Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Dinuclear Platinum(II) Complex Dominated by a Zig-Zag-Type Cyclometalated Ligand：An New Approach to Realize High-efficiency Near Infrared Emission

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Captions of Figures

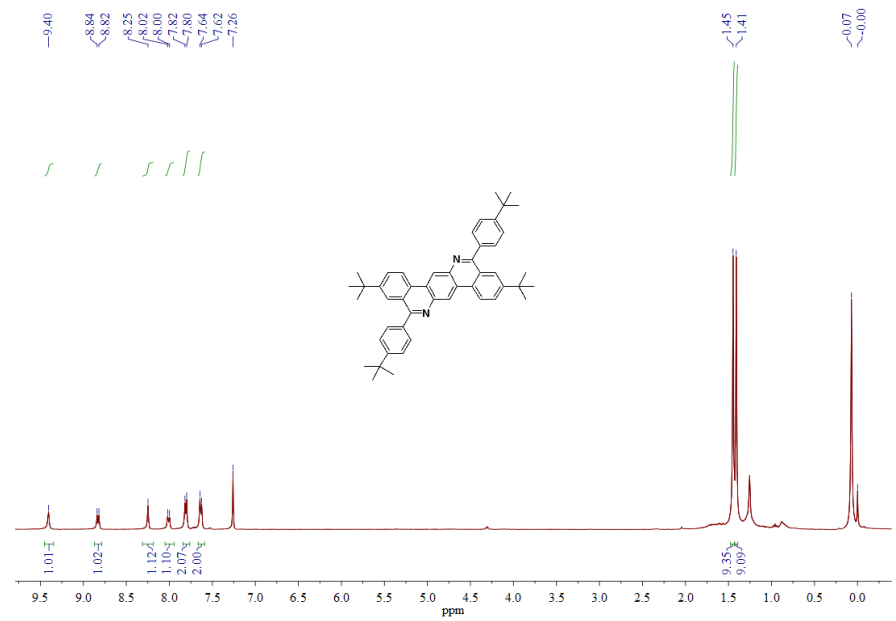


Fig. S1. ^{1}H NMR plot ofBuPh-BDIQ

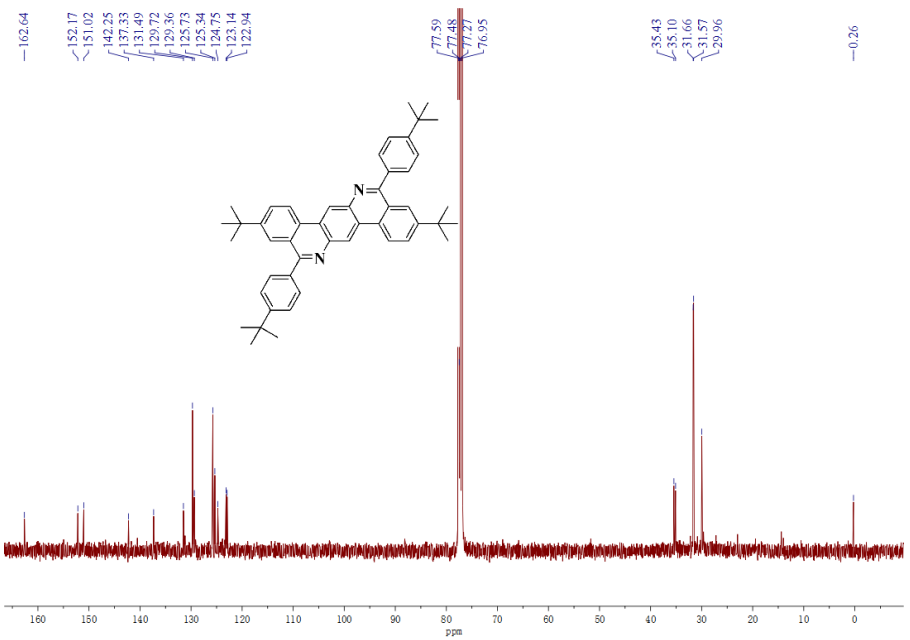


Fig. S2.^{13}C NMR plot ofBuPh-BDIQ

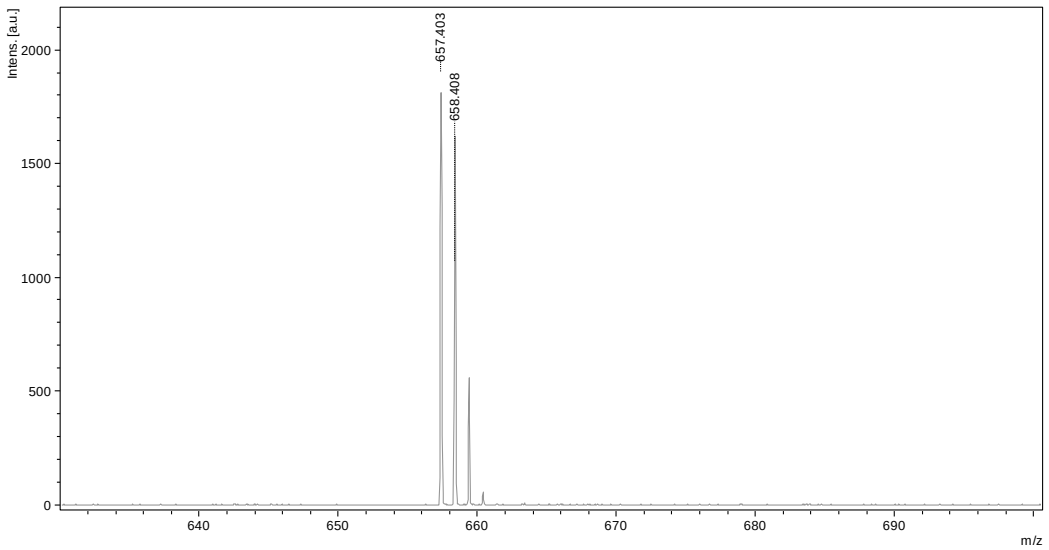


