominant transitions.

Supplementary Table 2 | Computed energy levels of 2PXZBN, 2PTZBN, BNSSe and BNSeSe using different methods.

Method	Energy level (eV)	2PXZBN	2PTZBN	BNSSe	BNSeSe
B3LYP/6-31G(d,p)	S ₁	2.7702	2.7808	2.7844	2.7879
	T ₁	2.3213	2.3816	2.3916	2.4040
	ΔE_{ST}	0.4489	0.3992	0.3928	0.3839
SCS-CC2/cc-pVDZ	S ₁	3.0447	3.0717	3.0793	3.0888
	T ₁	2.8827	2.9435	2.9537	2.9678
	ΔE_{ST}	0.1620	0.1280	0.1256	0.1210
ADC(2)/cc-pVDZ	S ₁	2.6891	2.7293	2.7376	2.7473
	T ₁	2.5330	2.6008	2.6106	2.6236
	ΔE_{ST}	0.1560	0.1284	0.1270	0.1238



Supplementary Figure 11 | Optimized structures of 2PXZBN, 2PTZBN, BNSSe and BNSeSe.

Crystallographic and thermal properties

General procedure for cultivation and analysis of single crystals

Single crystals of BNSSe and BNSeSe, suited for X-ray diffraction, were grown by slow diffusion of ethanol into the corresponding dichloromethane solution. The absolute configurations were confirmed using Bruker D8 Venture (for BNSSe) and Bruker APEX-II CCD (for BNSeSe) diffractometer using MoK radiation ($\lambda = 0.71073$) source. The frames were integrated with *SAINT* V8.40A software package; then, the structure was solved using SHELXL-97. CCDC codes: 2098121 for BNSSe and 2098120 for BNSeSe. Crystallographic data of 2PXZBN and 2PTZBN were downloaded from *the cambridge crystallographic data centre* through their CCDC codes reported in the previous work.³

General procedure for thermal measurements

A TGA Q50 (TA instrument) thermal analysis system was employed to analyze thermal gravimetric analysis (TGA) ranging from 50 °C to 800 °C with a heating rate of 10 K min⁻¹ under nitrogen flushing. The decomposition temperatures (T_d) of the emitters measured by TGA at 5% weight loss were observed at 394 °C (BNSSe) and 414 °C (BNSeSe).

Supplementary Table 3 | Crystallographic data collected for single crystals of BNSSe and BNSeSe.

	BNSSe	BNSeSe
Crystal data		
Chemical formula	C ₃₀ H ₁₇ BN ₂ SSe	C ₃₀ H ₁₇ BN ₂ Se ₂
M_r	527.28	574.18
Crystal system, space group	Monoclinic, $P2_1/n$	Monoclinic, $P2_1/n$
Temperature (K)	170	170
a, b, c (Å)	11.5775 (4), 17.4606 (6), 12.1758 (4)	11.6687 (5), 17.4073 (8), 12.2556 (5)
β (°)	113.941 (1)	114.033 (1)
V (Å ³)	2249.57 (13)	2273.56 (17)

<i>Z</i>	4	4
Radiation type	Mo <i>K</i> α	Mo <i>K</i> α
<i>m</i> (mm ⁻¹)	1.79	3.28
Crystal size (mm)	0.13 × 0.06 × 0.04	0.12 × 0.08 × 0.05
Data collection		
Diffractometer	Bruker D8 VENTURE	Bruker <i>APEX</i> -II CCD
Absorption correction	Part of the refinement model (<i>DF</i>) <i>SADABS2016/2</i> (Bruker,2016/2) was used for absorption correction. <i>wR2</i> (int) was 0.0830 before and 0.0607 after correction. The Ratio of minimum to maximum transmission is 0.8069. The 1/2 correction factor is Not present.	Multi-scan <i>SADABS2016/2</i> (Bruker,2016/2) was used for absorption correction. <i>wR2</i> (int) was 0.0921 before and 0.0683 after correction. The Ratio of minimum to maximum transmission is 0.8014. The 1/2 correction factor is Not present.
<i>T</i> _{min} , <i>T</i> _{max}	0.602, 0.745	0.597, 0.745
No. of measured, independent and observed [<i>I</i> > 2 <i>s</i> (<i>I</i>)] reflections	18475, 4535, 3571	19476, 4584, 3268
<i>R</i> _{int}	0.083	0.075
(sin <i>q/l</i>) _{max} (Å ⁻¹)	0.626	0.626
Refinement		
<i>R</i> [<i>F</i> ² > 2 <i>s</i> (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.049, 0.125, 1.05	0.039, 0.085, 1.04
No. of reflections	4535	4584
No. of parameters	311	316
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
Δ <i>ρ</i> _{max} , Δ <i>ρ</i> _{min} (e Å ⁻³)	1.04, -1.56	0.88, -0.54

Computer programs: *SAINT* V8.40A (Bruker, 2016), *XT* (Sheldrick, 2015), *SHELXL* (Sheldrick, 2015), *Olex2* (Dolomanov *et al.*, 2009).

Supplementary Table 4 | Selected bond lengths and angles (Å, °) from the crystal structure of BNSSe.

Bond lengths			
Se1—C1	1.853 (4)	C20—C21	1.390 (5)

Se1—C00F	1.845 (4)	C11—C12	1.398 (5)
S1—C11	1.865 (4)	C11—C10	1.378 (5)
S1—C14	1.825 (4)	C11—Se2	1.865 (4)
N1—C2	1.425 (4)	C14—C15	1.397 (5)
N1—C23	1.411 (4)	C14—Se2	1.825 (4)
N1—C007	1.434 (4)	C00F—C00R	1.392 (5)
N2—C13	1.430 (4)	C00F—S2	1.845 (4)
N2—C19	1.417 (4)	C19—C24	1.417 (4)
N2—C12	1.417 (4)	C7—C12	1.414 (5)
C2—C1	1.404 (5)	C7—C8	1.406 (5)
C2—C3	1.404 (5)	C7—B1	1.541 (5)
C23—C22	1.390 (5)	C24—B1	1.511 (5)
C23—C24	1.412 (5)	C6—C5	1.386 (5)
C007—C00F	1.394 (5)	C18—C17	1.393 (5)
C007—C00O	1.394 (5)	C4—C5	1.379 (5)
C1—C6	1.386 (5)	C00O—C00S	1.391 (5)
C1—S2	1.853 (4)	C8—C9	1.373 (5)
C3—C4	1.417 (5)	C00R—C00Y	1.374 (6)
C3—B1	1.538 (5)	C00S—C00Y	1.385 (6)
C22—C21	1.389 (5)	C10—C9	1.396 (6)
C13—C14	1.397 (5)	C17—C16	1.382 (6)
C13—C18	1.391 (5)	C16—C15	1.379 (7)
C20—C19	1.393 (5)		

