Supporting information

Investigation on voltage loss in organic triplet photovoltaic devices based on Ir complexes

Yingzhi Jin, ‡[a] Jie Xue, ‡[b] Juan Qiao,*[b], Fengling Zhang,*[a]

[a] *Department of Physics, Chemistry and Biology, Linköping University, Linköping SE-58183, Sweden.*

E-mail: fengling.zhang@liu.se

[b] *Key Lab of Organic Optoelectronics and Molecular Engineering of Ministry of Education, Department of Chemistry, Tsinghua University, Beijing 100084, China.*

E-mail: qjuan@mail.tsinghua.edu.cn,

Table S1 Photophysical Characteristics of $Ir(Ftbpa)_3$ and $Ir(FOtbpa)_3$.

	Degassed CH_2Cl_2 solution[a]					Neat film			
	λ_{abs}[nm] [ε ($\times 10^4$ L mol^{-1} cm^{-1})]	λ_{em} [nm]	Φ_{PL}[b] [%]	τ_p [ns]	K_r/K_{nr} [$\times 10^5$ s^{-1}]	λ_{em} [nm]	Φ_{PL}[b] [%]	τ_p [ns]	K_r/K_{nr} [$\times 10^5$ s^{-1}]
Ir(Ftbpa)$_3$	263 (12.3), 335 (3.5), 355 (3.6), 374 (3.3), 490 (2.3), 550 (1.8)	765, 820(s)	14.7	730	2.0/11.7	784	2.6	19	13.7/512.6
Ir(FOtbpa)$_3$	260 (10.8), 326 (3.0), 349 (2.9), 349 (2.8), 383 (2.1), 472 (1.9), 537 (1.1)	767, 827(s)	10.8	489	2.2/18.2	780	2.4	50	4.9/199.2

[a] The concentration of the solution is 2×10^{-5} M. ε denotes the molar extinction coefficients. [b] Φ_{PL} denotes the PLQY.

Table S2 Summary of photovoltaic parameters of T-OPVs based on Ftbpa and FOtbpa ligands.

Active layer	V_{oc} (V)	J_{sc} (mA/cm^2)	FF	PCE (%)
Ftbpa:$PC_{71}BM$	0.27	0.02	0.24	0.001
FOtbpa:$PC_{71}BM$	0.45	0.04	0.37	0.007

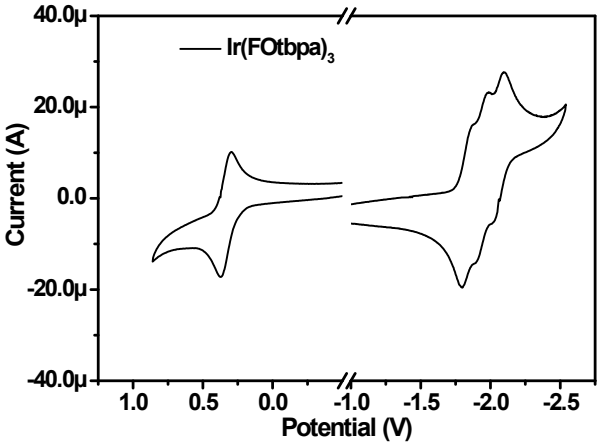

Fig. S1 CV of and $Ir(FOtbpa)_3$ recorded versus Fc^+/Fc in anhydrous DMF solutions at 298 K under a N_2 atmosphere;

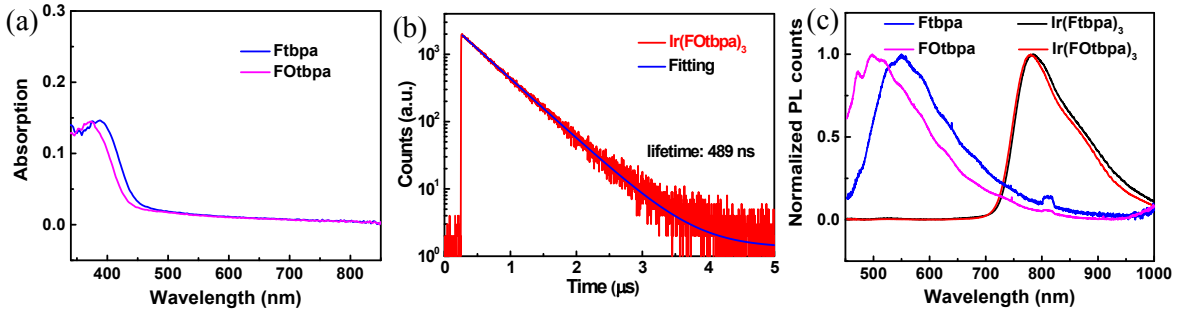

Fig. S2 (a) Absorption spectra of Ftbpa and FOtbpa films; (b) Transient PL decay curves of $Ir(FOtbpa)_3$ in degassed CH_2Cl_2 solution; (c) Normalized PL spectra of $Ir(Ftbpa)_3$, $Ir(FOtbpa)_3$, Ftbpa, and FOtbpa films; The films were excited by a 405 nm laser.