Fig. S3. MALDI-TOF-MS plot of BuPh-BDIQ

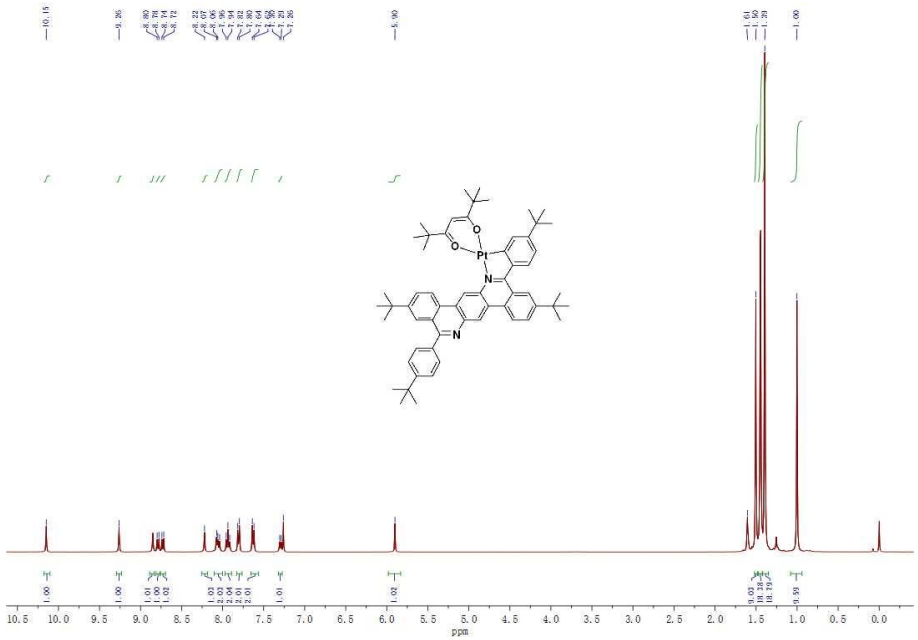


Fig. S4. ^{1}H NMR plot of (BuPh-BDIQ)Ptdpm

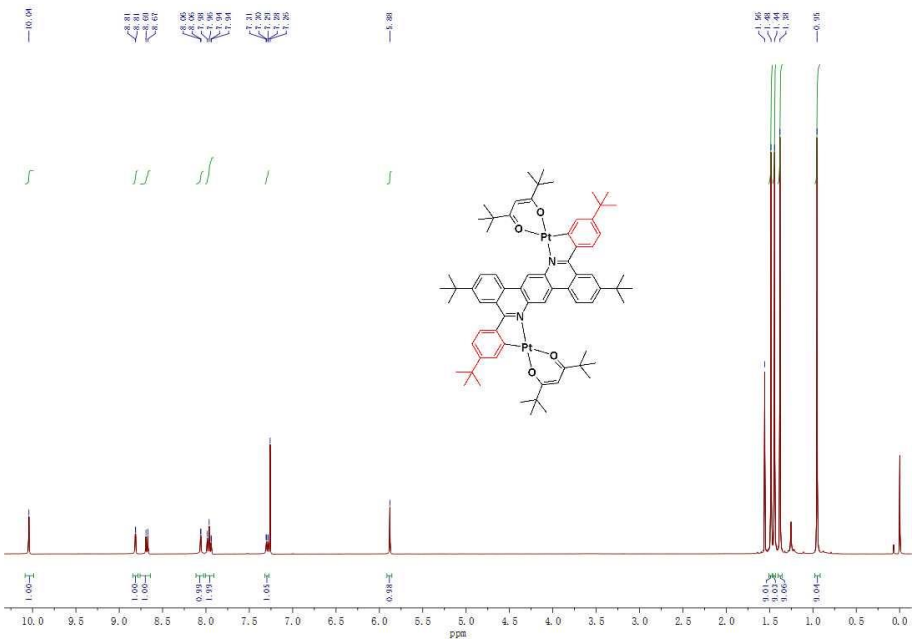


Fig. S5. ^{1}H NMR plot of (BuPh-BDIQ)$Pt_2(dpm)_2$

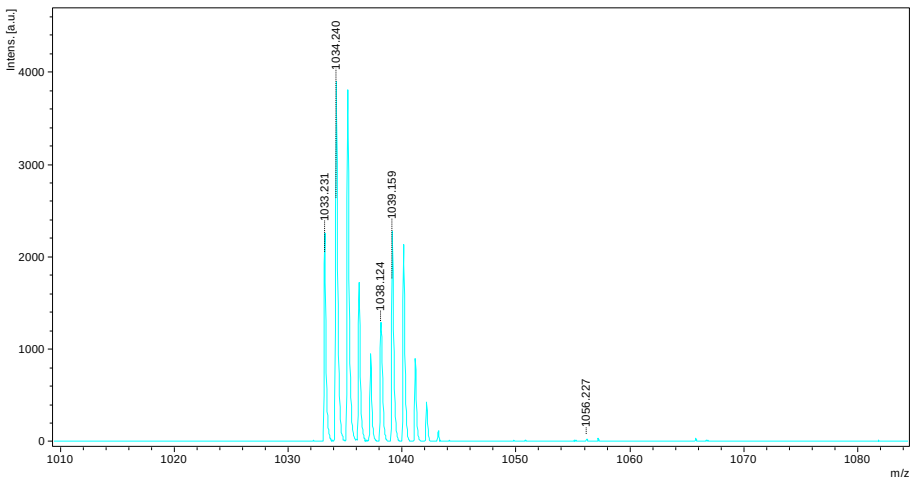


Fig. S6. MALDI-TOF-MS plot of (BuPh-BDIQ)Ptdpm

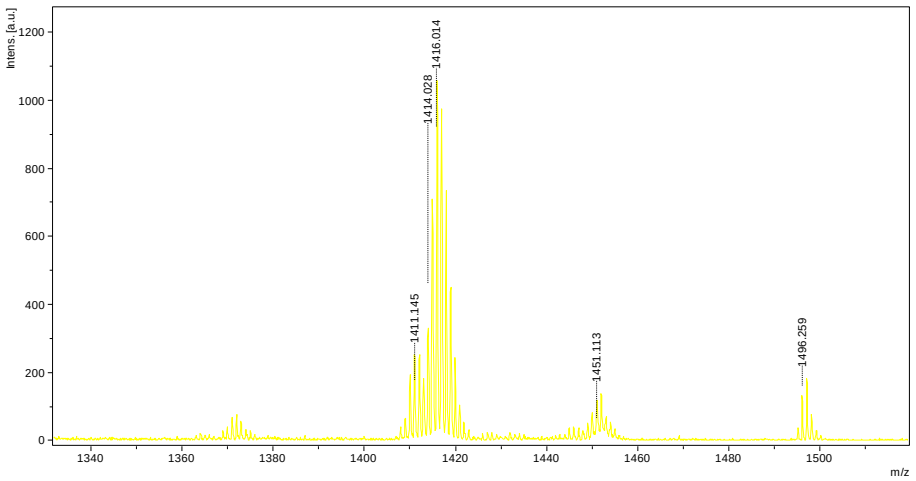


Fig. S7. MALDI-TOF-MS plot of (BuPh-BDIQ)$Pt_2(dpm)_2$

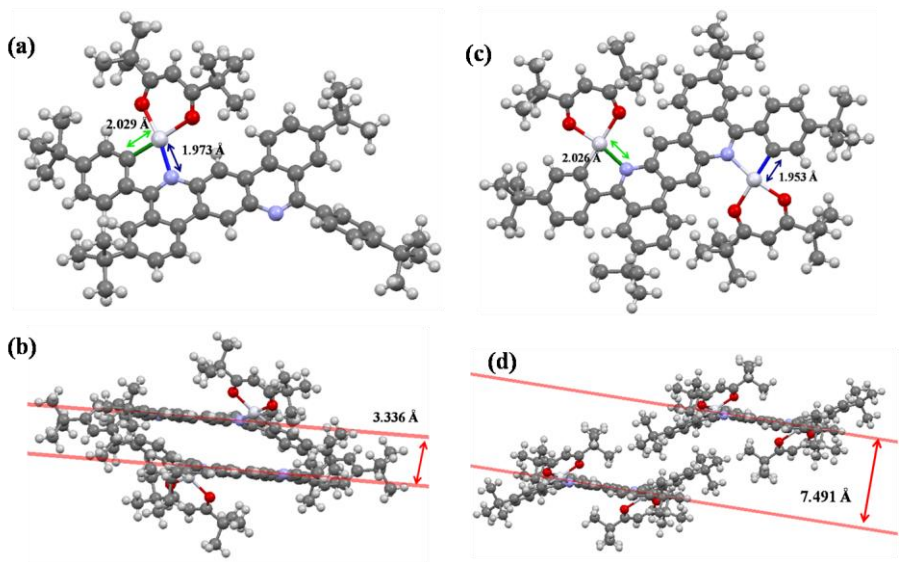


