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Materials characterization

^{1}H NMR was recorded using Avance 300 MHz and DRX 500MHz NMR Bruker spectrometers, and chemical shifts are reported in ppm units with tetramethylsilane as the internal standard. Thermogravimetric analysis (TGA) was performed under nitrogen on a TA Instruments 2050 thermogravimetric analyzer. The sample was heated at 10 °C**.**min^{-1} from 50 to 800 °C. The differential scanning calorimeter (DSC) was conducted under nitrogen in a TA Instruments 2100 differential scanning calorimeter. The sample was heated at 10 °C·min^{-1} from 30 to 350 °C. Mass spectra were measured using a Jeol JMS-700 mass spectrometer. UV−vis absorption spectra were measured using a Perkin-Elmer LAMBDA-900 UV−vis−NIR spectrophotometer and an LS-50B luminescence spectrophotometer, respectively. All of the devices were grown on glass substrates pre-coated with a 130 nm thick layer of indium tin oxide (ITO) with a sheet resistance of 15 Ω/square. The substrates were cleaned with ultra-purified water and organic solvents and then dry-cleaned for 30 min by exposure to a UV-ozone ambient. The organic compounds were successively deposited onto the ITO substrate under a vacuum (~10-5 Pa). LiF and Al were patterned using a shadow mask with an array of openings (2 mm × 2 mm) without breaking the vacuum (~10-5 Pa). All of the devices were encapsulated under a nitrogen atmosphere immediately after preparation using epoxy glue and glass lids. The PLQEs were measured on a Hamamatsu C9920-01 integral sphere system under nitrogen. The EL spectra were collected using an optical multichannel analyzer (Hamamatsu Photonics PMA-11). The current density–voltage and luminance–voltage characteristics were measured using a Keithley 2400 source measurement unit and a Minolta CS200 luminance-meter, respectively. The external quantum efficiencies were calculated from the front luminance, the current density, and the EL spectrum. The transient EL decay was measured with using a function generator (33220A, Agilent), an oscilloscope (DPO 3052, Tektronix), and an Si photodetector.

