Supporting Information for

Alkyl chain length effects on piezochromic luminescence of iridium(III)-based phosphors adopting 2-phenyl-1*H*-benzoimidazole type ligands

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Theoretical calculations

Calculation on the ground and excited electronic state of complexes were investigated by preforming DFT and TD-DFT at PBE0 level. The 6-31G* basis sets were employed for optimizing the C, H, N atoms and the LANL2DZ basis sets for Ir atom. An effective core potential (ECP) replaces the inner core electrons of iridium leaving the outer core $(5s)^2(5p)^6$ electrons and the $(5d)^6$ valence electrons of Ir(III). The geometry of the triplet states (T_1) was fully optimized and was calculated at the spin-unrestricted UPBE1PBE level with a spin multiplicity of 3. All expected values calculated for S^2 were smaller than 2.05.All calculations reported here were carried out with the Gaussian 09 software package.[1]

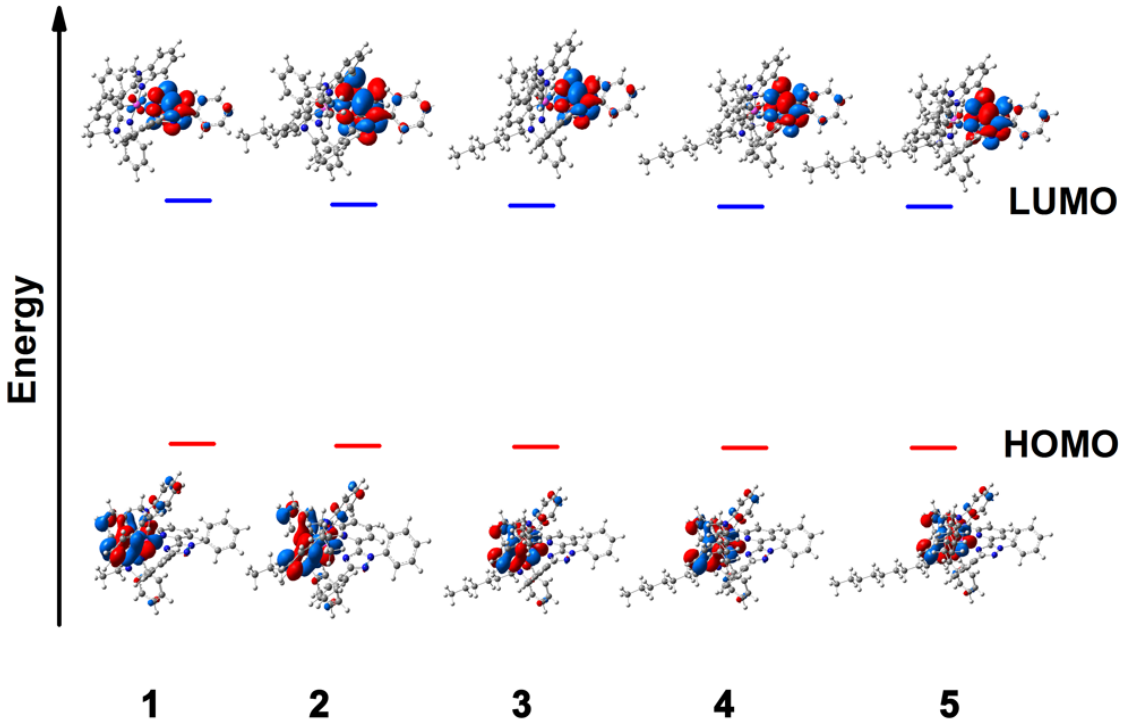

Fig. S1 HOMO and LUMO distributions of complexes **1–5**.

Table S1 Calculated energy levels of the lower-lying transitions of complexes **1–5**.

