Supplementary Material (ESI) for New Journal of Chemistry

Phosphole-based π-conjugated materials for OLEDs

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Table S1. Crystal data and structure refinement for derivative **3b** after the 'squeeze' treatment.

molecular formula	C44 H39 Au Cl P
molecular weight, g/mol	831.14
a, Å	11.2536(9)
b, Å	25.600(3)
c, Å	13.7924(14)
a, deg	90
b, deg	98.022(3)
g, deg	90
V, $Å^3$	3934.6(7)
Z	4
D_{calc}, g cm^{-3}	1.403
crystal system	Monoclinic
space group	P21/n
T, K	100(2)
wavelength Mo Ka, Å	0.71073
m, mm^{-1}	3.875
F(000)	1656
θ limit, deg	1.59 - 26.56
no. reflns collected	31372
no. ind reflns	8060
reflections [I > 2s(I)]	6332
data/restraints/parameters	8060 / 0 / 424
GOF on F^2	1.036
final R indices	R1 = 0.0461
[I > 2s(I)]	wR2 = 0.1266
largest diff peak	2.284
and hole (e $Å^{-3}$)	2.284 -2.328

Table S2. Crystal data and structure refinement for derivative **3b** before the 'squeeze' treatment.

molecular formula	C45 H41 Au Cl3 P
molecular weight, g/mol	916.06
α, Å	11.2536(9)
β, Å	25.600(3)
χ, Å	13.7924(14)
α, deg	90
β, deg	98.022(3)
γ, deg	90
V, $Å^3$	3934.6(7)
Z	4
D_{calc}, g cm^{-3}	1.543
crystal system	Monoclinic
space group	P21/n
T, K	100(2)
wavelength Mo Ka, Å	0.71073
μ, mm^{-1}	4.014
F(000)	1824
θ limit, deg	1.59 - 26.56
no. reflns collected	31372
no. ind reflns	8060
reflections [I > 2σ(I)]	6323
data/restraints/parameters	8060 / 0 / 469
GOF on F^2	1.092
final R indices	R1 = 0.0524
[I > 2σ(I)]	wR2 = 0.1347
largest diff peak	2.175
and hole (e $Å^{-3}$)	-2.430

Table S3 : Electrochemical data for **3a**,**b**, **4a**,**b** and $\mathbf{R_{AuCl}}$ /**Rs** (vs. SCE)

Compounds	E_{ox}/V^{a}	E_{ox}^{onset}/V	E_{red}/V^{a}	E_{red}^{onset}/V	HOMO/eV[b]	LUMO/eV[c]	DE^{EI}/eV^{d}
3a	+ 1.47	+ 1.26	-1.55	- 1.47	- 5.66	- 2.93	2.73
3b	+ 1.37	+ 1.28	-1.58	- 1.51	- 5.68	- 2.89	2.79
4a	+ 1.38	+ 1.18	-1.60	- 1.47	- 5.58	- 2.93	2.65
4b	+ 1.32	+ 1.12	-1.56	- 1.52	- 5.52	- 2.88	2.64
A	+ 1.95	+ 1.40	-1.64	- 1.60	- 5.80	- 2.80	3.00
B	+ 1.62	+ 1.37	-1.58	- 1.61	- 5.77	- 2.79	2.98

[a]All potentials were obtained during cyclic voltametric investigations in 0.2 M Bu_4NPF_6 in CH_2Cl_2. Platinum electrode diameter 1 mm, sweep rate: 200 mV s^{-1}. [b] Calculated from the onset oxidation potential E_{ox}^{onset}/V. [c]Calculated from the onset reduction potential E_{red}^{onset}/V. [d] Calculated as DE^{EI} = HOMO-LUMO from the redox data.

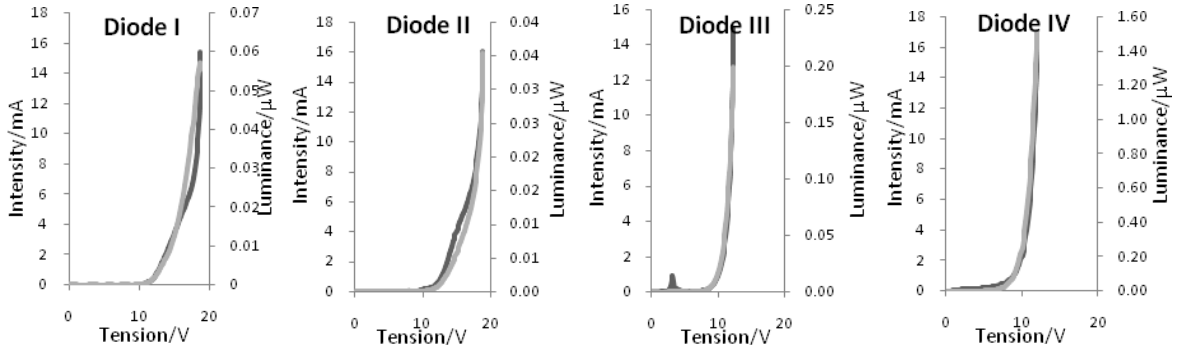

Figure S1 I-V-L characteristics of diodes **I-IV**.