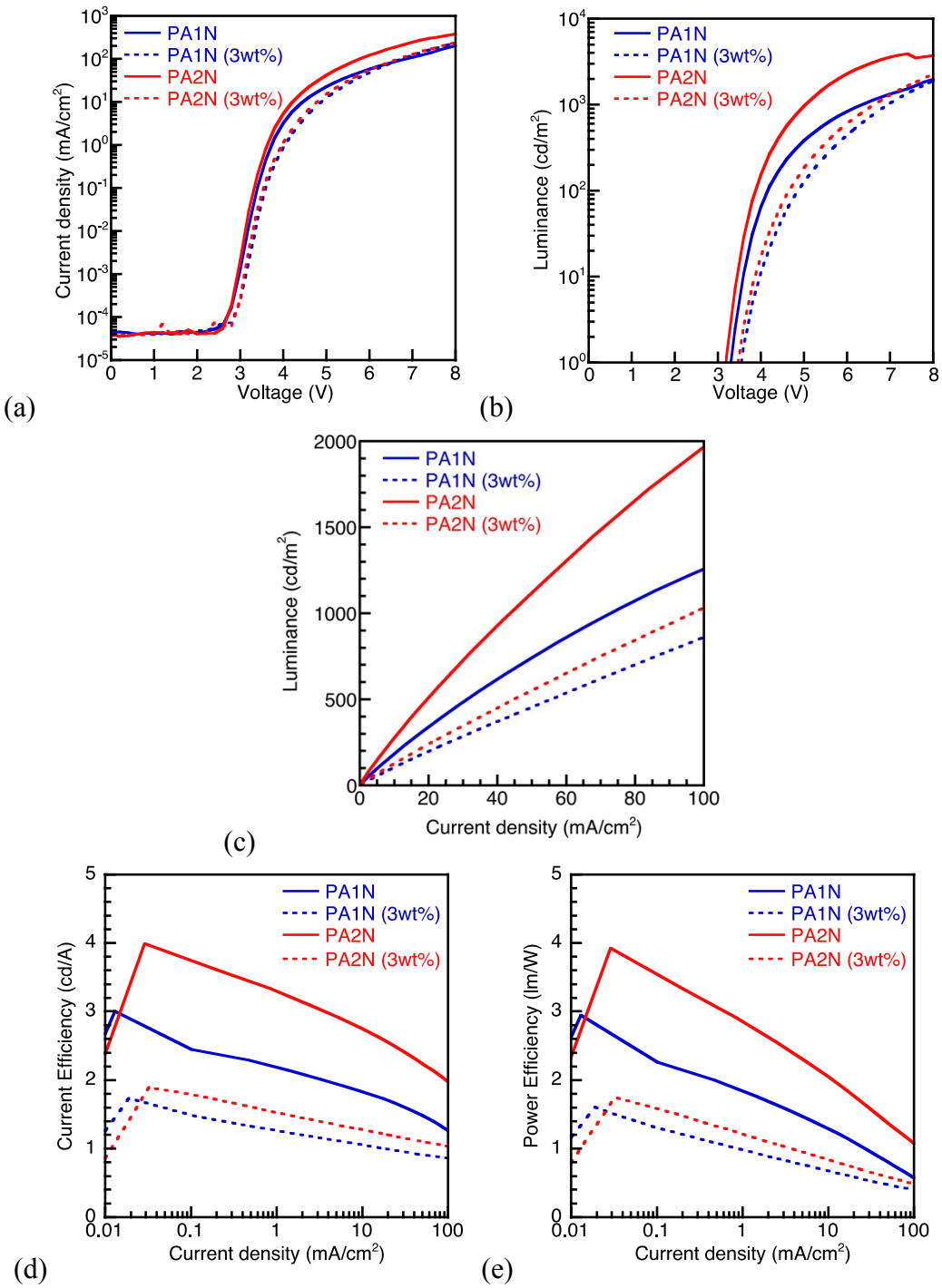
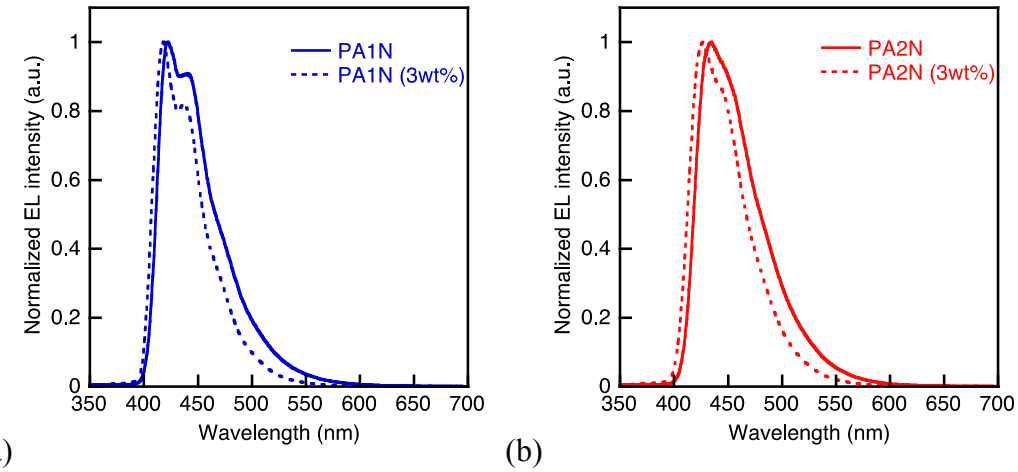
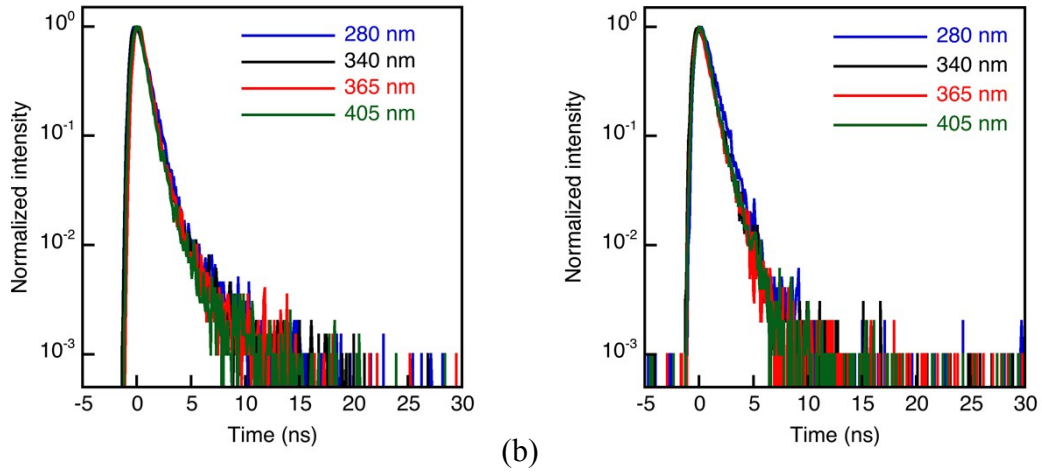


Figure S4. Characteristics of of the devices: (a) current density–voltage plot, (b) luminance–voltage plot, (c) luminance–current density plot, (d) current efficiency–current density plot, and (e) power efficiency–current density plot.