Fig. S8. Signal-crystal structures and molecular packing distance for (BuPh-BDIQ)Ptdpm (a and b) and (BuPh-BDIQ)$Pt_2(dpm)_2$ (c and d)

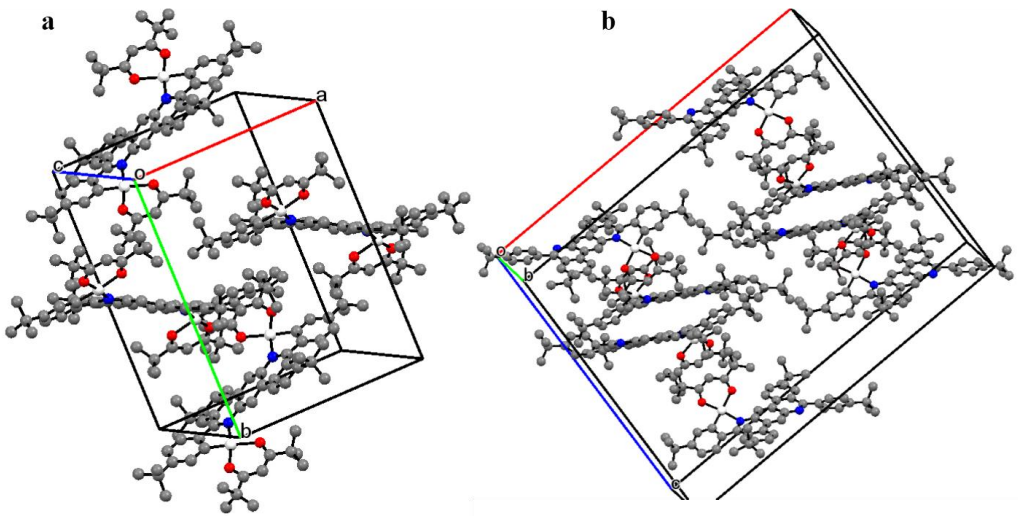


Fig. S9. Perspective view of (BuPh-BDIQ)$Pt_2(dpm)_2$ and (BuPh-BDIQ)Ptdpm

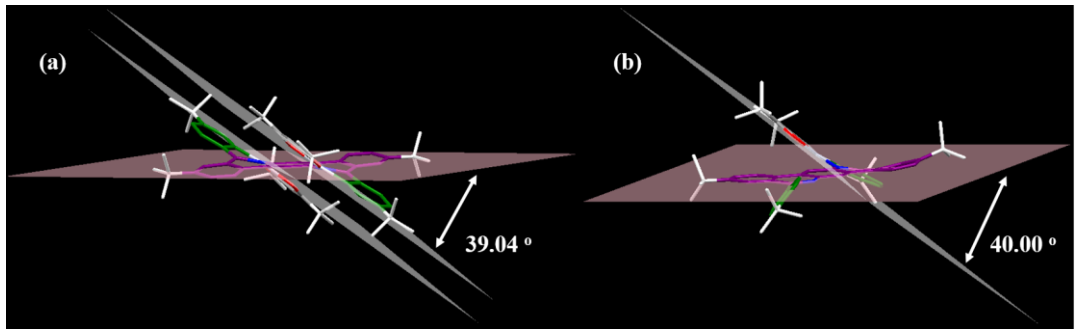


Fig. S10. The dihedral angles between the auxiliary ligand and the rigid main ligand plane for (a) (BuPh-BDIQ)$Pt_2(dpm)_2$ and (b) (BuPh-BDIQ)Ptdpm