Complex	States	Assignment	eV	*f*	Nature
1	T_1	H→L (88%)	2.27	0	^{3}MLCT/^{3}LLCT
2	T_1	H→L (88%)	2.27	0	^{3}MLCT/^{3}LLCT
3	T_1	H→L (87%)	2.27	0	^{3}MLCT/^{3}LLCT
4	T_1	H→L (88%)	2.27	0	^{3}MLCT/^{3}LLCT
5	T_1	H→L (88%)	2.27	0	^{3}MLCT/^{3}LLCT

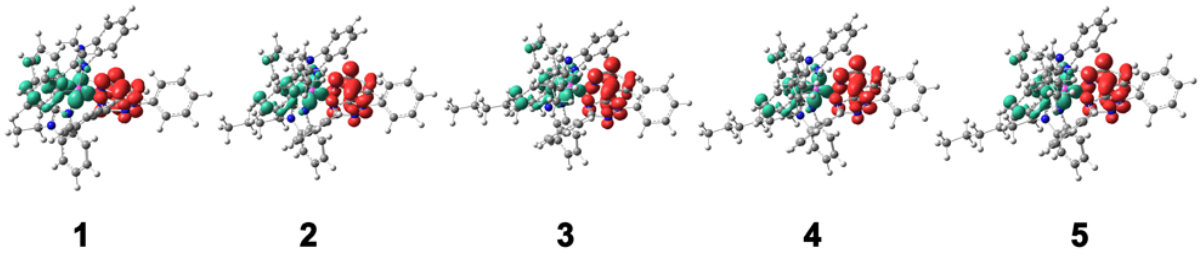

Fig. S2 Difference electron density computed by subtracting the electron densities of the T_1 and S_0 states for complex **1–5**. The charge goes from the green to the red areas.

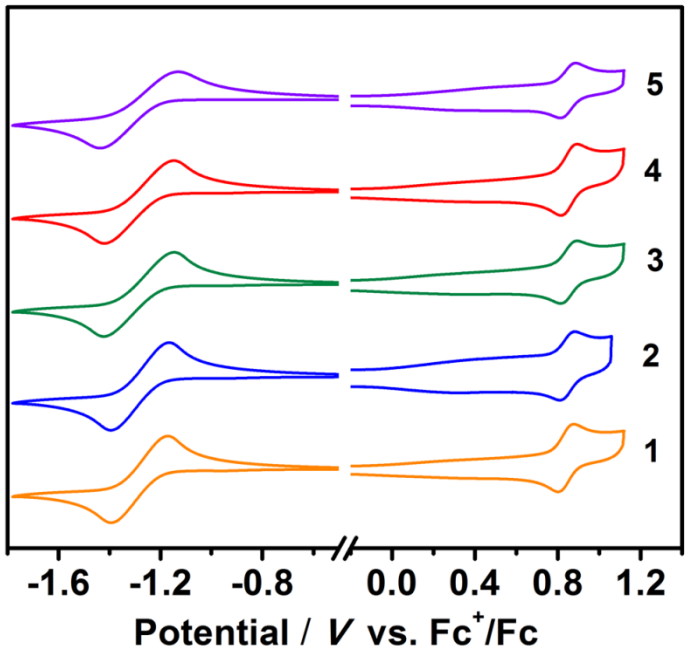

Fig. S3 Cyclic voltammograms of complexes **1–5** in CH_3CN solutions. Potentials were recorded versus Fc^+/Fc (Fc is ferrocene).

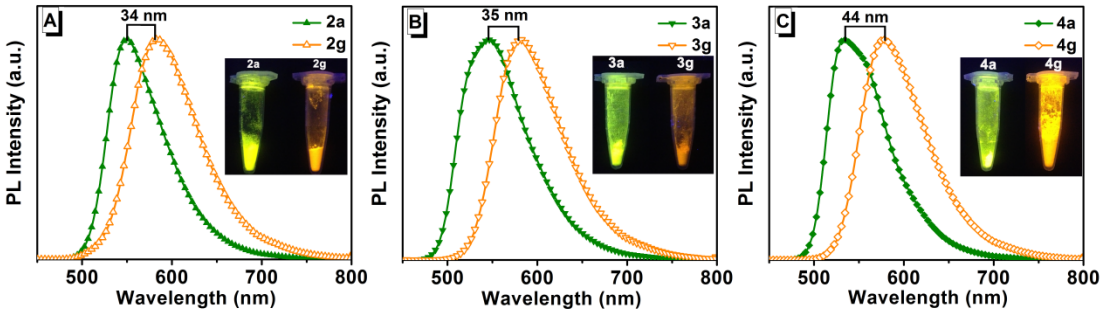

Fig. S4 Emission spectra of as-synthesized powders and ground samples for complexes **1** (A), **2** (B) and **3** (C) at room temperature (RT).

