Supplementary Information

3PTZ and 3PXZ small molecular hole-transporting materials in polymer light-emitting diodes

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1. C-V curves and UV-vis spectra of 3PXZ and 3PTZ.

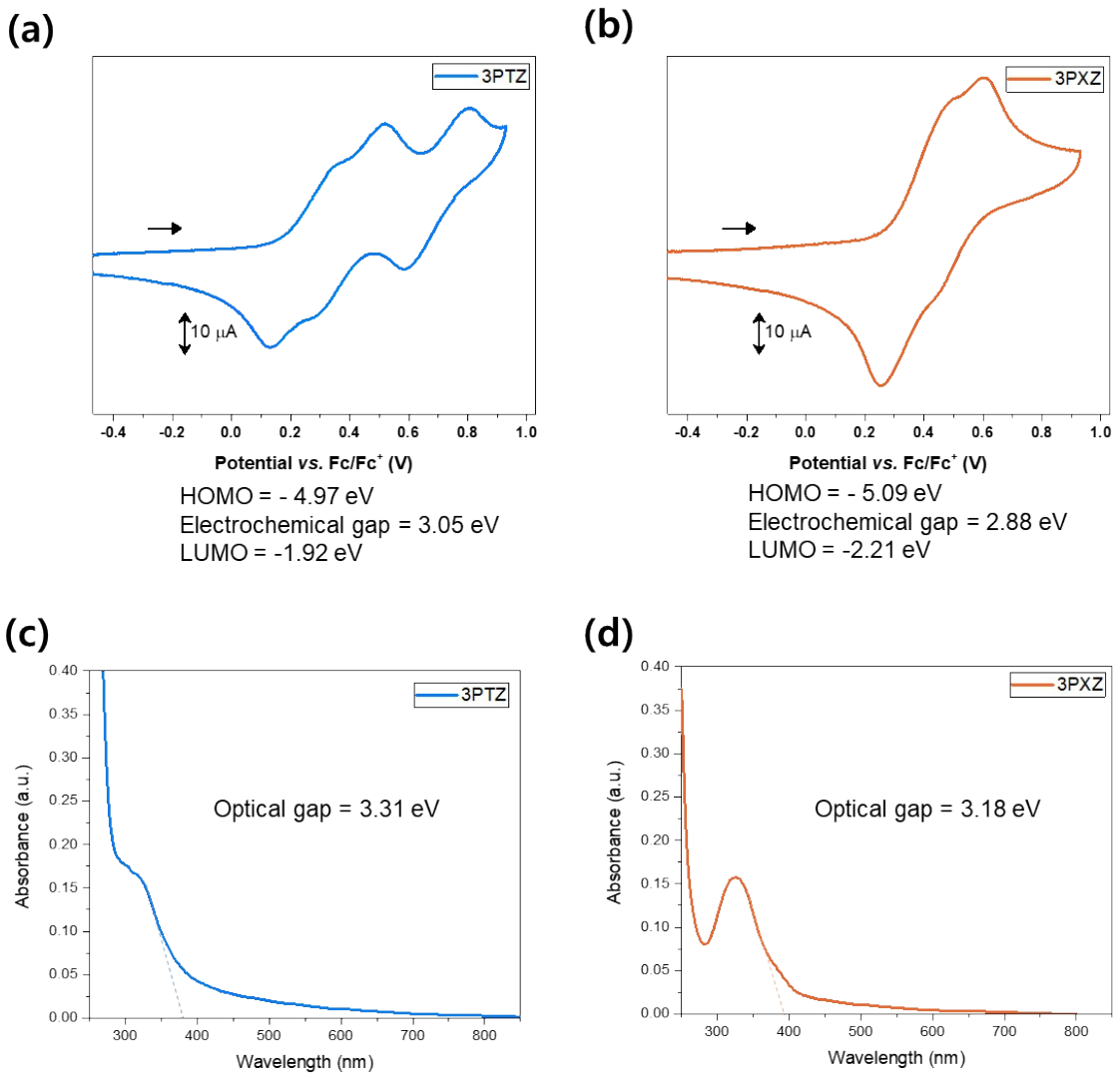

Figure S1. C-V curves (a, b) and UV-vis spectra (c, d) of 3PXZ and 3PTZ

Figure S1(a) and (b) show that the HOMO and LUMO levels of the 3PTZ and 3PXZ were obtained from a CV measurement at a scan rate of 20 $mV \cdot s^{-1}$. The HOMO and LUMO levels were calculated from the oxidation initiation potential (E_{ox}') and the reduction initiation potential (E_{red}'). The HOMO levels of the 3PTZ and 3PXZ were calculated to be 4.97 and 5.09 eV from the following equation:

$$E_{HOMO} = -I_P = -\left(E_{ox}' + 4.14\right)(eV),$$

where I_P is the ionization potential. The LUMO levels of the 3PTZ and 3PXZ were calculated

as 1.92 and 2.21 eV by the following equation:

$$E_{LUMO} = -E.A. = -\left(E_{red}^{'} + 4.14\right)(eV),$$

where E.A. is the electron affinity.

The optical gaps of the 3PTZ and 3PXZ were derived through the UV-vis spectra with Tauc plot equation to 3.31 and 3.18 eV as shown Figure S1(c) and (d).

2. AFM images of spin-coated and thermally evaporated 3PXZ films.

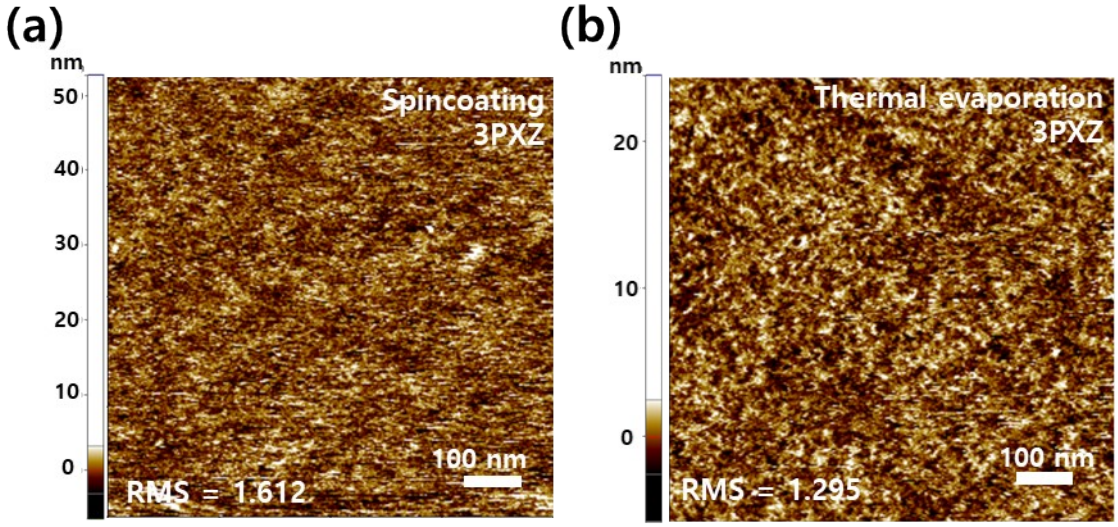

Figure S2. AFM images of (a) spin-coated and (b) thermally evaporated 3PTZ films.