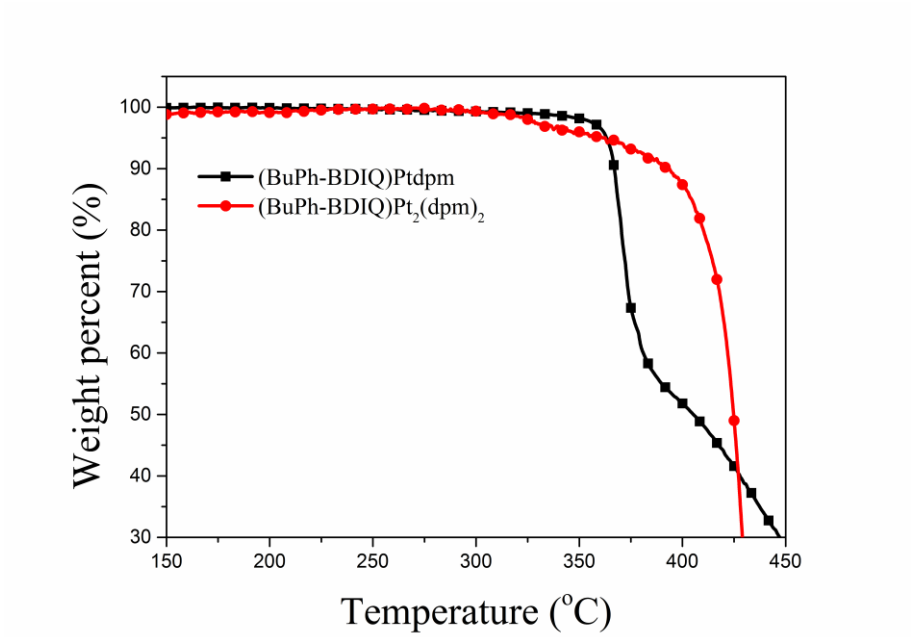


Fig. S11. TGA curves of (BuPh-BDIQ)Ptdpm and (BuPh-BDIQ)$Pt_2(dpm)_2$

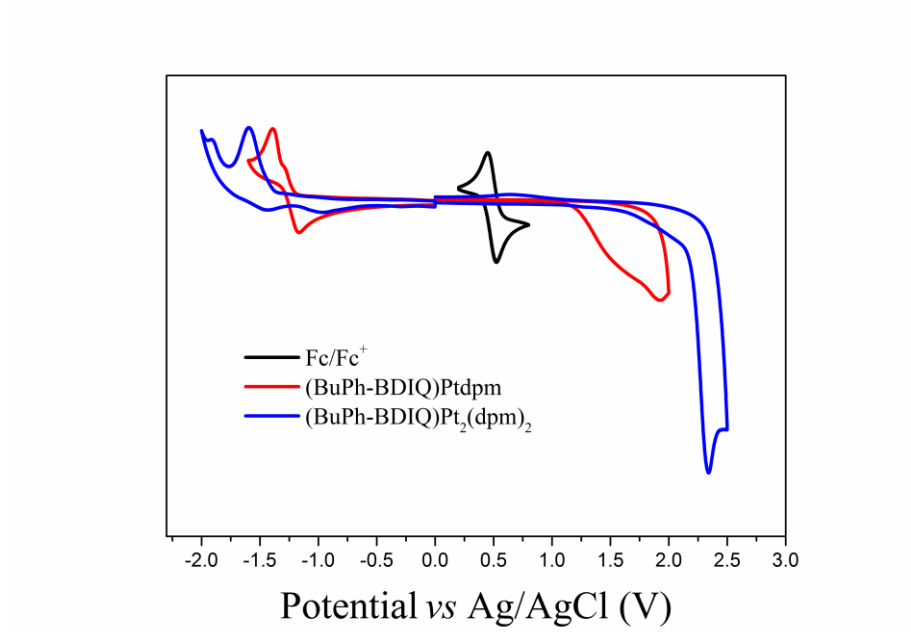


Fig. S12. CV curves of (BuPh-BDIQ)Ptdpm and (BuPh-BDIQ)$Pt_2(dpm)_2$

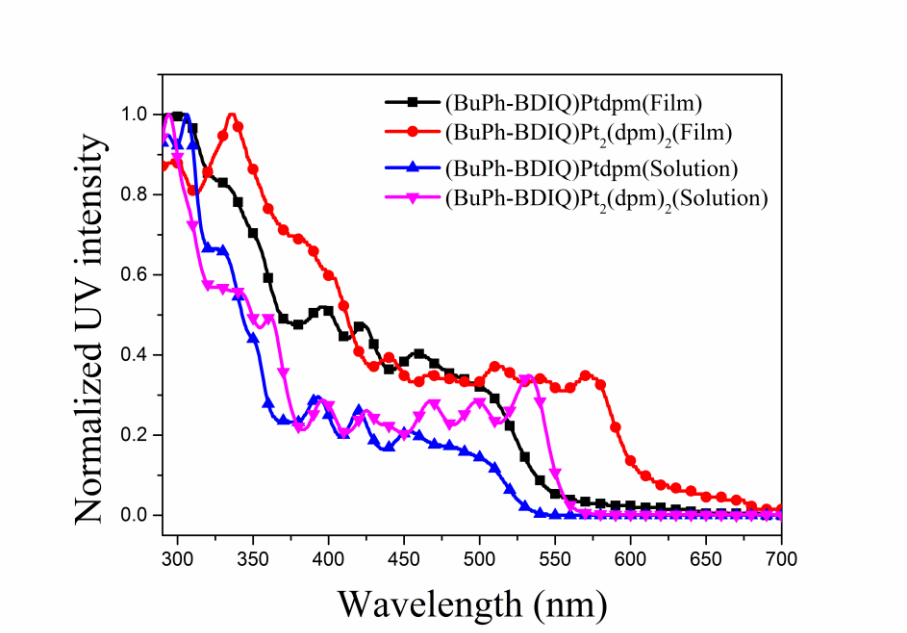


Fig. S13. Normalized UV-vis absorptions of (BuPh-BDIQ)Ptdpm and (BuPh-BDIQ)$Pt_2(dpm)_2$ in their toluene solutions and neat films.

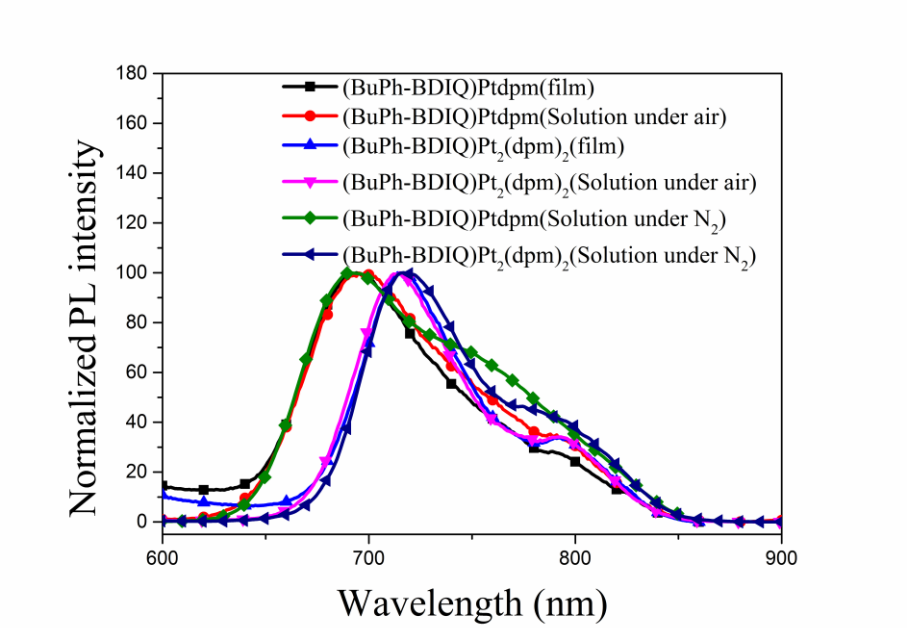


Fig. S14. PL spectra of (BuPh-BDIQ)Ptdpm and (BuPh-BDIQ)$Pt_2(dpm)_2$ in their toluene solutions and neat films under air and N_2 atmosphere