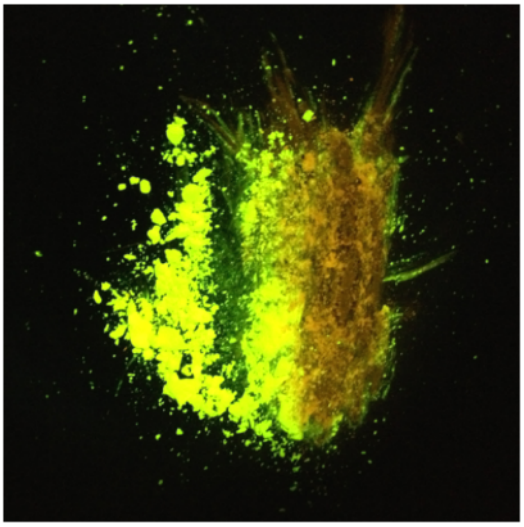

Fig. S5 Image of complex **5** powder after grinding the right-half with a pestle under UV irradiation.

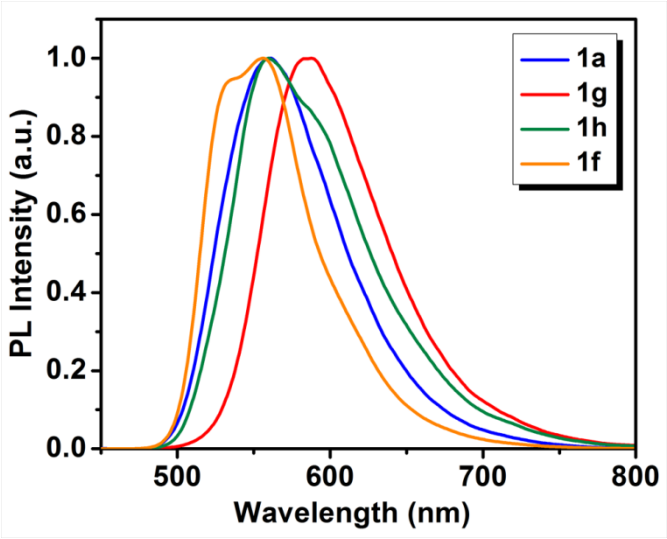

Fig. S6 Normalized emission spectra of as-synthesized powder for complex **1 (1a)**, upon grinding (**1g**), annealing (**1h**) and solvent-fuming (**1f**).

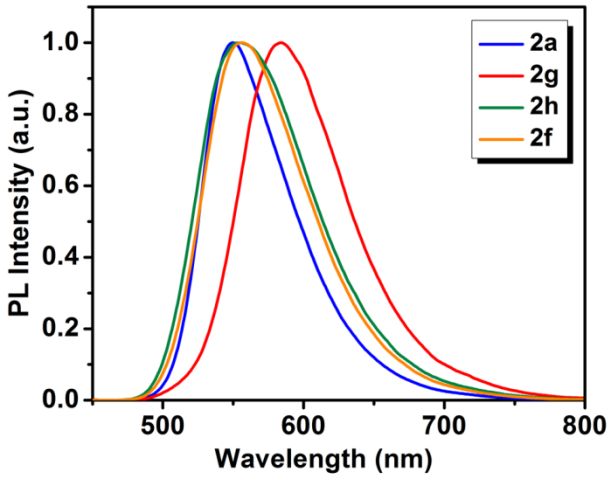

Fig. S7 Normalized emission spectra of as-synthesized powder for complex **2 (2a)**, upon grinding (**2g**), annealing (**2h**) and solvent-fuming (**2f**).