3. Schematic illustration of energy band diagram of PLEDs including poly-TPD.

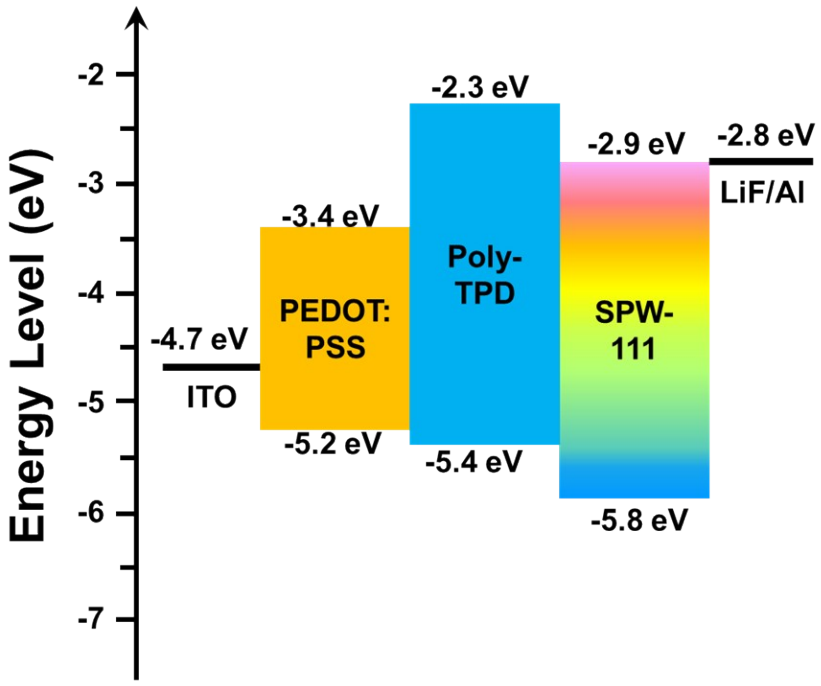

Figure S3. Schematic illustration of energy band diagram of PLED with poly-TPD HTL

