Electronic Supplementary Material (ESI) for Materials Chemistry Frontiers.

Supporting information

Purely Organic Phosphor Sensitization for Efficiency Improvement in Yellow Fluorescent Organic Light-Emitting Diode

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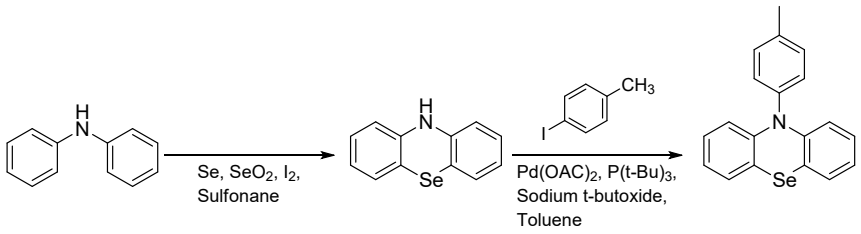
Synthesis and analysis

Materials and measurements

Selenium, diphenylamine, sulforane, sodium tert-butoxide, 1-iodo-4-methyl benzene, 9H-carbazole, N-bromosuccinimide (NBS), dimethylformamide (DMF), toluene, selenium dioxide, iodine, toluene (Samchun pure chemical Co.), palladium(II) acetate (GOM tech Co), and tri-tert-butyl phosphine (INCO) were used as received. The method of analysis is presented in a previous paper.[29]

Synthesis and analysis

The synthetic routes of 10-(P-tolyl)-10H-phenoselenazine have been described in previous work.[15]

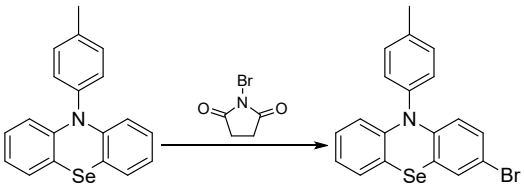


Scheme 1. Synthesis scheme of 10-(P-tolyl)-10H-phenoselenazine

Synthesis of 3-bromo-10-(p-tolyl)-10H-phenoselenazine

10-(P-tolyl)-10H-phenoselenazine (5g, 14.87 mmol) and NBS (3.18g, 17.84 mmol) were dissolved in DMF (20ml). The mixture was stirred overnight at room temperature. After the reaction, the mixture was purified by silica gel column chromatography using a n-hexane : MC as an eluent. Yield 40%,

^{1}H NMR (500 MHz, DMSO-d_6) δ 7.50 (d, J = 2.5 Hz, 1H), 7.41 (d, J = 8 Hz, 2H), 7.27 (m, 3H), 7.15 (m, 1H), 6.99 (m, 1H), 6.89 (m, 1H), 6.39 (m, 1H), 6.30 (d, J = 8.5 Hz, 1H), 2.39 (s, 3H).