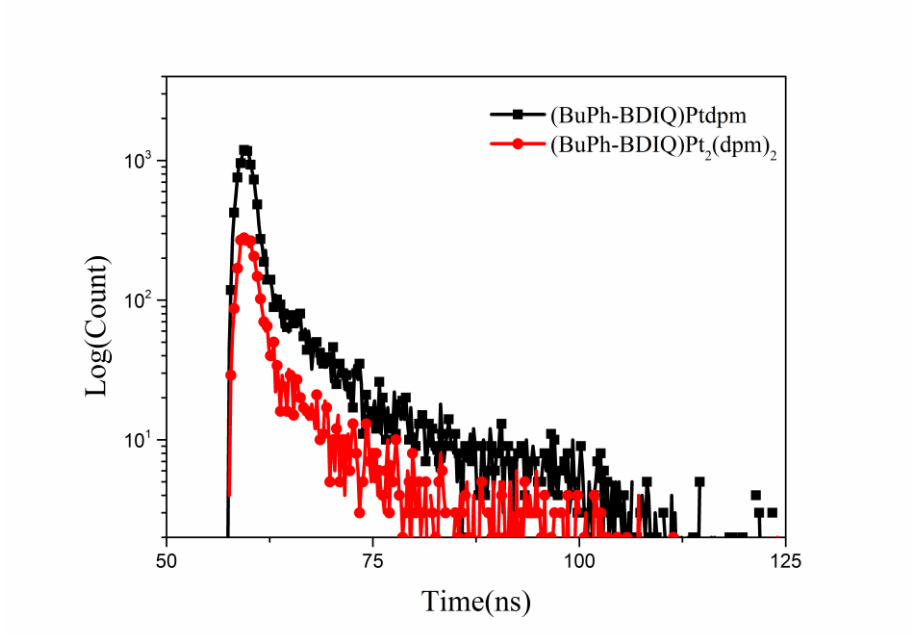


Fig. S15. Room-temperature decay curves of both platinum complexes in a dilute toluene solution