4. TEM image of 3PXZ

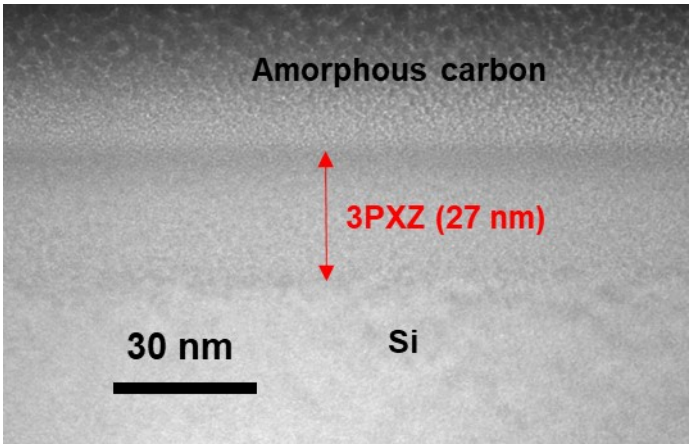

Figure S4. TEM image of 3PXZ on Si substrate

5. CIE coordinates of PLEDs.

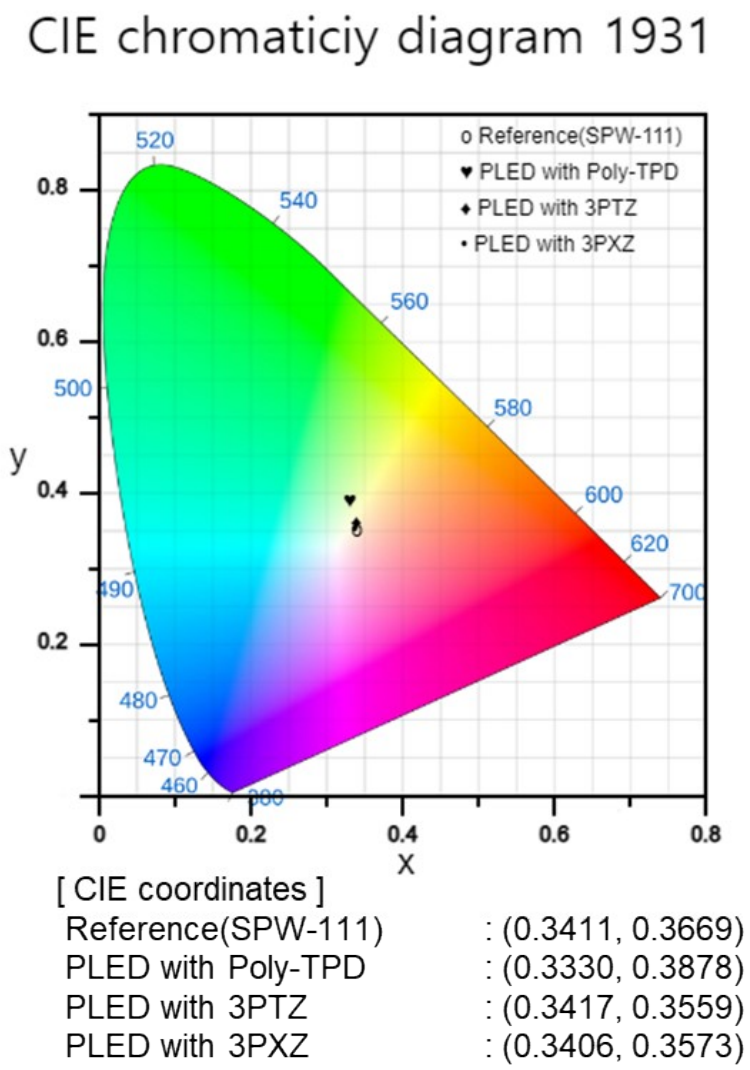

Figure S5. CIE coordinates of reference PLED, the PLED with poly-TPD, the PLED with 3PTZ, and the PLED with 3PXZ.

6. Calculated mobilities of 3PXZ and 3PTZ.

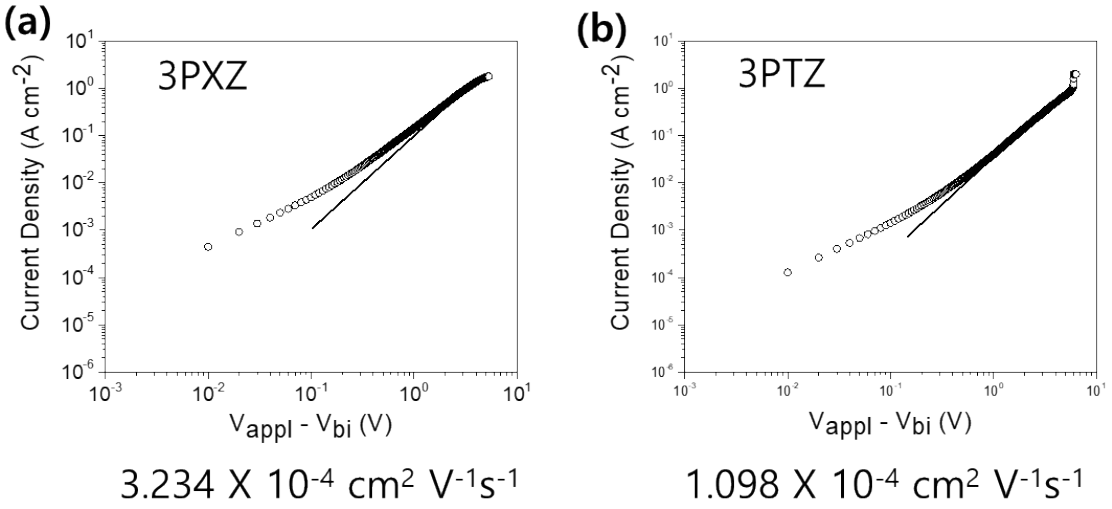

Figure S6. Calculated mobilities of (a) 3PXZ and (b) 3PTZ

In order to calculate the charge carrier mobilities of 3PXZ and 3PTZ, the J-V curves of organic devices(Glass/ITO/PEDOT:PSS/small molecular material/MoO_3/Ag) were investigated. The carrier mobilities of 3PXZ and 3PTZ are calculated using Mott-Gurney law (1) from SCLC of fitted J-V curve[1, 2]. The Mott-Gurney law is:

$$J = \frac{9}{8}\varepsilon\varepsilon_0\mu\frac{V^2}{L^3} \tag{1}$$

where J is the current density, ε is the relative dielectric constant of organic device, ε_0 is the permittivity of free space, μ is the charge carrier mobility, V is the voltage drop across the device ($V = V_{appl} - V_{bi}$, where V_{appl} is the applied voltage and V_{bi} is the built-in voltage), and L is the thickness of the device.