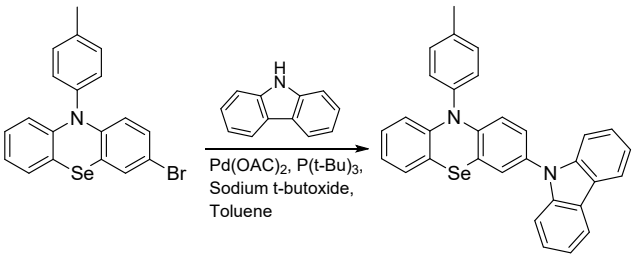


Scheme 2. Synthesis scheme of 3-bromo-10-(p-tolyl)-10H-phenoselenazine

Synthesis of 3-(9H-carbazol-9-yl)-10-(p-tolyl)-10H-phenoselenazine

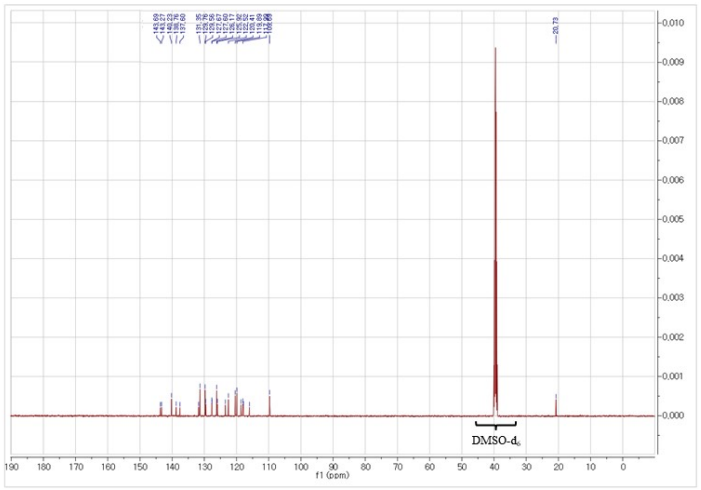
3-Bromo-10-(p-tolyl)-10H-phenoselenazine (0.50 g, 1.20 mmol), 9H-carbazole (0.24 g, 1.44 mmol), sodium tert-butoxide (0.29 g, 3 mmol), palladium(II) acetate (0.027 g, 0.12 mmol) and tri-tert-butyl phosphine (0.024 g, 0.12mmol) were dissolved in toluene (10 mL). The reaction mixture was refluxed under nitrogen at 300 °C for 24 h. Then, the mixture was purified by silica gel column chromatography using a n-hexane : MC. Yield 60%. HRMS (FAB): calcd for 502.0948m/z, found 502.0950 m/z.

^{1}H NMR (500 MHz, DMSO-d_6) δ 8.17 (d, J = 7.7 Hz, 2H), 7.53 (d, J = 2.5 Hz, 1H), 7.43 (d, J = 8.1 Hz, 2H), 7.39 – 7.33 (m, 4H), 7.32 – 7.26 (m, 3H), 7.25 – 7.17 (m, 3H), 7.04 – 6.97 (m, 1H), 6.89 (td, J = 7.4, 1.2 Hz, 1H), 6.60 (d, J = 8.7 Hz, 1H), 6.43 (dd, J = 8.3, 1.1 Hz, 1H), 2.39 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 144.24, 143.82, 140.78, 138.27, 138.15, 132.34, 131.89, 130.31, 130.11, 128.22, 128.15, 126.72, 126.47, 124.03, 123.07, 120.96, 120.44, 119.17, 118.54, 118.40, 116.52, 110.23.



Scheme 3. Synthesis scheme of 3-(9H-carbazol-9-yl)-10-(p-tolyl)-10H-phenoselenazine

(a)



(b)