Bond angles

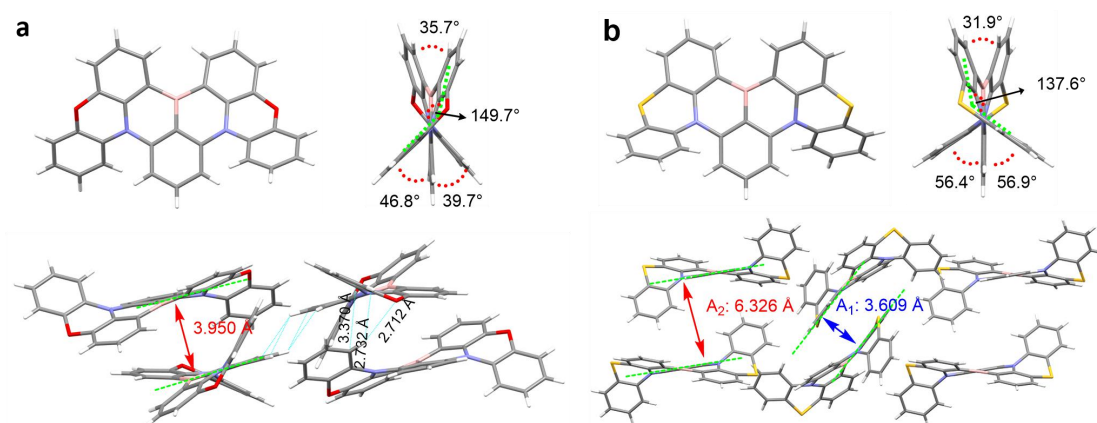
C00F—Se1—C1	94.20 (15)	C15—C14—Se2	119.6 (3)
C14—S1—C11	94.67 (16)	C007—C00F—Se1	120.5 (3)
C2—N1—C007	118.0 (3)	C007—C00F—S2	120.5 (3)
C23—N1—C2	120.7 (3)	C00R—C00F—Se1	118.7 (3)
C23—N1—C007	119.5 (3)	C00R—C00F—C007	120.8 (3)
C19—N2—C13	118.9 (3)	C00R—C00F—S2	118.7 (3)
C19—N2—C12	120.9 (3)	N2—C19—C24	118.8 (3)
C12—N2—C13	118.2 (3)	C20—C19—N2	120.2 (3)
C1—C2—N1	118.3 (3)	C20—C19—C24	121.0 (3)

C1—C2—C3	120.5 (3)	C12—C7—B1	117.6 (3)
C3—C2—N1	121.2 (3)	C8—C7—C12	117.5 (3)
N1—C23—C24	119.0 (3)	C8—C7—B1	124.6 (3)
C22—C23—N1	119.9 (3)	C22—C21—C20	122.1 (3)
C22—C23—C24	121.0 (3)	C23—C24—C19	118.2 (3)
C00F—C007—N1	120.6 (3)	C23—C24—B1	120.9 (3)
C00F—C007—C00O	118.6 (3)	C19—C24—B1	120.9 (3)
C00O—C007—N1	120.6 (3)	C1—C6—C5	120.6 (3)
C2—C1—Se1	121.9 (3)	C17—C18—C13	120.8 (4)
C2—C1—S2	121.9 (3)	C5—C4—C3	121.6 (3)
C6—C1—Se1	117.9 (3)	C11—C12—N2	118.3 (3)
C6—C1—C2	119.9 (3)	C11—C12—C7	120.0 (3)
C6—C1—S2	117.9 (3)	C7—C12—N2	121.6 (3)
C2—C3—C4	117.7 (3)	C00S—C00O—C007	120.2 (3)
C2—C3—B1	118.0 (3)	C9—C8—C7	122.5 (4)
C4—C3—B1	123.8 (3)	C4—C5—C6	119.7 (3)
C21—C22—C23	119.0 (3)	C00Y—C00R—C00	119.8 (4)
		F	
C14—C13—N2	120.4 (3)	C00Y—C00S—C00	120.3 (4)
		O	
C18—C13—N2	120.8 (3)	C11—C10—C9	120.8 (3)
C18—C13—C14	118.7 (3)	C16—C17—C18	120.1 (4)
C21—C20—C19	118.7 (3)	C15—C16—C17	119.6 (4)
C12—C11—S1	121.3 (3)	C8—C9—C10	118.8 (4)
C12—C11—Se2	121.3 (3)	C16—C15—C14	120.8 (4)
C10—C11—S1	118.2 (3)	C00R—C00Y—C00	120.1 (3)
		S	
C10—C11—C12	120.3 (3)	C3—B1—C7	129.9 (3)
C10—C11—Se2	118.2 (3)	C24—B1—C3	115.1 (3)
C13—C14—S1	120.4 (3)	C24—B1—C7	115.0 (3)
C13—C14—C15	119.9 (4)	C14—Se2—C11	94.67 (16)
C13—C14—Se2	120.4 (3)	C00F—S2—C1	94.20 (15)
C15—C14—S1	119.6 (3)		

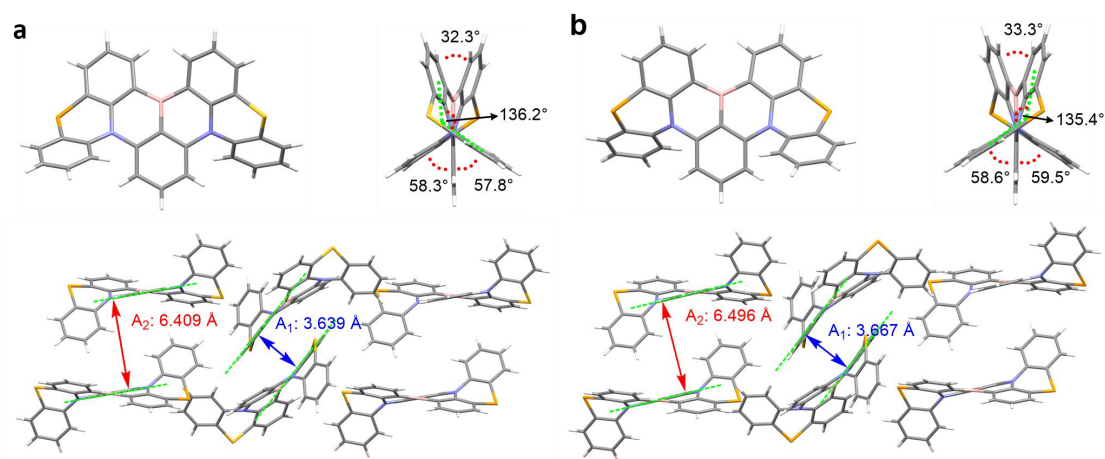
Supplementary Table 5 | Selected bond lengths and angles (Å, °) from the crystal structure of BNSeSe.

Bond lengths			
Se2—C7	1.905 (4)	C13—B1	1.541 (5)
Se2—C6	1.895 (4)	C1—C2	1.398 (5)
Se1—C17	1.908 (4)	C1—C6	1.390 (5)
Se1—C30	1.900 (4)	C7—C8	1.378 (5)
N1—C25	1.438 (4)	C18—C17	1.402 (5)
N1—C18	1.421 (4)	C19—C24	1.389 (5)
N1—C19	1.417 (4)	C23—C22	1.386 (5)
N2—C12	1.412 (4)	C23—C24	1.382 (5)
N2—C21	1.418 (4)	C14—C15	1.379 (5)
N2—C1	1.433 (4)	C17—C16	1.374 (5)
C12—C11	1.413 (5)	C10—C9	1.376 (5)
C12—C7	1.403 (5)	C30—C29	1.395 (5)
C21—C20	1.408 (5)	C8—C9	1.381 (5)
C21—C22	1.394 (5)	C2—C3	1.391 (5)
C11—C10	1.408 (5)	C26—C27	1.385 (5)
C11—B1	1.538 (5)	C29—C28	1.372 (5)
C25—C30	1.389 (5)	C6—C5	1.389 (5)
C25—C26	1.397 (5)	C16—C15	1.393 (6)
C20—C19	1.416 (5)	C28—C27	1.385 (5)
C20—B1	1.507 (5)	C3—C4	1.383 (6)
C13—C18	1.412 (5)	C5—C4	1.373 (6)
C13—C14	1.419 (5)		
Bond angles			
C6—Se2—C7	93.49 (15)	C17—C18—C13	119.9 (3)
C30—Se1—C17	93.75 (16)	C20—C19—N1	118.8 (3)
C18—N1—C25	118.7 (3)	C24—C19—N1	120.4 (3)
C19—N1—C25	118.5 (3)	C24—C19—C20	120.7 (3)
C19—N1—C18	120.8 (3)	C24—C23—C22	122.0 (3)
C12—N2—C21	120.4 (3)	C15—C14—C13	121.5 (4)
C12—N2—C1	118.6 (3)	C23—C22—C21	118.7 (3)

