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The influence of diphenylphosphoryl on the phosphorescent properties of heteroleptic Iridium (III) complexes and OLED performance: a theoretical study

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Table S1. the HOMO and energy gap between HOMO and LUMO of complex **FIrpicPO** at optimized S_0 geometry.

	TPSSh	PBE1PBE	B3LYP	Exp
HOMO/eV	-5.24	-5.87	-5.61	-5.47
Eg/eV	3.09	4.08	3.71	2.48

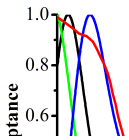

Fig. S1 The simulated absorption spectra of **FIrpicPO** calculated at B3LYP/PBE0/TPSSh functional in CH_2Cl_2 solution together with the experimental absorption spectra.

Table S2. Molecular orbital composition (%) of **FIrpic** at optimized T_1 geometry.

Orbital	Ir-d	dfppy1	dfppy2	pic
LUMO+2	3.31	87.03	4.30	4.40
LUMO+1	1.32	3.61	0.96	93.54
LUMO	3.35	4.87	88.95	1.48
HOMO	36.97	22.67	33.67	5.82
HOMO-1	33.54	27.54	29.60	9.20
HOMO-2	36.03	12.36	39.99	10.85

Table S3. Molecular orbital composition (%) of **FIrpicPO** at optimized T_1 geometry.

Orbital	Ir-d	Ph_2PO1	Ph_2PO2	dfppy1	dfppy2	Pic
LUMO+2	1.48	0.63	0.02	6.21	0.37	90.84
LUMO+1	2.42	4.77	0.24	87.12	3.00	1.62
LUMO	3.15	0.11	5.86	3.28	85.70	0.95
HOMO	37.80	0.20	0.50	23.86	30.14	6.57

HOMO-1	43.30	1.27	0.85	27.21	12.69	14.45
HOMO-2	25.96	0.09	2.70	8.37	55.51	6.74

Table S4. Molecular orbital composition (%) of **IrpicPO** at optimized T_1 geometry.

Orbital	Ir-d	Ph_2PO1	Ph_2PO2	ppy1	ppy2	pic
LUMO+2	1.41	0.01	0.03	0.57	0.83	96.60
LUMO+1	2.82	0.49	4.82	7.62	82.20	1.45
LUMO	2.76	4.64	0.46	81.62	8.15	0.98
HOMO	38.10	0.44	0.35	33.93	20.30	5.97
HOMO-1	53.54	0.65	1.08	19.53	8.71	15.94
HOMO-2	25.63	2.13	2.18	27.02	37.66	4.87