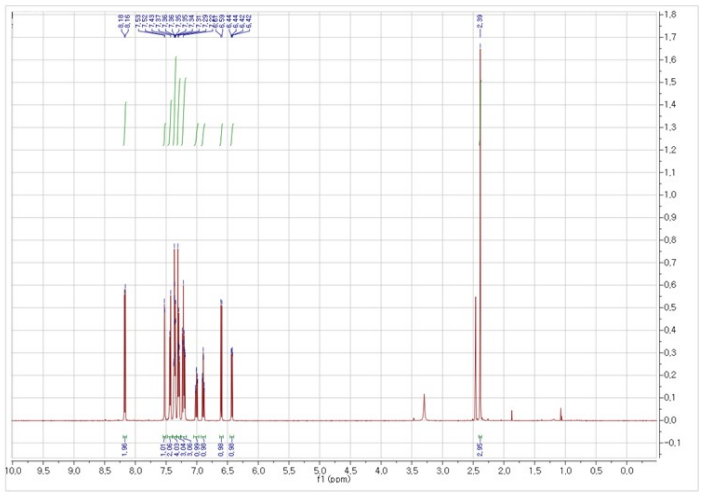


Figure S1. (a) 1H-NMR and (b) 13C-NMR spectra of PSez9Cz

Supplementary Figures

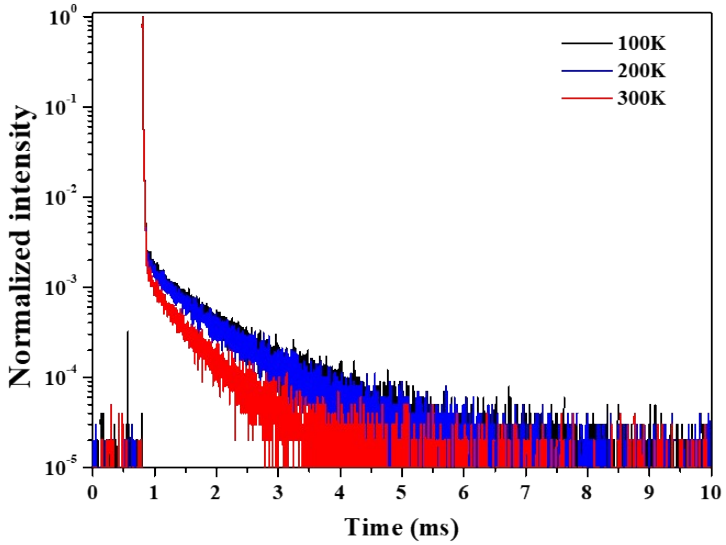


Figure S2. Temperature dependent TRPL curves of 10 w% PSez9Cz doped mixed host film Detection wavelength was 513 nm.

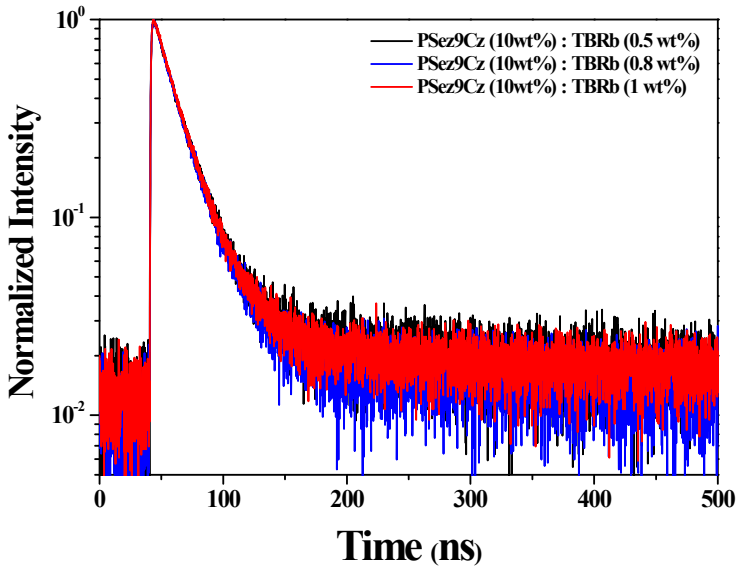


Figure S3. TRPL curves of 10 w% PSez9Cz doped film with and without TBRb dopant. Detection wavelength was 560 nm.