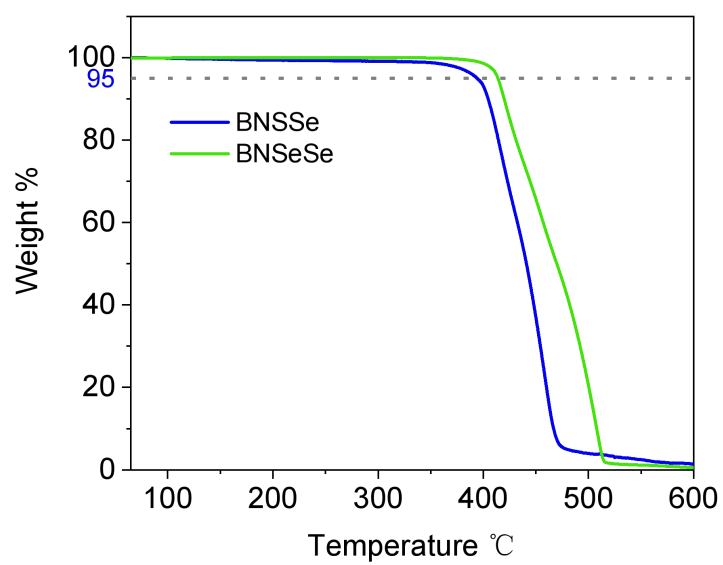
C21—N2—C1	118.7 (3)	C18—C17—Se1	120.7 (3)
N2—C12—C11	121.6 (3)	C16—C17—Se1	118.4 (3)
C7—C12—N2	119.0 (3)	C16—C17—C18	120.6 (4)
C7—C12—C11	119.3 (3)	C9—C10—C11	121.7 (4)
C20—C21—N2	119.2 (3)	C25—C30—Se1	119.0 (3)
C22—C21—N2	119.6 (3)	C25—C30—C29	120.4 (3)
C22—C21—C20	121.1 (3)	C29—C30—Se1	120.5 (3)
C12—C11—B1	117.4 (3)	C7—C8—C9	120.6 (4)
C10—C11—C12	118.1 (3)	C3—C2—C1	119.6 (4)
C10—C11—B1	124.1 (3)	C23—C24—C19	119.3 (3)
C30—C25—N1	121.4 (3)	C27—C26—C25	121.0 (4)
C30—C25—C26	118.4 (3)	C10—C9—C8	119.6 (4)
C26—C25—N1	120.1 (3)	C28—C29—C30	120.4 (4)
C21—C20—C19	118.1 (3)	C1—C6—Se2	119.7 (3)
C21—C20—B1	120.7 (3)	C5—C6—Se2	119.6 (3)
C19—C20—B1	121.2 (3)	C5—C6—C1	120.7 (4)
C18—C13—C14	117.7 (3)	C17—C16—C15	120.6 (4)
C18—C13—B1	118.0 (3)	C29—C28—C27	120.1 (4)
C14—C13—B1	123.8 (3)	C4—C3—C2	120.9 (4)
C2—C1—N2	120.3 (3)	C4—C5—C6	120.4 (4)
C6—C1—N2	120.8 (3)	C14—C15—C16	119.6 (4)
C6—C1—C2	118.8 (3)	C28—C27—C26	119.8 (4)
C12—C7—Se2	120.7 (3)	C11—B1—C13	129.8 (3)
C8—C7—Se2	118.4 (3)	C20—B1—C11	115.5 (3)
C8—C7—C12	120.7 (4)	C20—B1—C13	114.7 (3)
C13—C18—N1	121.3 (3)	C5—C4—C3	119.5 (4)
C17—C18—N1	118.8 (3)		



Supplementary Figure 12 | Single crystal structures and packing mode of 2PXZBN (a, CCDC: 2063408) and 2PTZBN (b, CCDC: 2063407).



Supplementary Figure 13 | Single crystal structures and packing mode of BNSSe (a, CCDC: 2098121) and BNSeSe (b, CCDC: 2098120).



Supplementary Figure 14 | TGA curves of BNSSe and BNSeSe.

Electrochemical and photophysical properties

General procedure for electrochemical measurements

Cyclic voltammograms (CV) were obtained in dichloromethane at room temperature with a CHI600 electrochemical workstation at 25 °C and a scan speed of 100 mV s⁻¹. The electrochemical oxidation potentials were collected by cyclic voltammetry measurements via a CHI660 electrochemical workstation (Chenhua, China) and ferroceniumferrocene (Fc/Fc⁺) was used as the internal reference, tetrabutylammonium hexafluorophosphate (0.1 M) was used as the supporting electrolyte. A platinum plate electrode was utilized as the working electrode, a platinum wire was utilized as the counter electrode and Ag/AgCl as reference electrode. The reduction potentials were calculated from $E_{\text{ox}} - E_{\text{g}}$, the optical bandgaps (E_{g}) were estimated from the onset of the absorption spectra.

General procedure for photophysical measurements

UV-vis absorption spectra and photoluminescence (PL) spectra were measured by a Shimadzu UV-2700 spectrophotometer (Shimadzu, Japan) and a Hitachi F-7100 fluorescence spectrophotometer (Hitachi, Japan), respectively. Phosphorescence spectra (Phos) were recorded on the Hitachi F-7100 fluorescence spectrophotometer at 77 K. The transient PL decay curves were obtained by FluoTime 300 (PicoQuant GmbH) with a Picosecond Pulsed UV-LASER (LASER375) as the excitation source. The photoluminescence quantum yields (Φ_{PLS}) were measured with a Hamamatsu UV-NIR absolute PL quantum yield spectrometer (C13534, Hamamatsu Photonics) equipped with a calibrated integrating sphere, the integrating sphere was purged with dry argon to maintain an inert atmosphere.

Determination of the emitting dipole orientation

The emitting dipole orientation of an emitting film was determined by angle-resolved and polarization-resolved PL measurements in a Hamamatsu's established molecular orientation measurement system (C14234-11, Hamamatsu Photonics). The sample consisted of a fused silica substrate with 15-nm-thick DMIC-TRZ film doped with 1 wt% emitter. The sample was attached to a fused silica half-cylinder prism by index matching liquid. The excitation of the samples was performed with the 360-nm line of the continuous-wave laser with a fixed excitation angle of 45°. The angle-dependent

p-polarized emission intensity at the peak wavelength of the PL spectrum of the emitting layer was detected. The emitting dipole orientation ($\Theta_{//}$) was then determined by least-square fitting of the measured angle-dependent *p*-polarized emission intensity with calculated results.

Analysis of rate constants

The rate constants of radiative decay ($k_{r,S}$) and nonradiative decay ($k_{nr,S}$) from S_1 to S_0 states, the rate constants of intersystem crossing (k_{ISC}) and reverse intersystem crossing (k_{RISC}) were calculated from the following six equations:

$$k_p = 1/\tau_p \dots \dots \dots \text{Eq.(1)}$$

$$k_d = 1/\tau_d \dots \dots \dots \text{Eq.(2)}$$

$$k_{r,S} = \Phi_p k_p + \Phi_d k_d \approx \Phi_p k_p \dots \dots \dots \text{Eq.(3)}$$

$$k_{nr,S} = \frac{1-\Phi_{PL}}{\Phi_{PL}} k_{r,S} \dots \dots \dots \text{Eq.(4)}$$

$$k_{ISC} = k_p - k_{r,S} - k_{nr,S} \dots \dots \dots \text{Eq.(5)}$$

$$k_{RISC} = (k_p k_d \Phi_d) / (k_{ISC} \Phi_p) \dots \dots \dots \text{Eq.(6)}$$