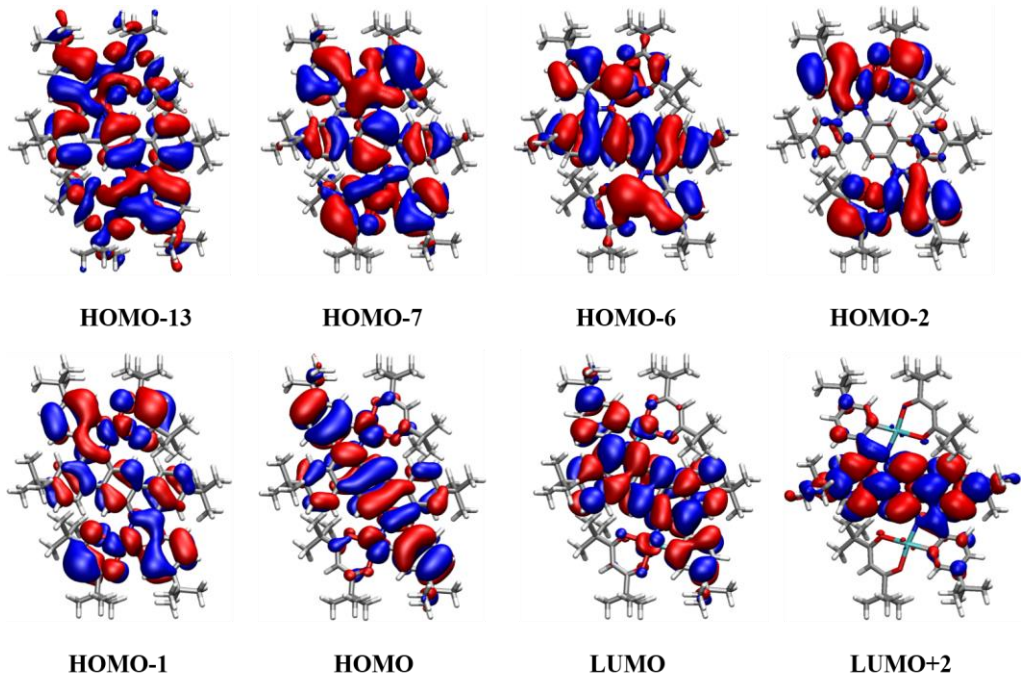


Fig. S16. Energy level diagram of (BuPh-BDIQ)$Pt_2(dpm)_2$

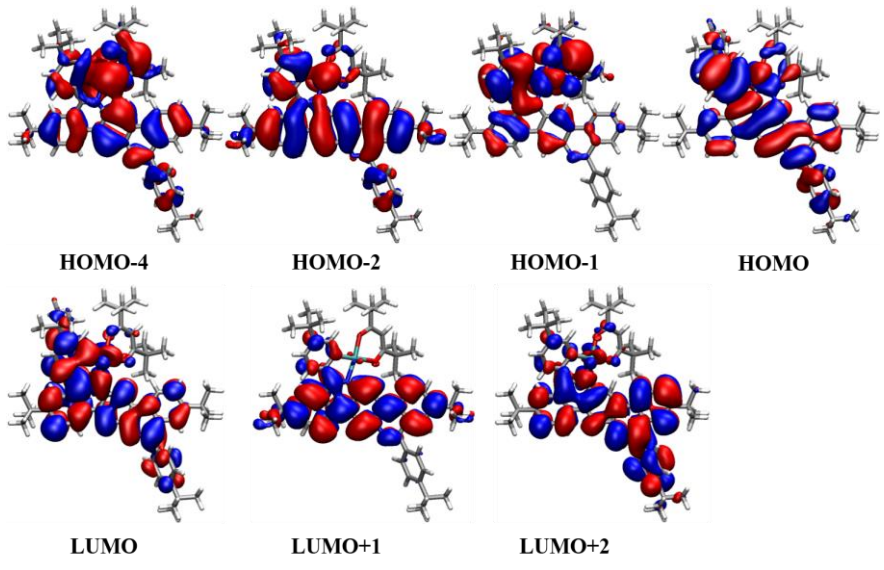


Fig. S17. Energy level diagram of (BuPh-BDIQ)Ptdpm

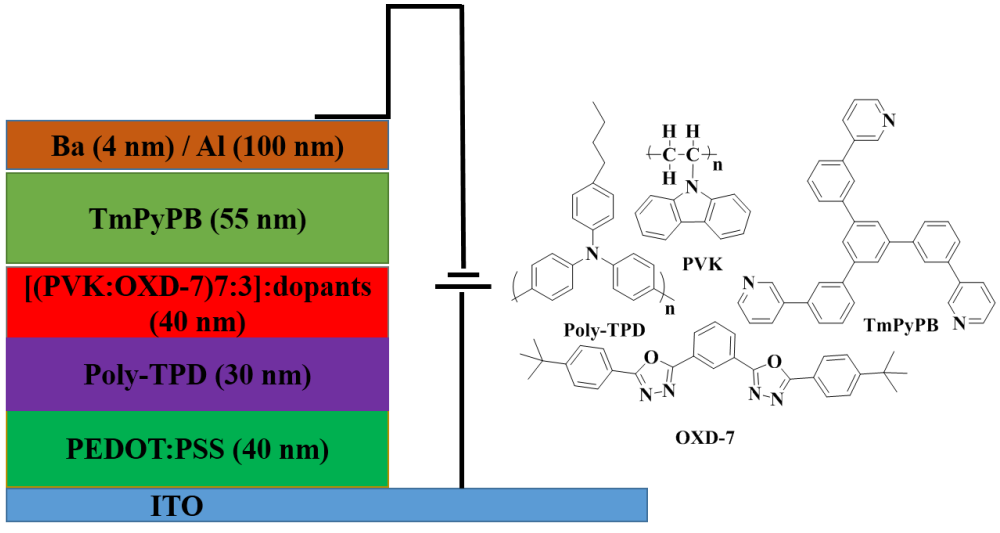


Fig. S18. Device structure of the (BuPh-BDIQ)Ptdpm and (BuPh-BDIQ)$Pt_2(dpm)_2$-doped devices

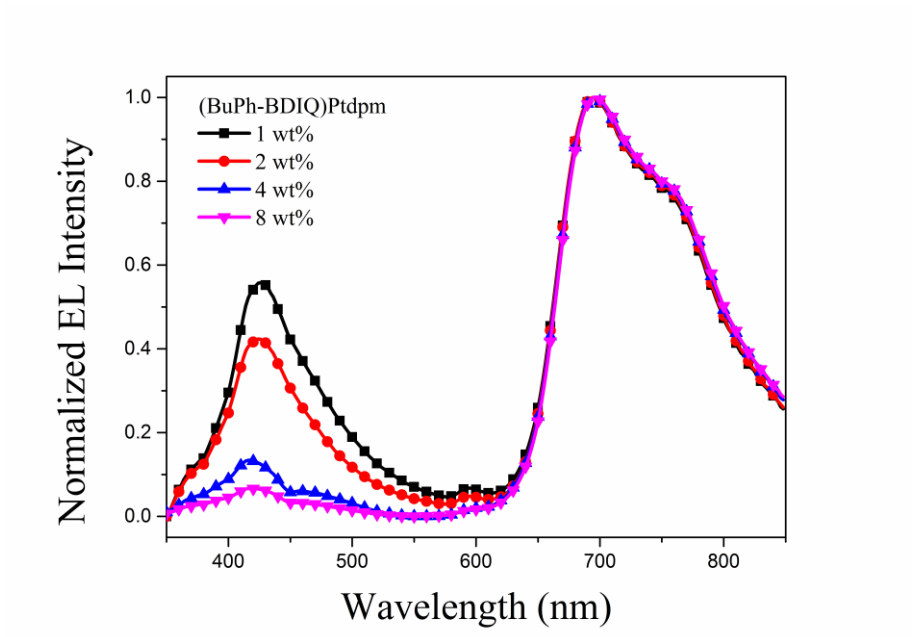


Fig. S19. EL spectra of the (BuPh-BDIQ)Ptdpm doped devices at different doping concentrations of 1wt%, 2 wt%, 4 wt% and 8 wt%

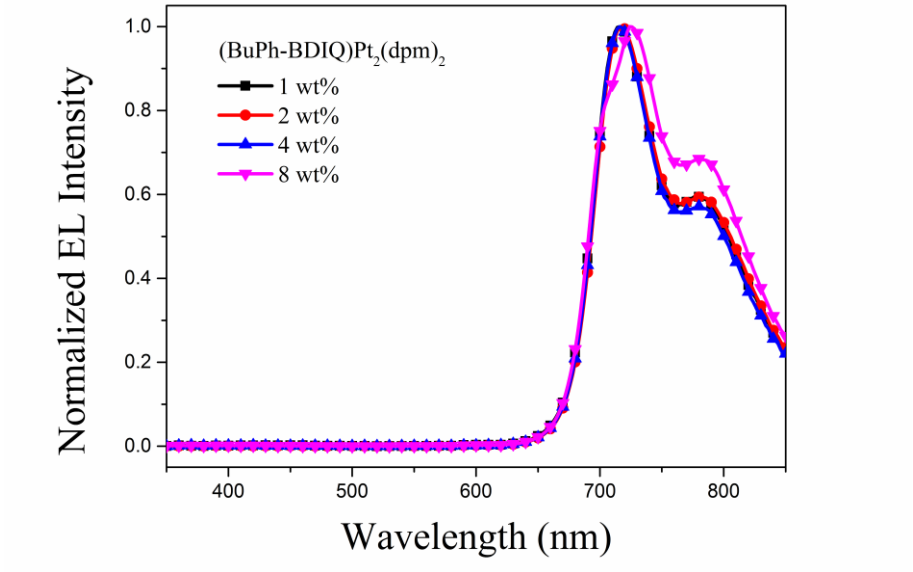


Fig. S20. EL spectra of the (BuPh-BDIQ)$Pt_2(dpm)_2$ doped PLEDs at different doping concentrations of 1wt%, 2 wt%, 4 wt% and 8 wt%