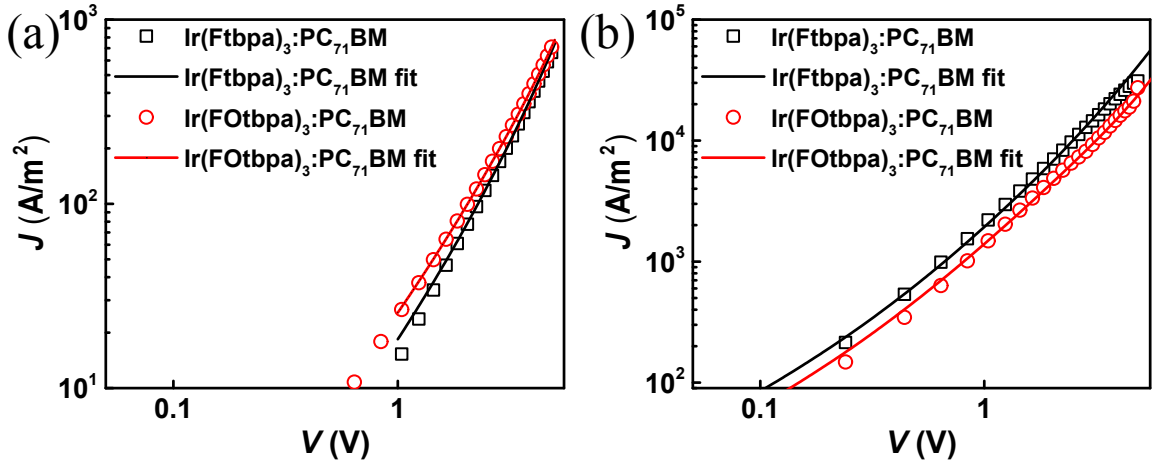

Fig. S3 *J–V* curves for hole (a) and electron (b) only devices based on Ir(Ftbpa)$_3$:PC$_{71}$BM and Ir(FOtbpa)$_3$:PC$_{71}$BM blends with a weight ratio of 1:1.5.

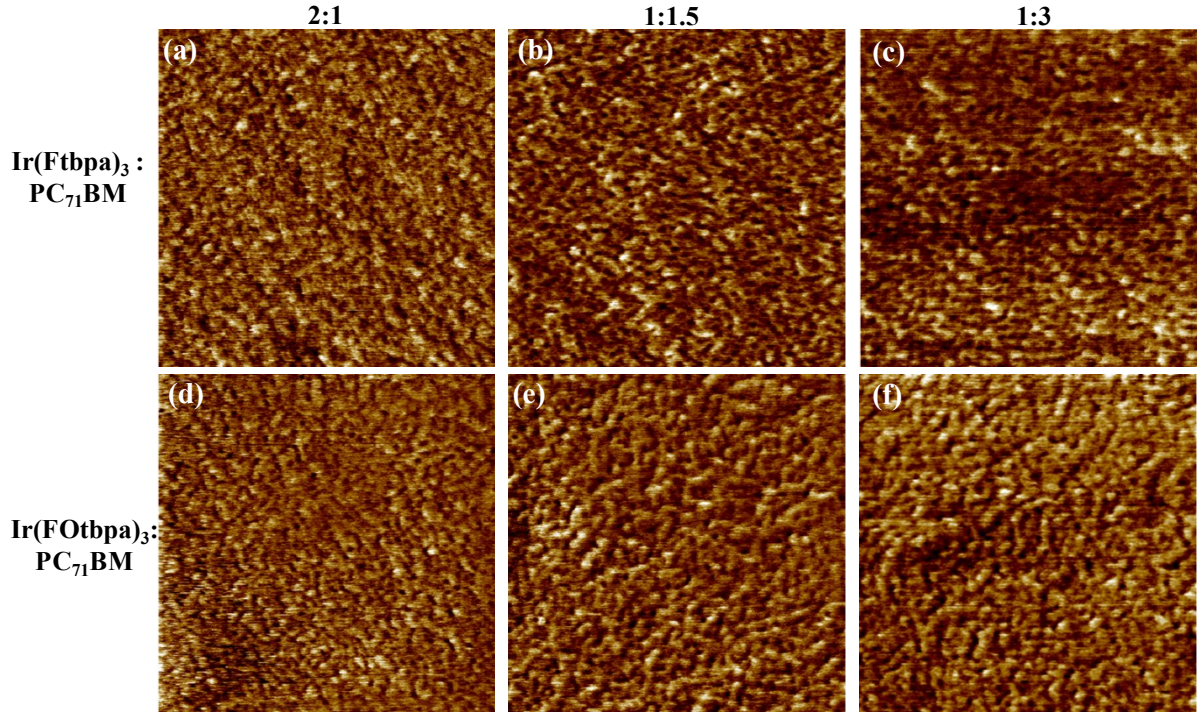

Fig. S4 AFM (2 μm × 2 μm) phase images of Ir(Ftbpa)$_3$:PC$_{71}$BM blends with weight ratio of 2:1 (a), 1:1.5 (b), 1:3 (c) and Ir(FOtbpa)$_3$:PC$_{71}$BM blends with weight ratio of 2:1 (d), 1:1.5 (e), 1:3 (f).