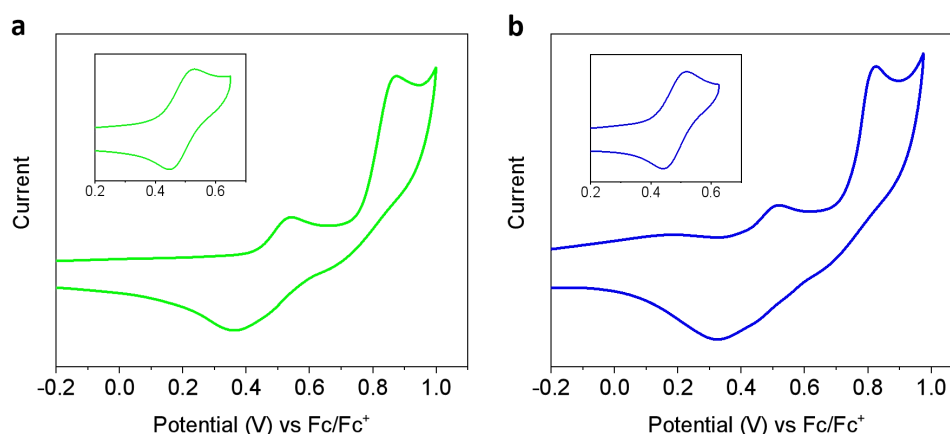
Where τ_p and τ_d represent the prompt and decay fluorescence lifetime, which determined from transient PL spectra. The k_p and k_d represent the decay rate constants for prompt and delayed fluorescence, respectively. Φ_p and Φ_d indicate prompt and delayed fluorescence components and can be distinguished from the total Φ_{PL} by comparing the integrated intensities of prompt and delayed components in the transient PL spectra.

Supplementary Table 6 | Photophysical and electrochemical properties of BNSSe and BNSeSe.

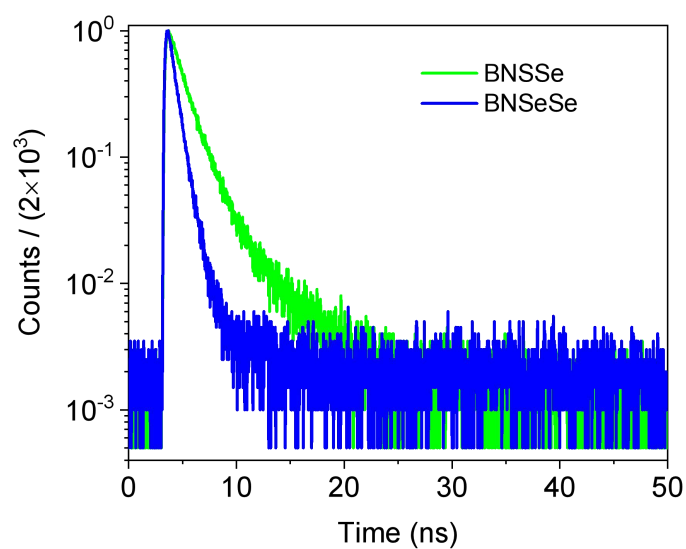
λ_{ab}^a	λ_{PL}^a	S_1^a	T_1^a	ΔE_{ST}^a	FWHM ^a	HOMO ^b	LUMO ^c	τ_{PF}^a	τ_{DF}^a
[nm]	[nm]	[eV]	[eV]	[eV]	[nm]	[eV]	[eV]	[ns]	[μs]

2PXZBN ^{ref}	475	504	2.60	2.41	0.19	34	-5.08	-2.62	4.9	11.6
2PTZBN ^{ref}	471	510	2.59	2.44	0.15	39	-5.19	-2.73	4.2	5.0
BNSSe	469	505	2.61	2.44	0.17	39	-5.22	-2.75	1.6	2.1
BNSeSe	467	502	2.63	2.46	0.17	38	-5.21	-2.72	0.76	1.9

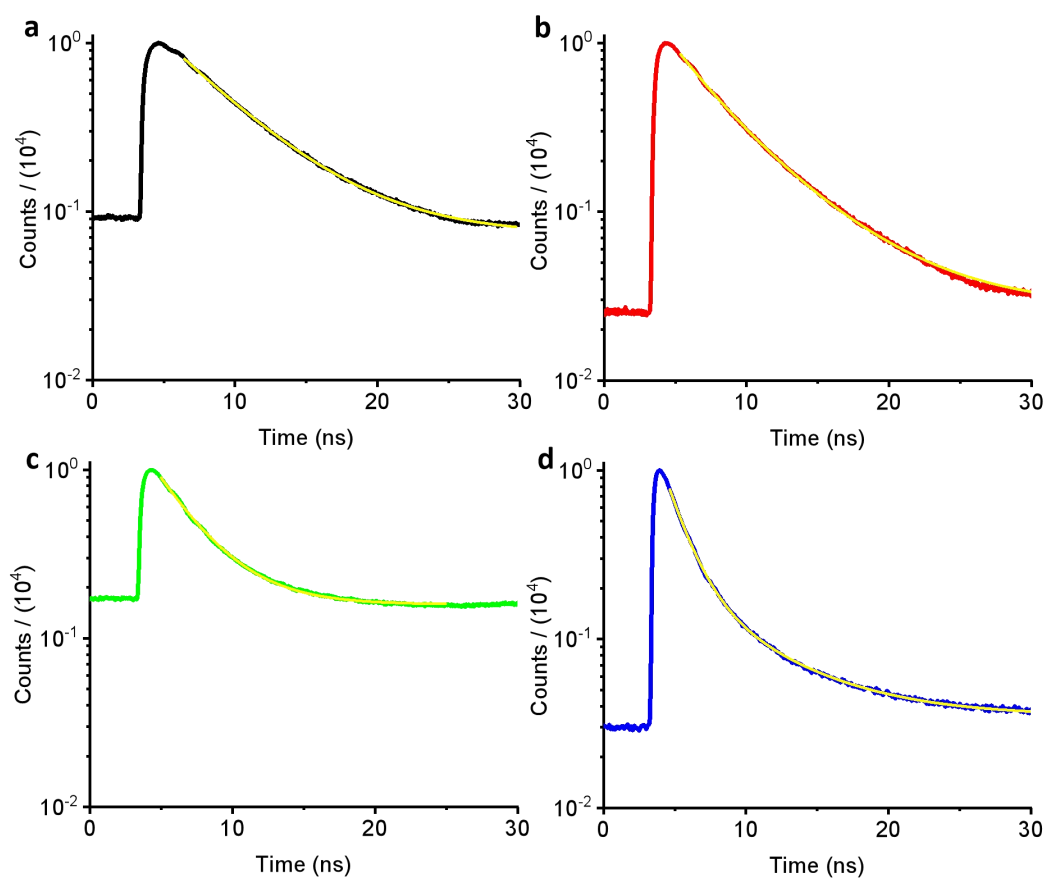
^a Measured in the toluene solution with a concentration of 10^{-5} mol L⁻¹. ^b Measured in dry dichloromethane with a concentration of 10^{-4} mol L⁻¹. ^c Calculated from $E_{\text{HOMO}} + E_{\text{g}}$, the optical bandgaps (E_{g}) were estimated from the onset of the absorption spectra.



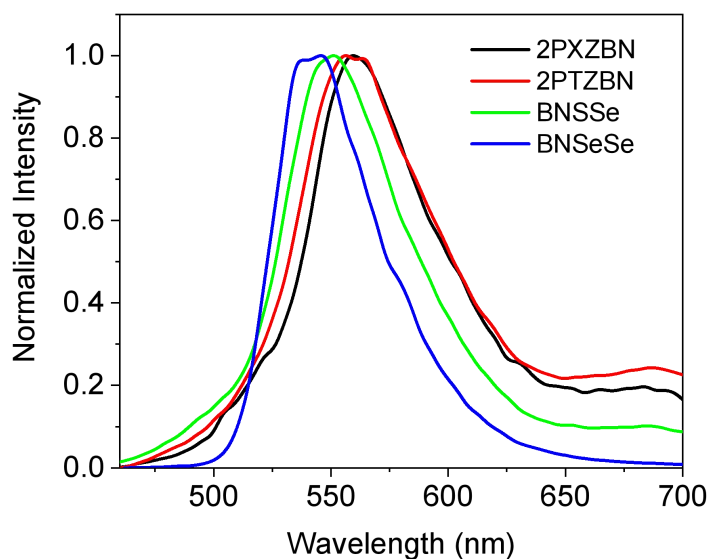
Supplementary Figure 15 | a, Cyclic voltammograms of the oxidation of BNSSe. Inset: first step oxidation of BNSSe. b, Cyclic voltammograms of the oxidation of BNSeSe. Inset: first step oxidation of BNSeSe. The potential scales correspond to the standard ferrocenium/ferrocene redox couple.