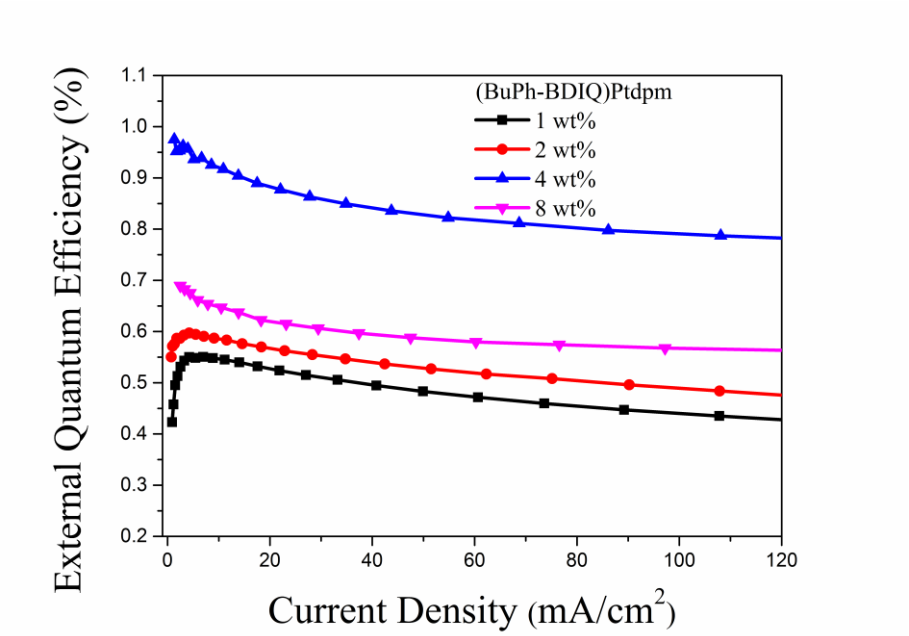


Fig. S21. *EQE-J* curves of the (BuPh-BDIQ)Ptdpm doped PLEDs at different doping concen- trations of 1wt%, 2 wt%, 4 wt% and 8 wt%

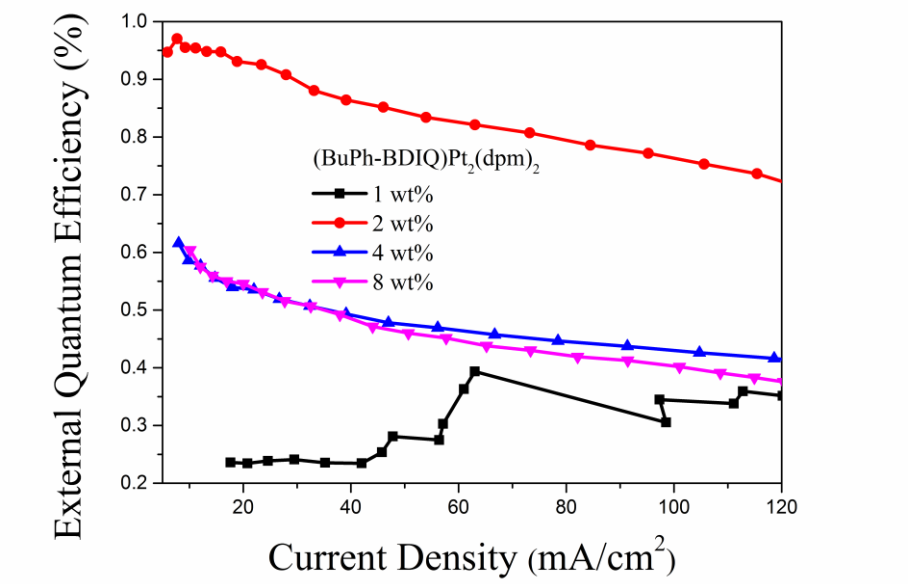


Fig. S22. *EQE-J* curves of the (BuPh-BDIQ)$Pt_2(dpm)_2$ doped PLEDs at different doping concentrations of 1wt%, 2 wt%, 4 wt% and 8 wt%

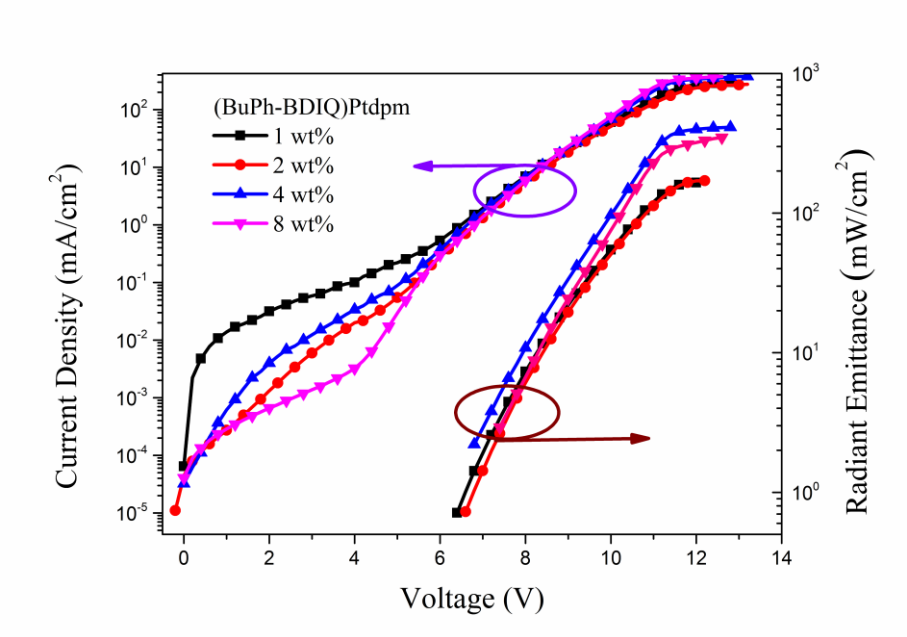


Fig. S23. *J-V-R* curves of the (BuPh-BDIQ)Ptdpm doped PLEDs at different doping concentrations of 1wt%, 2 wt%, 4 wt% and 8 wt%