[1] C. Goh, R. J. Kline, M. D. McGehee, E. N. Kadnikova, J. M. Frechet, Molecular-weight-dependent mobilities in regioregular poly(3-hexyl-thiophene) diodes, J. Appl. Phys. Lett. 2005, 86 (2005) 122110, https://doi.org/10.1063/1.1891301

[2] P. W. M. Blom, M. J. M. de Jong, M. G. van Munster, Electric-field and temperature dependence of the hole mobility in poly(p-phenylene vinylene), Phys. Rev. B 55 (1997) R656(R), https://doi.org/10.1103/PhysRevB.55.R656

Table 1. Work function, HOMO, and LUMO results of 3PTZ and 3PXZ by using UPS and IPES measuring equipment.

	3PXZ	3PTZ
Work Function	4.516 eV	4.473 eV
E_F – HOMO	0.846 eV	0.952 eV
E_F – LUMO	2.605 eV	2.614 eV
(Transport) Band Gap	3.451 eV	3.566 eV
HOMO (IE)	5.362 eV	5.425 eV
LUMO (EA)	1.911 eV	1.859 eV

Table S1. Work function, HOMO, and LUMO results of 3PTZ and 3PXZ by using UPS and IPES

Table 2. Optical properties of PLEDs with 3PTZ and 3PXZ with different thickness

	Maximum luminance (cd/m^2)	Current efficiency (cd/A)	Power efficiency (lm/W)	Quantum efficiency
20 nm of 3PTZ	2672 @ 11 V	0.47 @ 8.5 V	0.18 @ 7.5 V	0.22 @ 8.5 V
27 nm of 3PTZ	2808 @ 12.5 V	1.07 @ 9.5 V	0.38 @ 8 V	0.53 @ 9.5 V
40 nm of 3PTZ	3023 @ 11 V	0.63 @ 8.5 V	0.26 @ 7 V	0.31 @ 8.5 V
20 nm of 3PXZ	1158 @ 18 V	0.72 @ 14 V	0.17 @ 12.5 V	0.39 @ 14 V
27 nm of 3PXZ	2755 @ 13 V	0.97 @ 10 V	0.33 @ 8.5 V	0.49 @ 10 V
40 nm of 3PXZ	1319 @ 19.5 V	0.89 @ 14 V	0.22 @ 11 V	0.50 @ 14 V

Table S2. Optical properties of PLEDs with 3PTZ and 3PXZ with different thickness.

Table 3. CIE coordinates of reference PLED, PLED with poly-TPD, PLED with 3PTZ, and PLED with 3PXZ with applied voltages.

	voltage (V)	x	Y
Reference PLED	6	0.3699	0.3929
	8	0.3541	0.3955
	10	0.3468	0.3941
	12	0.3421	0.3862
	14	0.328	0.3582
PLED with Poly-TPD	6	0.3224	0.3848
	8	0.311	0.3719
	10	0.3117	0.3531
	12	0.3037	0.274
	14	0.2959	0.2959
PLED with 3PTZ	6	0.3614	0.3855
	8	0.3499	0.3858
	10	0.3416	0.3853
	12	0.3397	0.3788
	14	0.3516	0.3564
PLED with 3PXZ	6	0.3633	0.3846
	8	0.3483	0.3853
	10	0.3398	0.3843
	12	0.3375	0.3778
	14	0.3462	0.3528

Table S3. CIE coordinates of reference PLED, PLED with poly-TPD, PLED with 3PTZ, and PLED with 3PXZ with applied voltages.