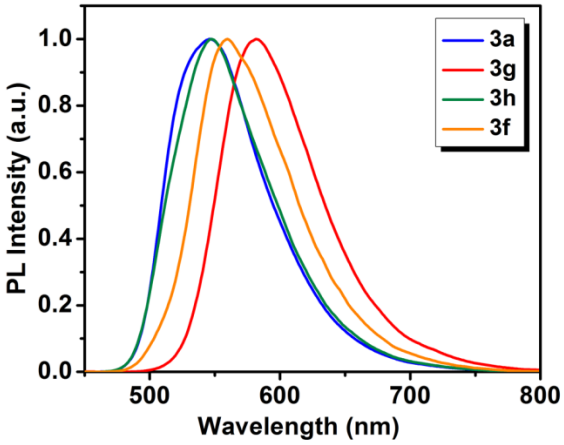

Fig. S8 Normalized emission spectra of as-synthesized powder for complex **3 (3a)**, upon grinding (**3g**), annealing (**3h**) and solvent-fuming (**3f**).

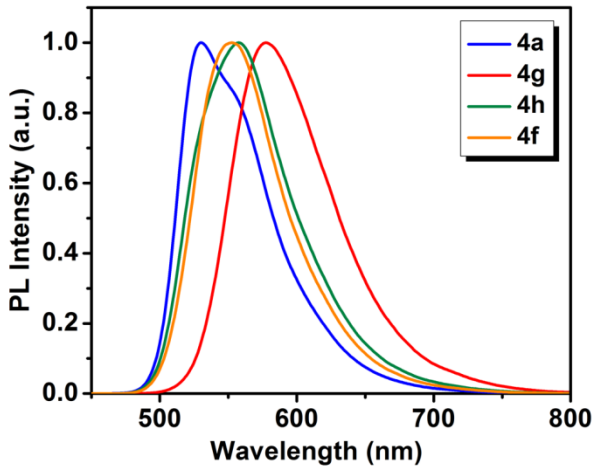

Fig. S9 Normalized emission spectra of as-synthesized powder for complex **4 (4a)**, upon grinding (**4g**), annealing (**4h**) and solvent-fuming (**4f**).

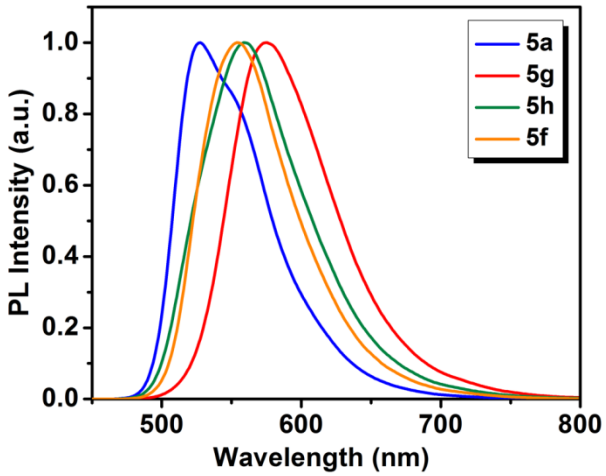

Fig. S10 Normalized emission spectra of as-synthesized powder for complex **5 (5a)**, upon grinding (**5g**), annealing (**5h**) and solvent-fuming (**5f**).