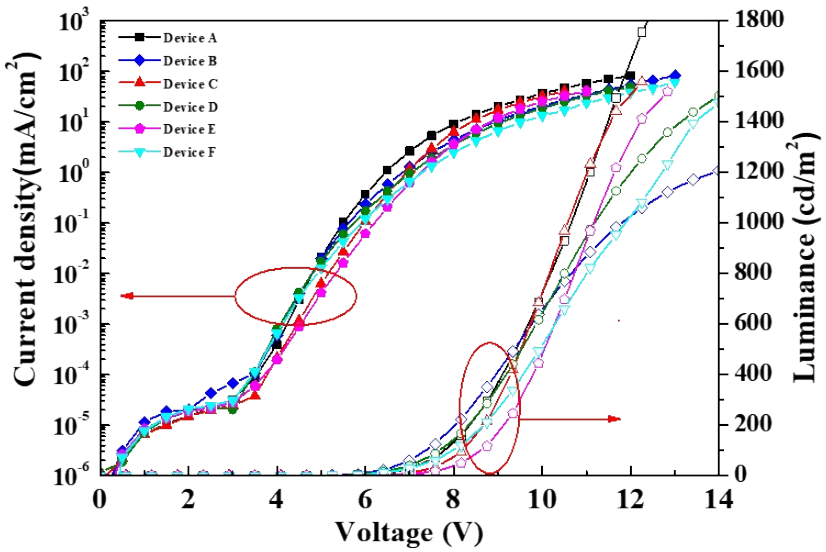
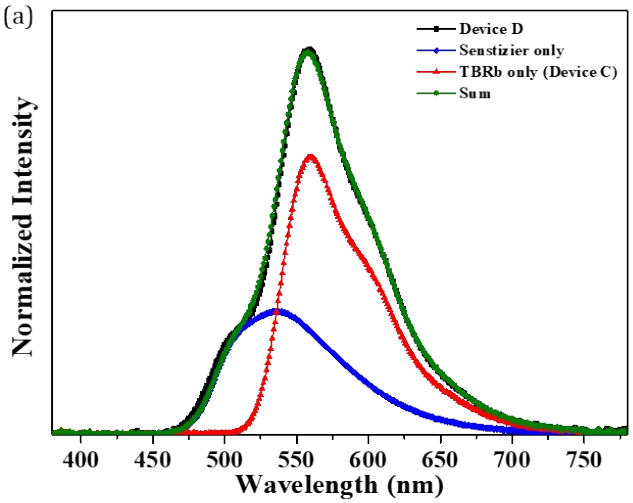


Figure S4. Current density and luminance - voltage curves of RTPH sensitized yellow hyperfluorescent OLEDs



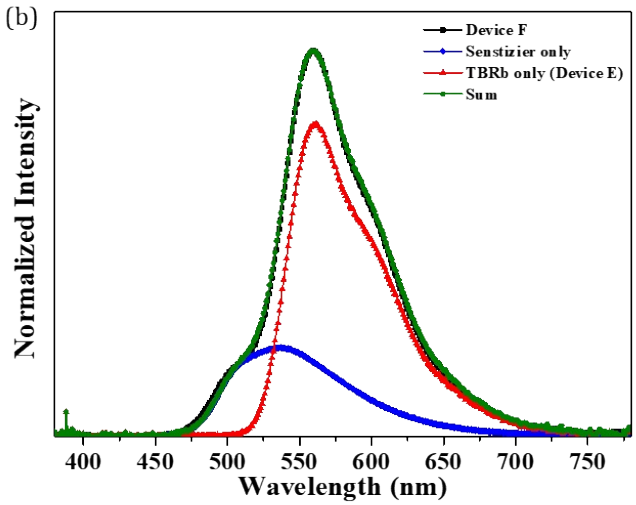


Figure S5. Deconvoluted EL spectrum of (a) Device D and (b) Device F

Table S1. Comparison between experimental EQE and calculated EQE from area of the deconvoluted spectra.

	Sensitizer only	0.8 wt%	1.0 wt%
Sensitizer only Max. EQE (%)	11.4	-	-
TBRb only Max. EQE (%)	-	2.8	2.8
Sensitizer area ratio (%)	-	36.9	27.1
TBRb area ratio (%)	-	63.1	72.9
Sum of EQE (%)[(a)]	-	6.0	5.1
Experimental Max. EQE (%)	11.4	8.1	7.6

(a) Sum of EQE = (Maximum EQE of the sensitizer only device multiplied by sensitizer area ratio) + (Maximum EQE of the TBRb only device multiplied by TBRb area ratio)