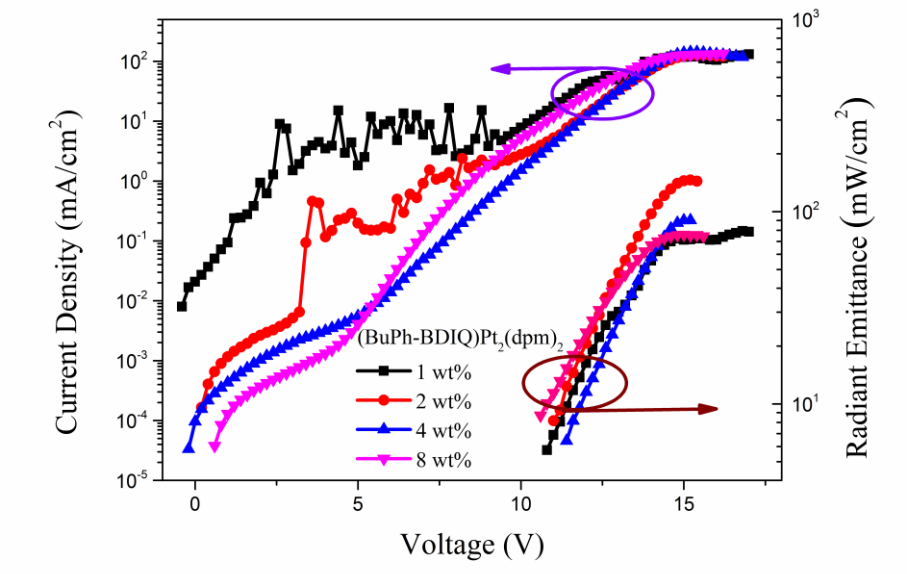


Fig. S24. *J-V-R* curves of the (BuPh-BDIQ)$Pt_2(dpm)_2$ doped PLEDs at different dop -ing concentrations of 1wt%, 2 wt%, 4 wt% and 8 wt%

Table S1. Rate constants K_r and K_{nr} of (BuPh-BDIQ)Ptdpm and (BuPh-BDIQ)$Pt_2(dpm)_2$

Complexes	K_r [10^5 s^{-1}] [a]	K_{nr} [10^5 s^{-1}] [a]
(BuPh-BDIQ)Ptdpm	0.0237	6.555
(BuPh-BDIQ)$Pt_2(dpm)_2$	0.2129	5.635

[a]Rate constants K_r and K_{nr} are calculated using the equations $K_r = \Phi_f/\tau$ and $K_{nr} = (1-\Phi_f)/\tau$.

Table S2. Selected TD-DFT results of (BuPh-BDIQ)$Pt_2(dpm)_2$

NO.	State	λ/nm	f	Transition
1	S1	517	0.3377	HOMO-2→LUMO +1(2.1%) HOMO-1→LUMO (4.9%) HOMO→LUMO (88.9%)
2	S3	468	0.1087	HOMO-1→LUMO (90.7%) HOMO→LUMO (4.8%)
3	S7	412	0.0921	HOMO-7→LUMO (2.4%) HOMO-6→LUMO (52.7%) HOMO-4→LUMO (21.4%) HOMO→LUMO+2 (16.6%)
4	S12	371	0.1820	HOMO-6→LUMO (6.7%) HOMO-4→LUMO (9.0%) HOMO-3→LUMO+1 (10.4%) HOMO→LUMO+2 (68.1%)
5	S15	353	0.2119	HOMO-2→LUMO+2 (96.1%)
6	S27	327	0.1062	HOMO-13→LUMO (43.0%) HOMO-10→LUMO (8.9%) HOMO-8→LUMO+1 (2.7%) HOMO-4→LUMO+2 (5.8%) HOMO-2→LUMO+4 (4.7%) HOMO→LUMO+3 (25.2%)
7	S40	298	0.5285	HOMO-15→LUMO (8.7%) HOMO-7→LUMO+2 (49.8%) HOMO-6→LUMO+2 (7.9%) HOMO-4→LUMO+2 (11.8%)

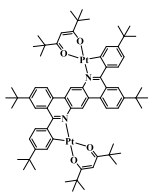
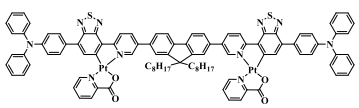
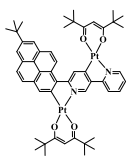
Table S3. Selected TD-DFT results of (BuPh-BDIQ)Ptdpm

NO.	State	λ/nm	f	Transition
1	S1	482	0.1902	HOMO-1→LUMO (11.7%) HOMO→LUMO (80.9%)
2	S2	449	0.1012	HOMO-1→LUMO (85.1%) HOMO→LUMO (9.7%)
3	S4	403	0.1501	HOMO-4→LUMO (8.2%) HOMO-3→LUMO (8.9%) HOMO-2→LUMO (62.2%) HOMO→LUMO+1 (13.1%)
4	S5	390	0.1800	HOMO-4→LUMO (51.2%) HOMO-3→LUMO (38.0%) HOMO→LUMO (4.0%) HOMO→LUMO+1 (2.4%)
5	S8	346	0.1983	HOMO-5→LUMO (12.0%) HOMO-2→LUMO (2.3%) HOMO-1→LUMO+1 (75.6%) HOMO→LUMO+2 (2.6%)
	S9			HOMO-1→LUMO+1 (4.8%) HOMO→LUMO+1 (2.4%) HOMO→LUMO+2 (80.3%)

Table S4. The *EQE* and *J-V-R* data of the (BuPh-BDIQ)Ptdpm and (BuPh-BDIQ)$Pt_2(dpm)_2$ doped PLEDs

Complexes	Doping concentrations	V_{on} (V)	λ_{EL} (nm)	R ($\mu W/cm^2$)	EQE_{max} (%)
(BuPh-BDIQ)Ptdpm	1 wt%	6.4	694	165	0.55
	2 wt%	6.6	694	171	0.60
	4 wt%	6.8	696	412	0.97
	8 wt%	7.4	696	348	0.69
(BuPh-BDIQ)$Pt_2(dpm)_2$	1 wt%	11.0	716	79	0.39
	2 wt%	11.2	718	146	0.97
	4 wt%	11.6	724	90	0.62
	8 wt%	10.8	716	76	0.60

Table S5. The maximum of EL wavelength, *EQE* and irradiance summary of the representative NIR dinuclear platinum complexes

Compound	Structure	EL_{max} (nm)	EQE_{max} (%)	R_{max} $\mu W/cm^2$	Ref.
This work: $(BuPh\text{-}BDIQ)Pt_2(dpm)_2$		785	0.97	146	-
$Fl(TPA\text{-}BTPy)_2Pt_2(pic)_2$		780	0.02	59	1
$(BuPyrDPy)[Pt(dpm)]_2$		762	0.31	26.9	2

1 Y. M. Zhang, F. Meng, J. H. Tang, Y. Wang, C. You, H. Tan, Y. Liu, Y. W. Zhong, S. Su and W. Zhu, Dalton Trans, 2016, **45**, 5071-5080.

2 Z. Hao, F. Meng, P. Wang, Y. Wang, H. Tan, Y. Pei, S. Su and Y. Liu, Dalton Trans, 2017, **46**, 16257-16268.