

Electronic Supplementary Information (ESI)

Low efficiency roll-off and high performance OLEDs employing alkyl groups modified iridium(III) complexes as emitters

Li-Li Wen,^a Jing Yu,^b Guo-Gang Shan,^{a,*} Hai-Zhu Sun,^a Wen-Fa Xie,^{b,*} Zhong-Min Su^{a,*}

^a *Institute of Functional Materials Chemistry & National and Local United Engineering Lab for Power Battery, Faculty of Chemistry, Northeast Normal University, Changchun 130024, P. R. China.*

Fax: +86-431-85684009 Tel.: +86-431-85099108

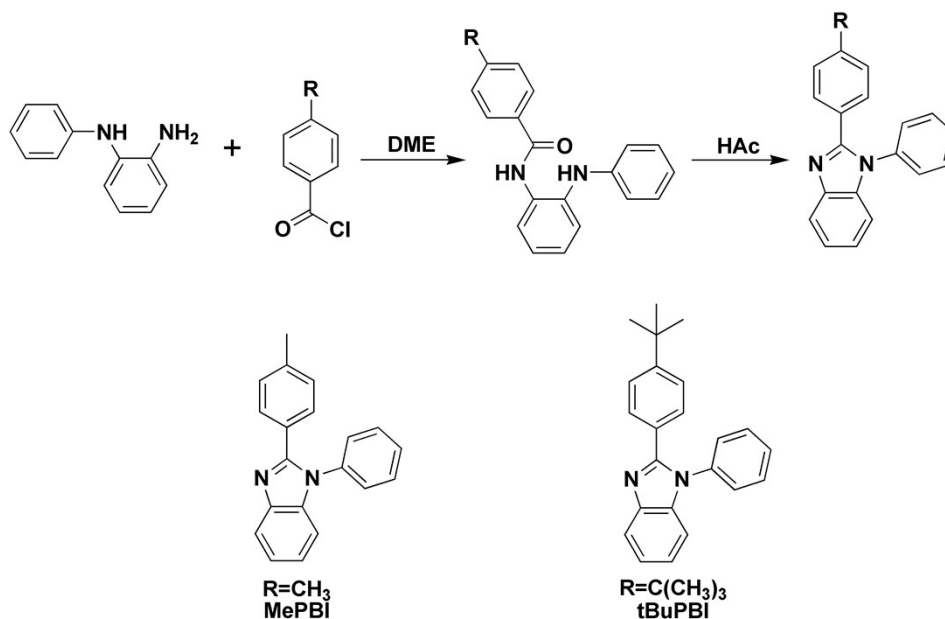
E-mail: shangg187@nenu.edu.cn (G. Shan); zmsu@nenu.edu.cn (Z. Su)

^b *State Key Laboratory on Integrated Optoelectronics, College of Electronic Science and Engineering, Jilin University, Changchun, Jilin 130012, P. R. China*

Tel: +86-13844907598, E-mail: xiewf@jlu.edu.cn (W. Xie)

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Scheme S1. Synthetic route and structures of cyclometalated ligands.

MePBI. The *N*-phenyl-*o*-phenylenediamine (9.21 g, 50.00 mmol) was dissolved in *N,N*-dimethylacetamide (20 mL), 4-methylbenzoyl chloride (7.70 g, 50.00 mmol) was added slowly under nitrogen atmosphere, and the mixture was stirred for 1 h at room temperature. After addition of water, the precipitated solid was filtered off and washed with water and methanol. The solid was recrystallized from a *N,N*-dimethylacetamide/water mixture and then added into acetic acid (25 mL) under reflux. The solvent was evaporated and purified by column chromatography on silica gel. White solid (9.23 g, 32.48 mmol) were obtained with the yield of 65%. ^1H NMR (500 MHz, CDCl_3 , δ [ppm]): 7.89 (d, $J = 8.0$ Hz, 1H), 7.52–7.45 (m, 5H), 7.35–7.31 (m, 3H), 7.27–7.23 (m, 2H), 7.11 (d, $J = 8.0$ Hz, 2H), 2.34 (s, 3H).

tBuPBI. White solid (9.62 g, 29.50 mmol) were obtained with the yield of 65%. Synthesis of tBuPBI was similar to MePBI. ^1H NMR (500 MHz, CDCl_3 , δ [ppm]): 7.88 (d, $J = 8.0$ Hz, 1H), 7.53–7.48 (m, 5H), 7.35–7.30 (m, 5H), 7.26–7.21 (m, 2H),

2.29 (s, 9H).