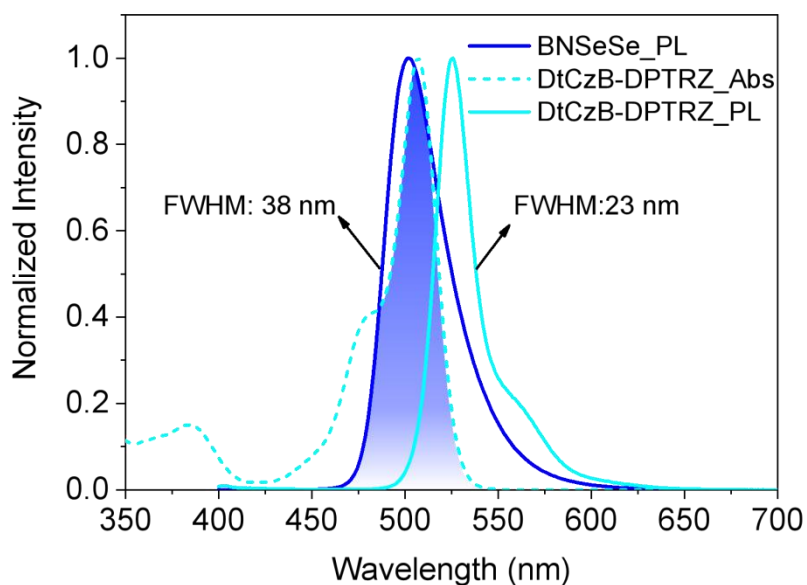
Supplementary Figure 16 | Prompt PL transient decay of BNSSe and BNSeSe in degassed toluene.



Supplementary Figure 17 | Transient PL decay of prompt fluorescence of 2PXZBN, 2PTZBN, BNSSe and BNSeSe in 1 wt% DMIC-TRZ doped film under Ar atmosphere.



Supplementary Figure 18 | Phosphorescence spectra at 77 K of 2PXZBN, 2PTZBN, BNSse and BNSseSe in 1 wt% DMIC-TRZ doped film.



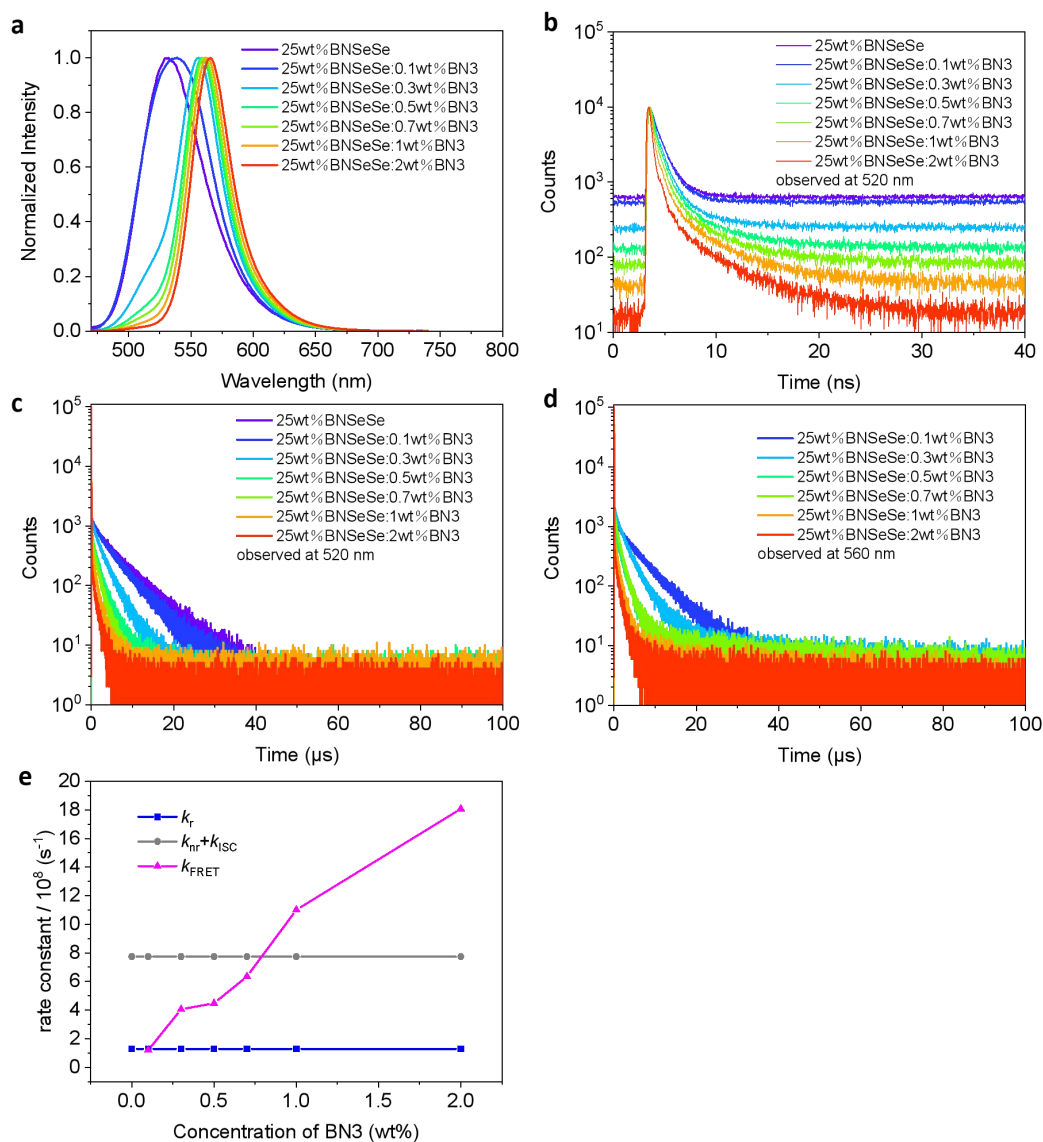
Supplementary Figure 19 | Emission spectrum of BNSseSe and UV-vis absorption and emission spectrum at 298 K of DtCzB-DPTRZ in toluene solution with a concentration of 10^{-5} mol L⁻¹.