(a) (b)

Figure S5. (a) EL spectra of the PA1N device, and (b) EL spectra of the PA2N device.



(a) (b)

Figure S6. Fluorescence lifetime of (a) PA1N and (b) PA2N at several emission wavelength.

Table S1. Calculated energy levels, oscillator strengths (f), and orbital transition analyses for PA1N.

excited state	E_g (eV)	E_g (nm)	f	transition (An: anthracene unit, Py: pyrene unit, Np: Naphthalene unit)			CI coefficient
S_1	3.0552	405.81	0.2287	An: HOMO	–>	An: LUMO	0.69974
S_2	3.2623	380.05	0.0000	An: HOMO	–>	Py: LUMO+1	0.70653
S_3	3.3318	372.12	0.0002	Py: HOMO-1	–>	An: LUMO	0.70678
S_4	3.3976	364.91	0.0001	An: HOMO	–>	Np: LUMO+2	0.70494
S_5	3.4518	359.19	0.0002	Np: HOMO-2	–>	An: LUMO	0.70283
S_6	3.5308	351.15	0.4275	Py: HOMO-1	–>	Py: LUMO+1	0.67759
				HOMO-3	–>	LUMO+3	-0.18399
S_7	3.6756	337.32	0.0009	HOMO-3	–>	Py: LUMO+1	0.49523
				Py: HOMO-1	–>	LUMO+3	0.49250
S_8	3.7381	331.67	0.0010	HOMO-4	–>	An: LUMO	-0.45613
				An: HOMO	–>	LUMO+3	0.13208
				An: HOMO	–>	LUMO+4	0.48403
				An: HOMO	–>	LUMO+8	-0.13619
S_9	3.9555	313.45	0.0066	An: HOMO	–>	LUMO+5	0.69788
S_{10}	3.9757	311.85	0.0000	Np: HOMO-2	–>	Py: LUMO+1	0.70675
T_1	1.7299	716.73	0.0000	An: HOMO	–>	An: LUMO	0.69885
				An: HOMO	<–	An: LUMO	0.13229
T_2	2.0839	594.95	0.0000	HOMO-8	–>	LUMO+7	0.10657
				HOMO-3	–>	LUMO+3	-0.11802
				Py: HOMO-1	–>	Py: LUMO+1	0.68651
				Py: HOMO-1	<–	Py: LUMO+1	0.11195
T_3	2.6847	461.82	0.0000	HOMO-11	–>	LUMO+15	0.12084
				Np: HOMO-2	–>	Np: LUMO+2	0.67603
				Np: HOMO-2	<–	Np: LUMO+2	0.10187
T_4	3.2138	385.79	0.0000	HOMO-9	–>	An: LUMO	-0.29878
				HOMO-7	–>	An: LUMO	-0.28540
				HOMO-5	–>	An: LUMO	-0.23690
				Np: HOMO-2	–>	An: LUMO	-0.25724
				An: HOMO	–>	Py: LUMO+1	-0.10318
				An: HOMO	–>	LUMO+6	-0.21955
				An: HOMO	–>	LUMO+11	0.31126
T_5	3.2625	380.03	0.0000	An: HOMO	–>	Py: LUMO+1	0.69759
T_6	3.3315	372.16	0.0000	Py: HOMO-1	–>	An: LUMO	0.70364
T_7	3.3684	368.08	0.0000	HOMO-3	–>	Py: LUMO+1	0.56132
				Py: HOMO-1	–>	LUMO+3	-0.40333
T_8	3.3828	366.51	0.0000	HOMO-4	–>	An: LUMO	-0.23742
				An: HOMO	–>	Np: LUMO+2	0.58117
				An: HOMO	–>	LUMO+4	-0.24054
				An: HOMO	–>	LUMO+8	0.12300
T_9	3.4009	364.56	0.0000	HOMO-5	–>	An: LUMO	0.12433
				HOMO-4	–>	An: LUMO	0.37725
				Np: HOMO-2	–>	An: LUMO	-0.2570
				An: HOMO	–>	Np: LUMO+2	0.39038
				An: HOMO	–>	LUMO+4	0.29385
				An: HOMO	–>	LUMO+8	-0.13910
T_{10}	3.4733	356.96	0.0000	HOMO-7	–>	An: LUMO	-0.10342
				Np: HOMO-2	–>	An: LUMO	0.55961
				An: HOMO	–>	LUMO+4	0.31703
				An: HOMO	–>	LUMO+6	-0.13126
				An: HOMO	–>	LUMO+8	-0.10240
				An: HOMO	–>	LUMO+11	0.10836