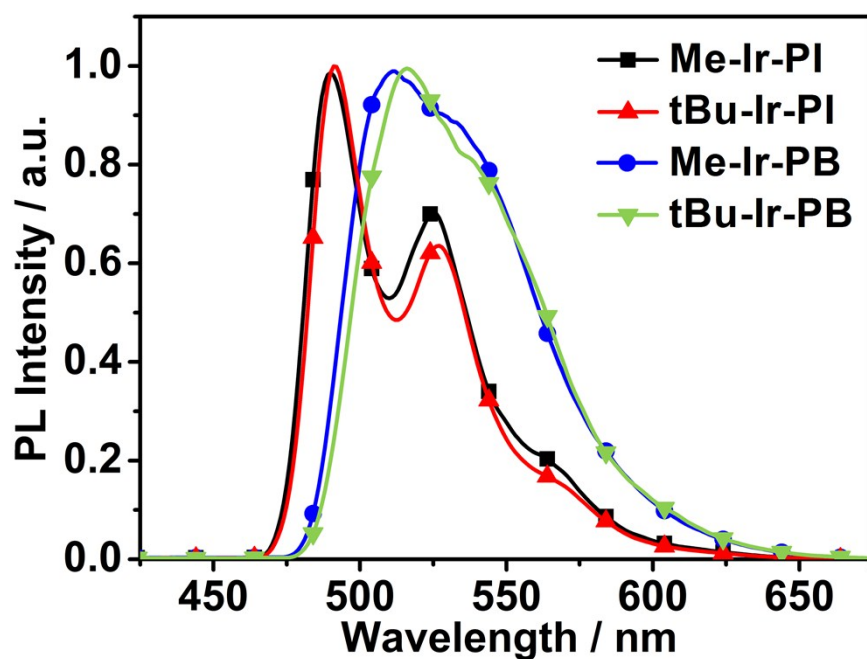


Figure S1 Photoluminescence spectra of all complexes in CH_2Cl_2 solutions at 77 K.

Table S1 The calculated energy levels of the lower-lying transitions of all complexes.

Complex	State	eV	f	Assignment	Character
Me-Ir-PI	T_1	2.12	0.00	H→L (81%)	$^3\text{MLCT}/^3\text{LLCT}/^3\text{LC}$
tBu-Ir-PI	T_1	2.12	0.00	H→L (82%)	$^3\text{MLCT}/^3\text{LLCT}/^3\text{LC}$
Me-Ir-PB	T_1	2.18	0.00	H→L (82%)	$^3\text{MLCT}/^3\text{LLCT}/^3\text{LC}$
tBu-Ir-PB	T_1	2.18	0.00	H→L (83%)	$^3\text{MLCT}/^3\text{LLCT}/^3\text{LC}$