Supplementary Table7 | The life-times of the PL decay curves of the DMIC-TRZ:25

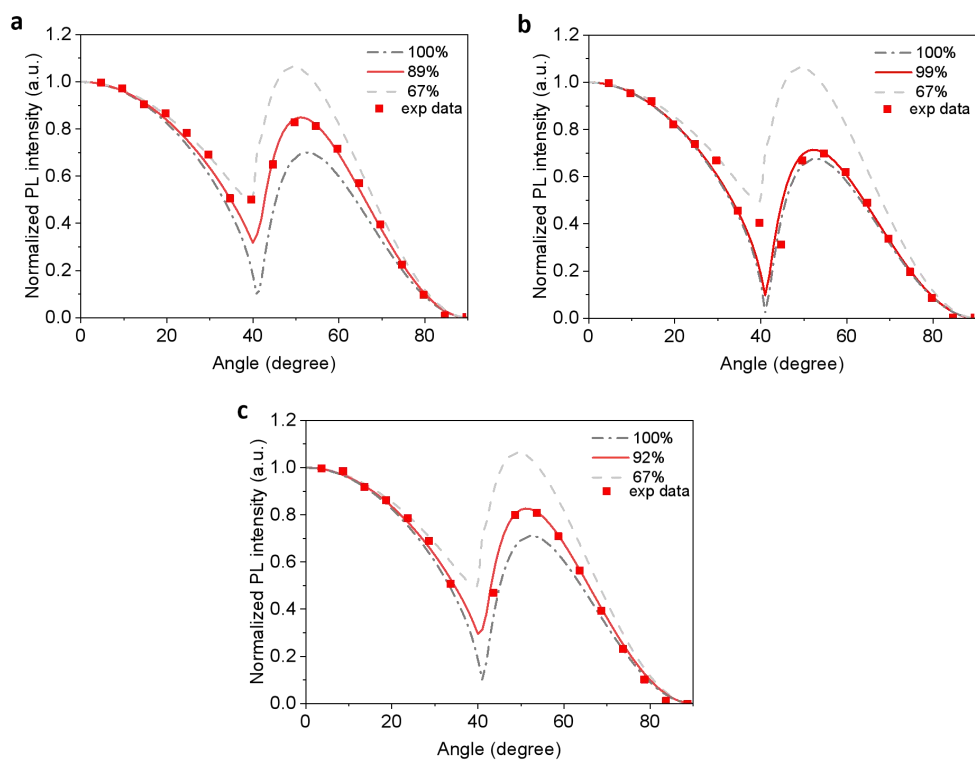
wt% BNSeSe:x wt% BN3 films.

x^a	τ_p^b [ns]	k_{FRET}^c [s ⁻¹]	k_r^d [s ⁻¹]	$k_{\text{nr}}+k_{\text{ISC}}^e$ [s ⁻¹]	Ratio of prompt part
0	1.11	-	1.29×10^8	7.74×10^8	17.24%
0.1	0.98	1.20×10^8	1.29×10^8	7.74×10^8	18.40%
0.3	0.76	4.06×10^8	1.29×10^8	7.74×10^8	30.12%
0.5	0.74	4.48×10^8	1.29×10^8	7.74×10^8	50.22%
0.7	0.65	6.35×10^8	1.29×10^8	7.74×10^8	54.46%
1	0.50	1.01×10^9	1.29×10^8	7.74×10^8	66.11%
2	0.37	1.81×10^9	1.29×10^8	7.74×10^8	82.53%

^a Doping concentration of BN3. ^b Prompt fluorescence lifetime of DMIC-TRZ:25 wt% BNSeSe:x wt% BN3 films. ^c The rate constant of Förster resonance energy transfer process between BNSeSe and BN3. ^d The radiate decay rate constant of BNSeSe. ^e Sum of nonradiate decay rate constant and the rate constant of intersystem crossing process of BNSeSe.



Supplementary Figure 19 | a, The PL spectra of the DMIC-TRZ:25 wt% BNSeSe:x wt% BN3 films. b, The PL decay of prompt fluorescence of the DMIC-TRZ:25 wt% BNSeSe:x wt% BN3 films observed at 520 nm. c, The PL decay of delayed fluorescence of the DMIC-TRZ:25 wt% BNSeSe:x wt% BN3 films observed at 520 nm. d, The PL decay of delayed fluorescence of the DMIC-TRZ:25 wt% BNSeSe:x wt% BN3 films observed at 560 nm. e, The values of k_r , $k_{nr}+k_{ISC}$ and k_{FRET} of the DMIC-TRZ:25 wt% BNSeSe:x wt% BN3 films. x = 0, 0.1, 0.3, 0.5, 0.7, 1 and 2, respectively.



Supplementary Figure 21 | The characterizations of horizontal dipole orientation by angle-dependent p-polarized PL spectra. Measured horizontal transition dipole moment ratios for BNSeSe (a), BN3 (b) and DtCzB-DPTRZ (c) 1 wt%-doped films in DMIC-TRZ.

Device performances

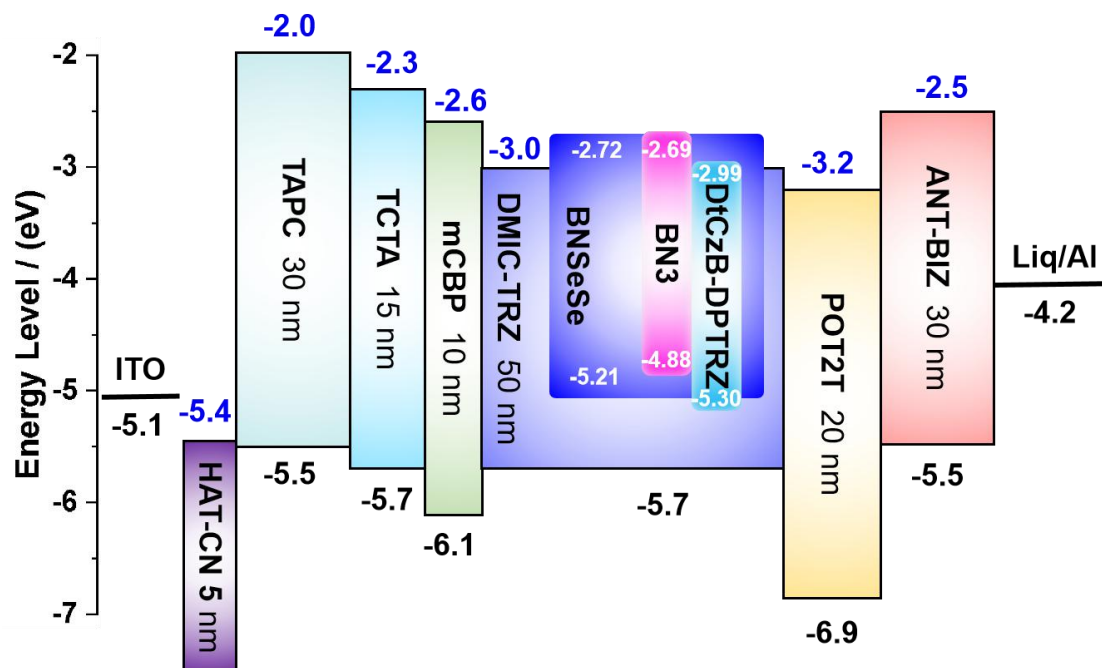
The ITO coated glass substrates with a sheet resistance of $15 \Omega \text{ square}^{-1}$ were consecutively ultrasonicated with acetone/ethanol and dried with nitrogen gas flow, followed by 20 min ultraviolet light-ozone (UVZ) treatment in a UV-ozone surface processor (PL16 series, Sen Lights Corporation). Then the sample was transferred to the deposition system. Both 8-hydroxyquinolinolato-lithium (Liq) as electron injection layer and aluminum (Al) as cathode layer were deposited by thermal evaporation at $5 \times 10^{-5} \text{ Pa}$. Additionally, the organic layers were deposited at the rates of 0.2-3 Å/s. After the organic film deposition, Liq and Al layer were deposited with rates of 0.1 and 3 Å/s, respectively. The emitting area of the device is about 0.09 cm^2 . The current density-voltage-luminance (J - V - L), L - EQE curves and electroluminescence spectra were measured using a Keithley 2400 source meter and an absolute EQE measurement system (C9920-12, Hamamatsu Photonics, Japan).

Supplementary Table 8 | Summary of device performances for A–H.