Table S2. Calculated energy levels, oscillator strengths (f), and orbital transition analyses for PA2N.

excited state	E_g (eV)	E_g (nm)	f	transition (An: anthracene unit, Py: pyrene unit, Np: Naphthalene unit)			CI coefficient
S_1	3.0695	403.93	0.2422	An: HOMO	–>	An: LUMO	0.69971
S_2	3.2626	380.01	0.0000	An: HOMO	–>	Py: LUMO+1	0.70657
S_3	3.3465	370.49	0.0001	Py: HOMO-1	–>	An: LUMO	0.70681
S_4	3.4256	361.93	0.0027	An: HOMO	–>	Np: LUMO+2	0.69616
S_5	3.5310	351.13	0.4301	HOMO-3	–>	LUMO+3	0.18474
				Py: HOMO-1	–>	Py: LUMO+1	0.67763
S_6	3.5879	345.56	0.0003	Np: HOMO-2	–>	An: LUMO	0.69862
S_7	3.6756	337.32	0.0009	HOMO-3	–>	Py: LUMO+1	0.49530
				Py: HOMO-1	–>	LUMO+3	-0.49387
S_8	3.7683	329.02	0.0003	HOMO-4	–>	An: LUMO	0.45405
				An: HOMO	–>	LUMO+3	0.13747
				An: HOMO	–>	LUMO+4	-0.27898
				An: HOMO	–>	LUMO+5	0.39266
				An: HOMO	–>	LUMO+8	0.13622
S_9	3.9637	312.80	0.0013	An: HOMO	–>	LUMO+4	0.57717
				An: HOMO	–>	LUMO+5	0.40139
S_{10}	3.9759	311.84	0.0000	Py: HOMO-1	–>	Np: LUMO+2	0.70684
T_1	1.7359	714.24	0.0000	An: HOMO	–>	An: LUMO	0.69889
				An: HOMO	<–	An: LUMO	0.13256
T_2	2.0841	594.91	0.0000	HOMO-8	–>	LUMO+7	-0.10651
				HOMO-3	–>	LUMO+3	0.11853
				Py: HOMO-1	–>	Py: LUMO+1	0.68653
				Py: HOMO-1	<–	Py: LUMO+1	0.11195
T_3	2.7208	455.69	0.0000	HOMO-5	–>	LUMO+6	0.14526
				Np: HOMO-2	–>	Np: LUMO+2	0.66698
T_4	3.2168	385.43	0.0000	HOMO-9	–>	An: LUMO	0.29631
				HOMO-7	–>	An: LUMO	0.32522
				HOMO-5	–>	An: LUMO	-0.14537
				Np: HOMO-2	–>	An: LUMO	-0.15970
				An: HOMO	–>	Np: LUMO+2	0.25599
				An: HOMO	–>	LUMO+6	0.12865
				An: HOMO	–>	LUMO+8	-0.18605
				An: HOMO	–>	LUMO+10	0.15319
				An: HOMO	–>	LUMO+11	0.25634
				An: HOMO	–>	LUMO+15	0.10870
T_5	3.2623	380.06	0.0000	An: HOMO	–>	Py: LUMO+1	0.69644
T_6	3.3434	370.83	0.0000	HOMO-7	–>	An: LUMO	-0.13289
				HOMO-4	–>	An: LUMO	0.23147
				Np: HOMO-2	–>	An: LUMO	0.12346
				An: HOMO	–>	Np: LUMO+2	0.47459
				An: HOMO	–>	LUMO+4	0.18523
				An: HOMO	–>	LUMO+5	-0.28940
				An: HOMO	–>	LUMO+8	-0.12220
T_7	3.3463	370.52	0.0000	Py: HOMO-1	–>	An: LUMO	0.69641
T_8	3.3685	368.07	0.0000	HOMO-3	–>	Py: LUMO+1	0.55949
				Py: HOMO-1	–>	LUMO+3	0.40320
T_9	3.4805	356.23	0.0000	HOMO-5	–>	An: LUMO	-0.12100
				HOMO-4	–>	An: LUMO	0.54073
				Np: HOMO-2	–>	An: LUMO	0.12416
				An: HOMO	–>	Np: LUMO+2	-0.36296
T_{10}	3.5041	353.82	0.0000	HOMO-8	–>	Py: LUMO+1	-0.43670
				Py: HOMO-1	–>	LUMO+3	-0.11077
				Py: HOMO-1	–>	LUMO+7	0.50335