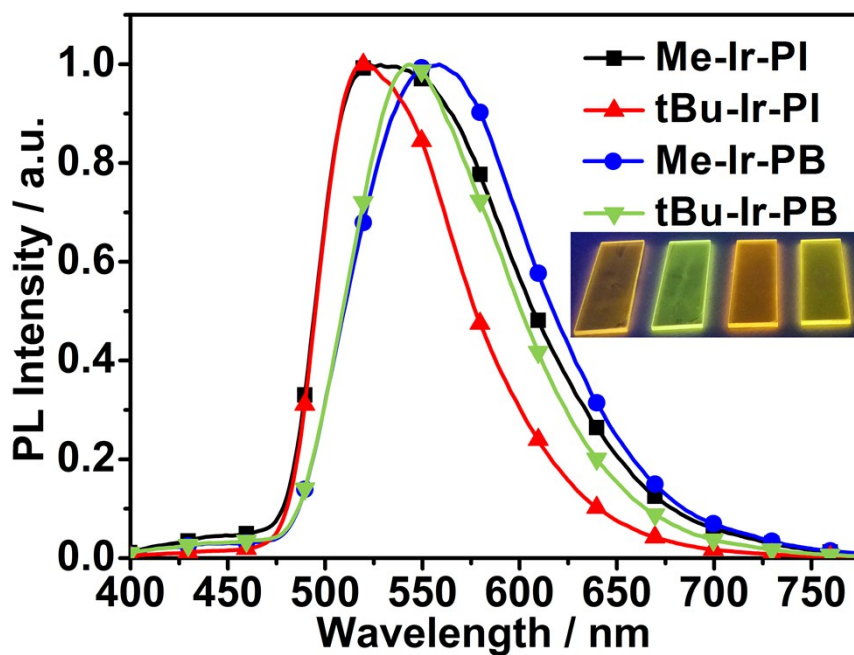


Figure S2 Photoluminescence spectra of all complexes in neat films. Insert: Image of neat films based on **Me-Ir-PI**, **tBu-Ir-PI**, **Me-Ir-PB**, and **tBu-Ir-PB** in accordance with the order from left to right, taken under UV irradiation.

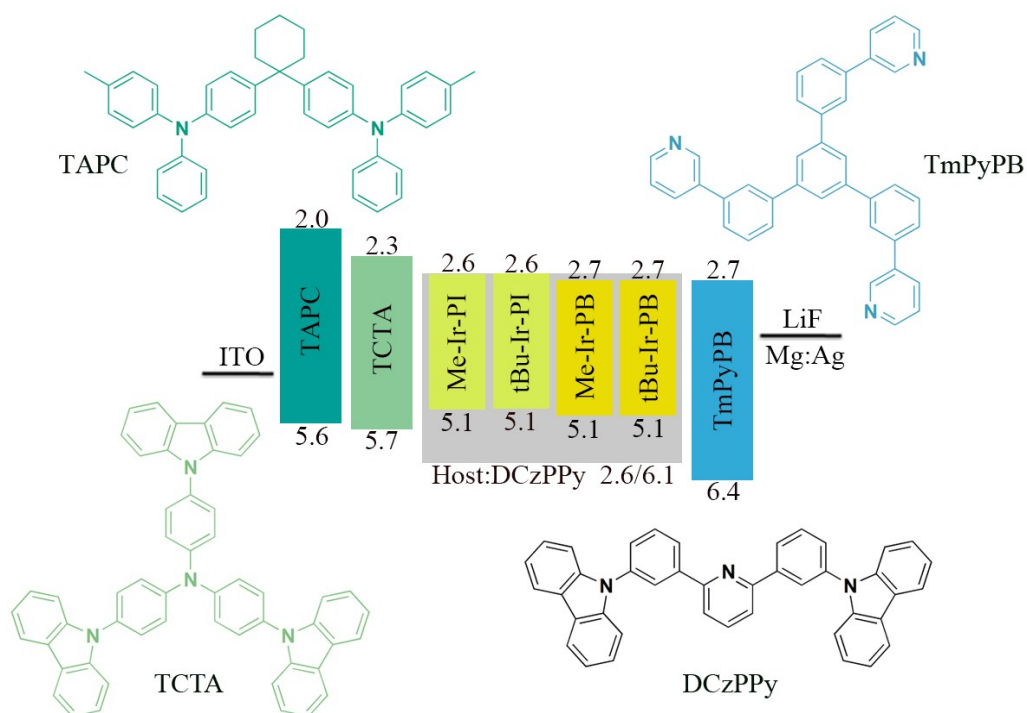


Figure S3 Energy levels and chemical structures of the materials used in OLEDs.