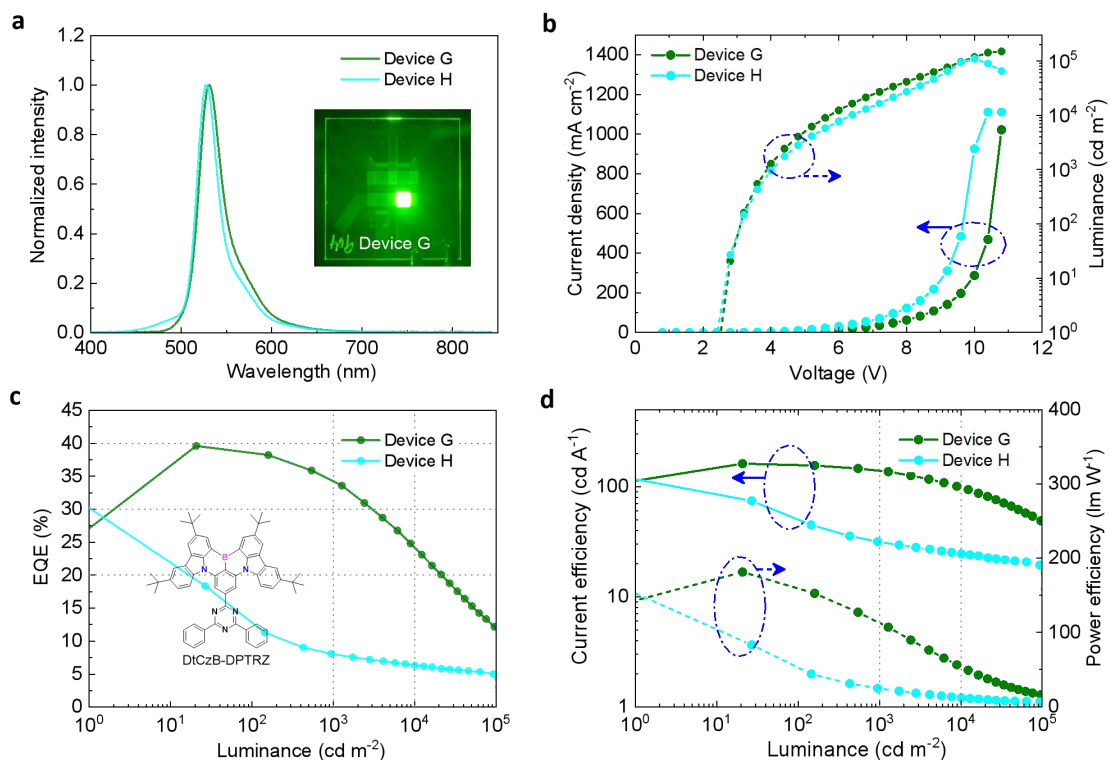
Device (emitter)	λ_{EL} [nm]	V_{on} [V]	FWHM [nm]	$L_{\text{max}}^{\text{a}}$ [cd m ⁻²]	LT_{50}^{b} [h]	CIE ^c [x, y]
A (2PXZBN)	517	2.48	49 (49.37±0.25)	120321 (118302±8236)	158	0.23, 0.67
B (2PTZBN)	520	2.40	52 (51.69±0.63)	128576 (118183±5462)	5.6	0.24, 0.67
C (BNSSe)	515	2.40	50 (49.91±0.22)	113881 (109771±5200)	4.8	0.22, 0.66
D (BNSeSe)	512	2.40	48 (48.26±0.20)	108188 (103425±3298)	4.1	0.19, 0.66
E (HF BN3)	558	2.40	40 (39.87±0.48)	191023 (184543±8106)	51.1	0.41, 0.58
F (BN3)	560	2.57	38 (37.96±0.16)	154424 (147157±8885)	-	0.43, 0.56
G (HF DtCzB-DPTRZ)	531	2.51	31 (31.39±0.20)	149376 (151545±3986)	32.4	0.29, 0.68
H (DtCzB-DPTRZ)	527	2.42	28 (28.26±0.53)	109026 (102297±8019)	-	0.26, 0.68

^a Maximum luminance. ^b LT_{50} are recorded at an initial luminance of 1000 cd m^{-2} . ^c Commission International de l'Eclairage, value taken at 1000 cd m^{-2} . The average device parameters in parentheses are based on the measurement of over fifteen independent

devices.

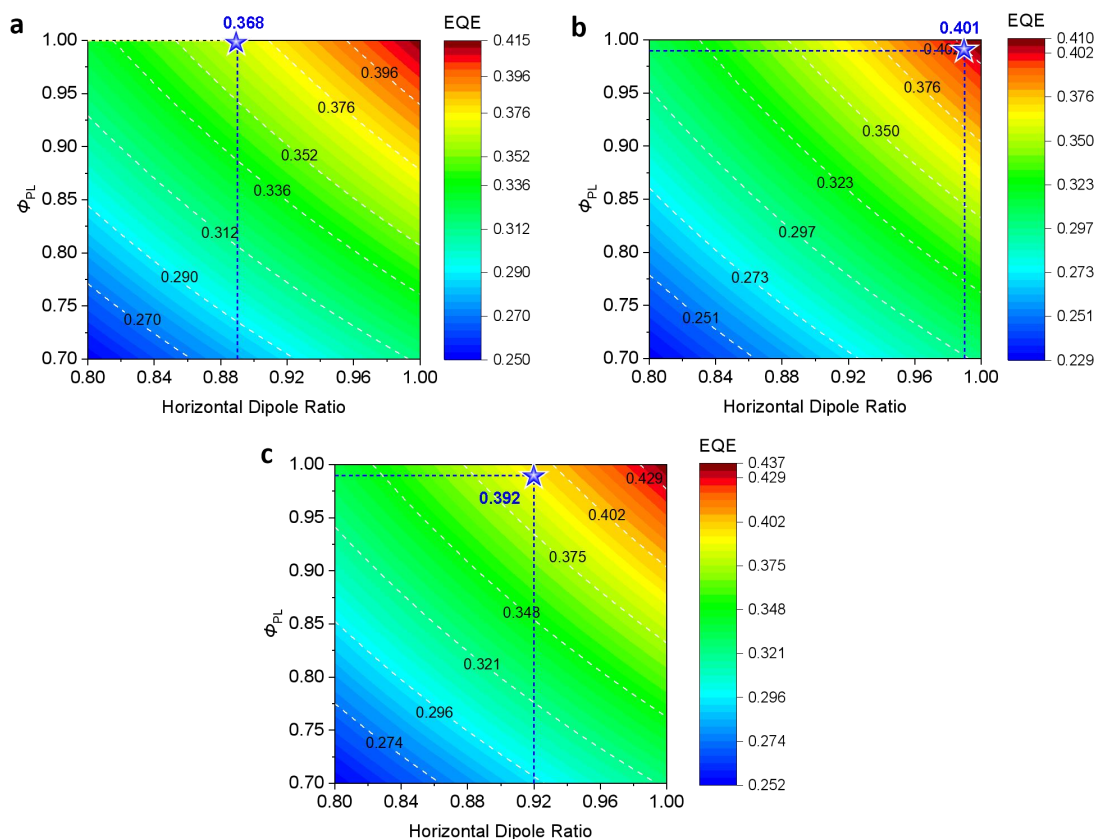


Supplementary Figure 22 | Device structure of hyperfluorescent devices E and G.



Supplementary Figure 23 | a, Normalized EL spectra at 1000 cd m⁻² of DTCzB-DPTRZ

in Device G and H, respectively. Inset: photograph of device G. b, Current density and luminance versus driving voltage characteristics. c, EQE versus luminance characteristics. d, Current and power efficiency versus luminance characteristics.