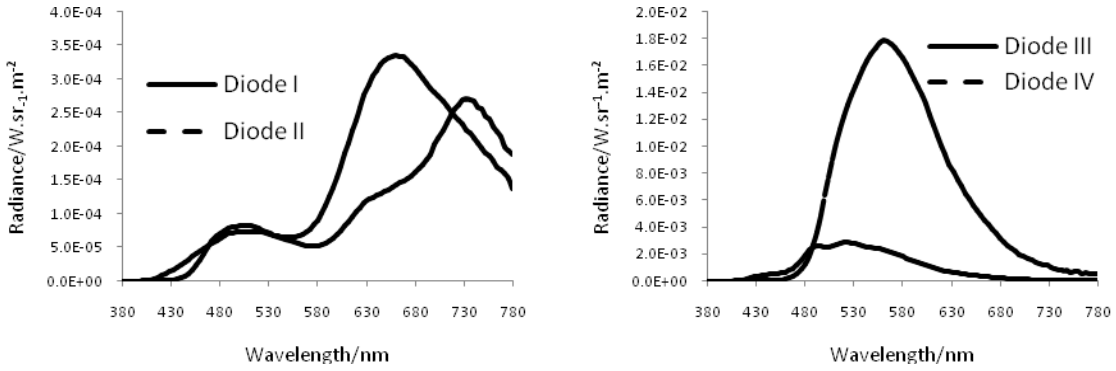

Figure S2 EL spectra of the devices **I-IV** recorded at 30 mA/cm².

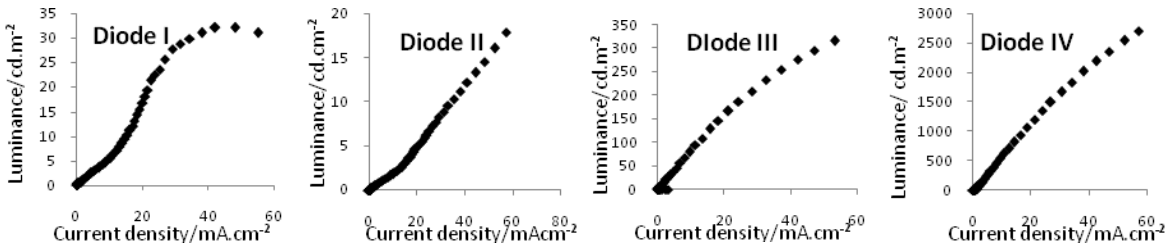

Figure S3 Luminance-current density characteristics of diodes **I-IV**

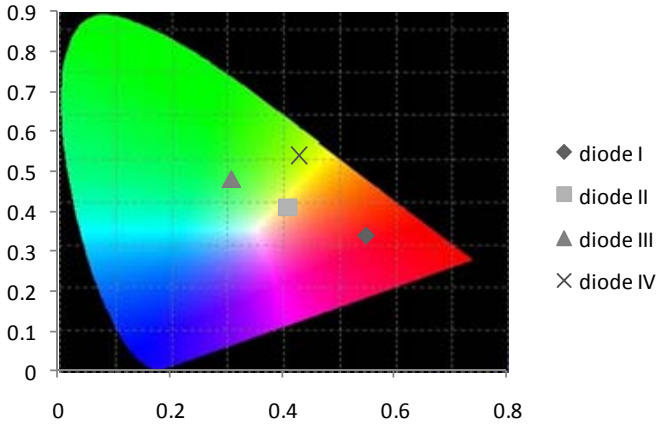

Figure S4 CIE coordinates of diodes **I-IV**.

Compounds	Diodes		B_1 [a]/cd.m^{-2}	B_1 [b]/cd.m^{-2}
		1	28.4	21.1
4a	**III**	2	23.6	17.0
		3	26.2	20.6
		1	120.1	114.3
4b	**IV**	2	118.9	110.5
		3	109.4	97.6

[a] brigthness at 1 mA, measured before IVL measurement; [b] brigthness at 1 mA, measured after IVL measurement

Figure S5 Measurements of the Brigthness at 1 mA before and after IVL Characterizations