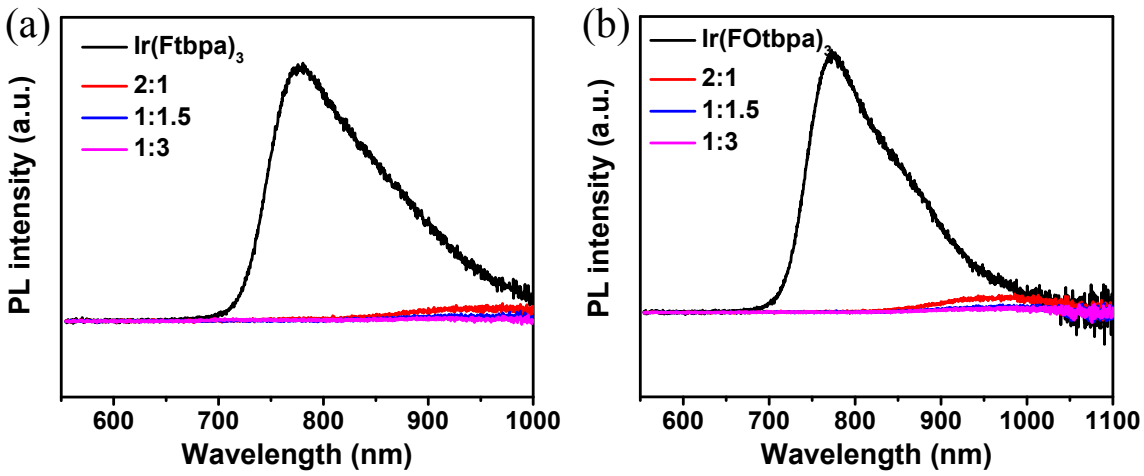

Fig. S5 (a) PL spectra of the pristine Ir(Ftbpa)$_3$ and blended films with different weight ratios. (b) PL spectra of the pristine Ir(FOtbpa)$_3$ and blended films with different weight ratios. The PL intensities are corrected by their absorptions at the excitation wavelength (532 nm).

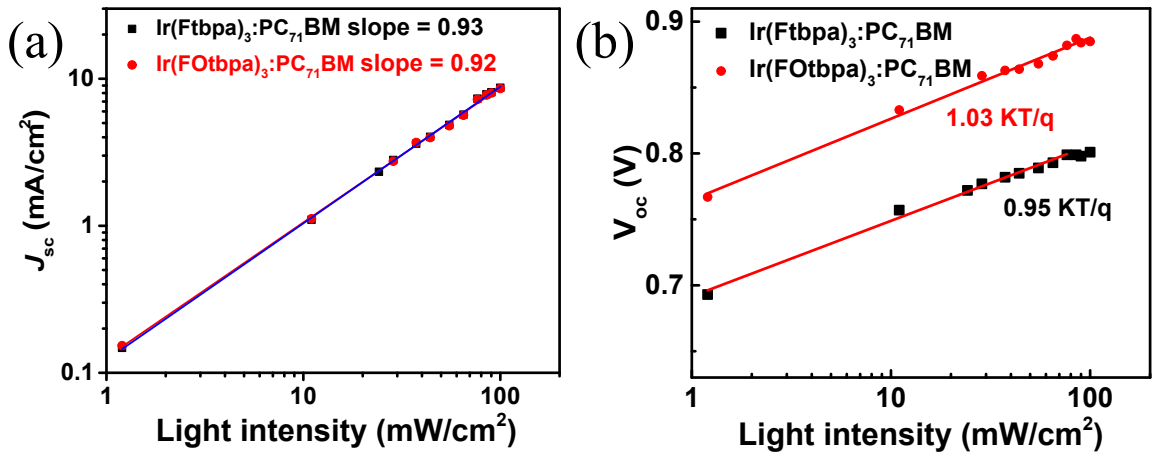

Fig. S6 (a) J_{sc} and (b) V_{oc} versus light intensity for T-OPVs based on Ir(Ftbpa)$_3$:PC$_{71}$BM blends (1:1.5) and Ir(FOtbpa)$_3$:PC$_{71}$BM blends (1:1.5).