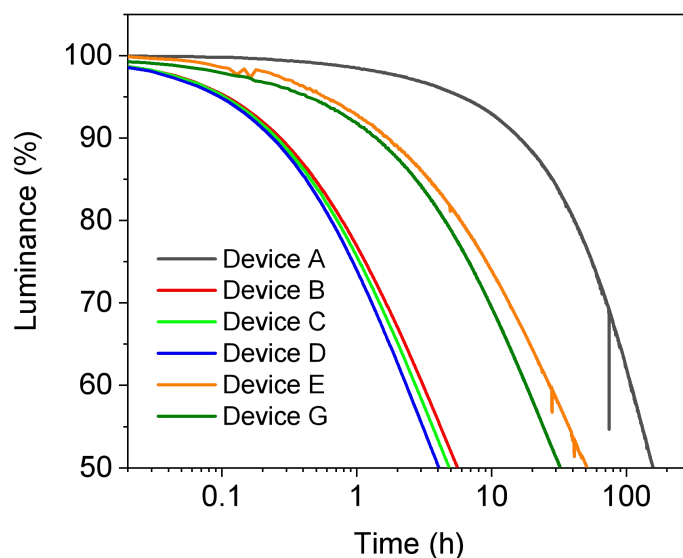
Supplementary Figure 24 | The calculated maximum EQE according to the molecular orientation factor and Φ_{PL} for BNSeSe-based device (a), BN3-based HF device (b) and DtCzB-DPTRZ-based HF device (c).

Supplementary Table 9 | Summary of optical simulation results of device D, HF device E and G.

Device (EML)	Φ_{PL}	$\theta_{//}$	Simulated EQE _{max} ^a	Experimental EQE _{max}
D (DMIC-TRZ:1 wt% BNSeSe)	1.00	0.89	0.368	0.368
E (DMIC-TRZ:25 wt% BNSeSe:1 wt% BN3)	0.99	0.99	0.401	0.405

G						
(DMIC-TRZ:25 wt% BNSeSe:1 wt% DtCzB-DPTRZ)	0.99	0.92	0.392	0.396		

^a Theoretical device efficiency with respect to Φ_{PL} and horizontal orientation factor via optical simulation.



Supplementary Figure 25 | Luminance changes versus time of device A-E and device G at an initial luminance of 1000 cd m⁻².

Supplementary Table 10 | Summary of the reported k_{RISC} s, EQEs, PE_{max} and L_{max} of MR-TADF emitters.

Emitter	k_{RISC} (s ⁻¹)	EQE (%)			PE_{max} (lm W ⁻¹)	L_{max} (cd m ⁻²)	Ref.
		Max	@1000	@10000			
2PXZBN	4.3×10^4	30.7 (29.95±0.30)	24.0 (23.43±0.22)	11.6 (11.56±0.25)	123.4 (120.3±1.3)	120321 (118302±8236)	This work
2PTZBN	1.9×10^5	34.6 (33.83±0.83)	29.5 (28.17±0.61)	15.4 (13.88±0.78)	157.7 (154.8±4.1)	128576 (118183±5462)	
BNSeSe	6.0×10^5	35.7 (35.02±0.44)	32.0 (31.06±0.55)	18.9 (17.65±0.75)	156.2 (152.0±3.1)	113881 (109771±5200)	
BNSeSe	2.0×10^6	36.8 (36.40±0.22)	34.0 (33.34±0.28)	21.9 (21.19±0.51)	146.3 (147.6±2.5)	108188 (103425±3298)	
BN3 (HF)	-	40.5 (40.03±0.40)	32.4 (31.32±0.81)	23.3 (22.62±0.60)	205.8 (197.7±8.7)	191023 (184543±8106)	

DtCzB-DPT RZ (HF)	-	39.6 (37.85±0.99)	34.5 (33.09±0.86.)	24.3 (23.27±0.70)	181.3 (174.2±6.6)	149376 (151545±3986)	
DABNA-1	9.9×10^3	13.5	-	-	8.3	< 1000	4
DABNA-2	1.48×10^4	20.2	-	-	15.1	< 1000	
TBN-TPA	-	32.1	13.9	-	30.0	16593	5
t-DABNA	2.4×10^3	25.1	-	-	14.7	< 1000	6
ν-DABNA	2.0×10^5	34.4	26.0	-	25.6	< 4000	7
ν-DABNA (HF)	-	33.8	29.1	-	-	< 20000	8
2F-BN	2.4×10^4	22.0	15.0	-	69.8	20000	9
3F-BN	3.9×10^4	22.7	21.1	-	72.3	20000	
4F-BN	4.4×10^4	20.9	16.4	-	51.3	20000	
ADBNA-Me- Mes	7.6×10^3	16.2	-	-	19.3	< 1000	10
ADBNA-Me- Tip	9.0×10^3	21.4	-	-	28.7	< 1000	
AZA-BN	7.53×10^3	28.2	19.1	-	121.7	10000	11
m-Cz-BNCz	$\sim 1.0 \times 10^6$	31.4	17.5	-	127.4	26230	12
BBCz-DB	1.9×10^4	29.3	-	-	-	< 2000	13
BBCz-SB	1.4×10^4	27.8	-	-	-	< 3000	
BBCz-G	1.8×10^5	31.8	-	-	-	< 20000	
BBCz-Y	1.0×10^5	29.3	-	-	-	< 20000	
BBCz-R	1.2×10^4	22.0	-	-	-	< 1000	14
3-Ph-QAD	1.2×10^4	19.1	-	-	32.9	4975	
7-Ph-QAD	6.4×10^3	18.7	-	-	28.2	2944	15
DiKTa	4.6×10^4	14.7	3.3	-	-	10385	
Mes₃DiKTa	3.1×10^4	21.1	4.5	-	-	12949	3
2PXZBN	1.0×10^5	17.7	7.4	-	58.3	11910	
2PTZBN	2.8×10^5	25.5	17.2	-	86.6	16720	16
ν-DABNA-O- Me	1.6×10^5	29.5	26.9	-	22.7	< 20000	
R-BN	6.7×10^4	28.1	-	-	-	-	17
R-TBN	4.5×10^4	27.6	-	-	-	-	
BN1	1.9×10^5	24.3	12.9	-	65.3	6636	18
BN2	1.5×10^5	24.5	7.6	-	83.1	6286	
BN3	1.4×10^5	24.7	8.9	-	106.4	5004	
DABNA-NP- TB	1.4×10^4	19.5	12.0	-	16.1	< 10000	19
Cz2DABNA- NP-M/TB	7.3×10^4	21.8	14.9	-	26.0	< 10000	
CzB2-M/P	5.1×10^4	26.7	18.0	-	62.6	< 10000	
BSBS-N1	1.9×10^6	21.0	-	-	-	< 4000	20
DtCzB-DPT	1.0×10^3	24.6	4.7	-	92.7	16180	21

RZ							
DtCzB-TPT RZ	1.1×10^4	29.8	12.4	-	98.8	16550	
DtCzB-PPm	1.0×10^4	28.6	10.2	-	92.1	13280	
DtCzB-CNP m	1.4×10^3	25.0	5.7	-	107.4	13390	
CNCz-BNCz	4.2×10^5	23.0	5.4	-	65.4	-	
CNCz-BNCz (HF)	-	33.7	16.4	-	117.8	-	22
BN-DMAC	9.6×10^4	21.1	12.5	-	43.4	< 10000	
BN-DPAC	1.3×10^5	28.2	19.2	-	63.2	< 10000	23
(R)-OBN-2C N-BN	9.5×10^3	29.4	8.1	-	70.5	6617	
(R)-OBN-4C N-BN	8.3×10^3	24.5	2.1	-	74.1	2982	
(R)-OBN-2C N-BN (HF)	-	29.8	21.2	-	79.8	27200	24
(R)-OBN-4C N-BN (HF)	-	24.7	13.1	-	81.1	9052	
(+)-BN4	1.6×10^5	20.6	10.7	-	38.6	3334	
(-)-BN4		19.0	10.1	-	35.2	3037	
(+)-BN5	7.4×10^4	22.0	10.9	-	36.5	2950	
(-)-BN5		26.5	11.1	-	44.5	3062	25
DtBuCzB	1.8×10^4	27.5	24.1	-	-	< 30000	
S-Cz-BN	1.8×10^4	30.5	26.2	-	-	< 30000	26
D-Cz-BN	3.0×10^4	37.2	34.3	-	-	< 50000	
BN-CP1	1.56×10^4	40.0	18.5	-	109.7	54753	
BN-CP2	1.43×10^4	36.4	19.2	-	108.1	57582	27

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