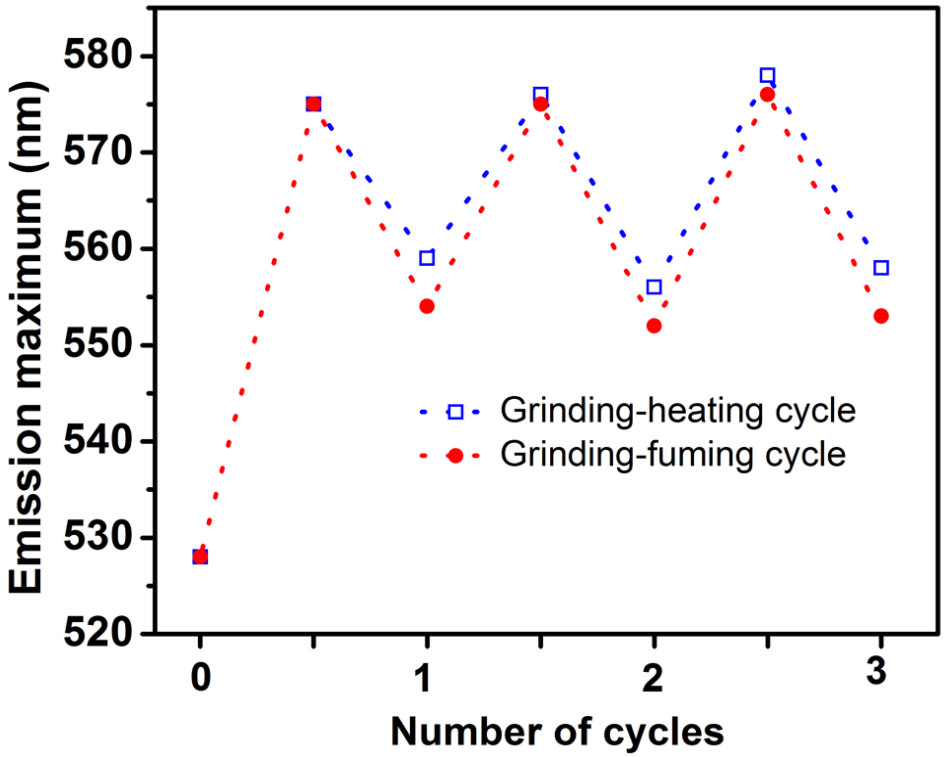

Fig. S11 Reversible switching of emission maximum of complex **5** by repeated grinding-heating (□) or grinding-fuming (●) cycle.

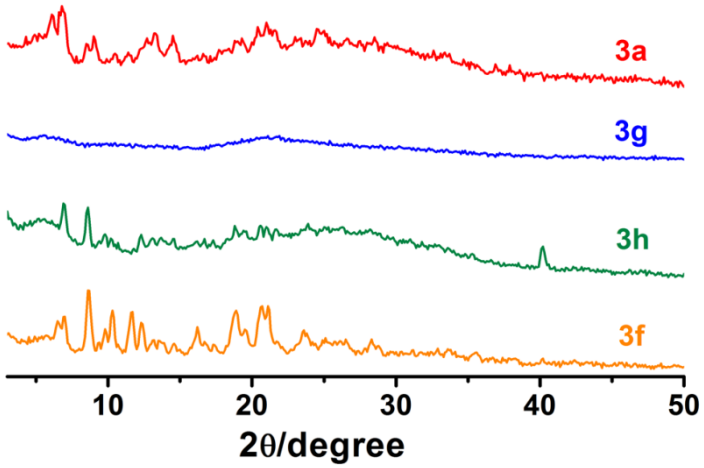

Fig. S12 PXRD curves of complex **3** in different states. The letter "a", "g" "h" and "f" represent as-synthesized powder, ground sample, heated sample and solvent-fumed sample, respectively.

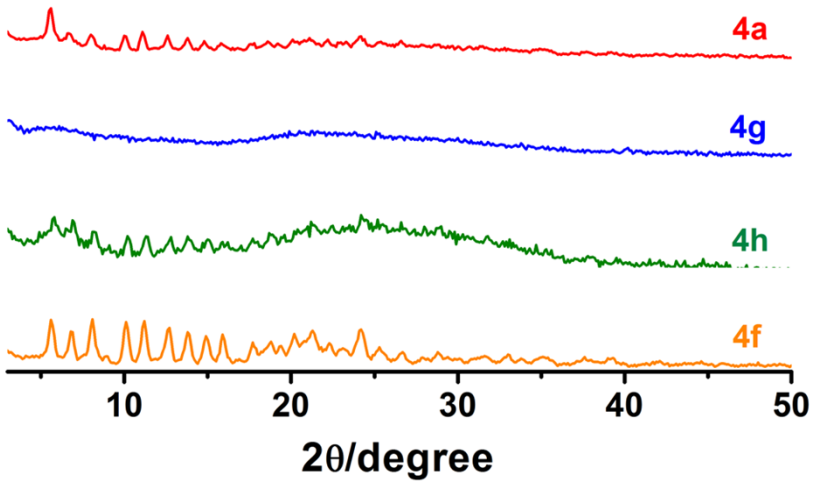

Fig. S13 PXRD curves of complex **4** in different states.

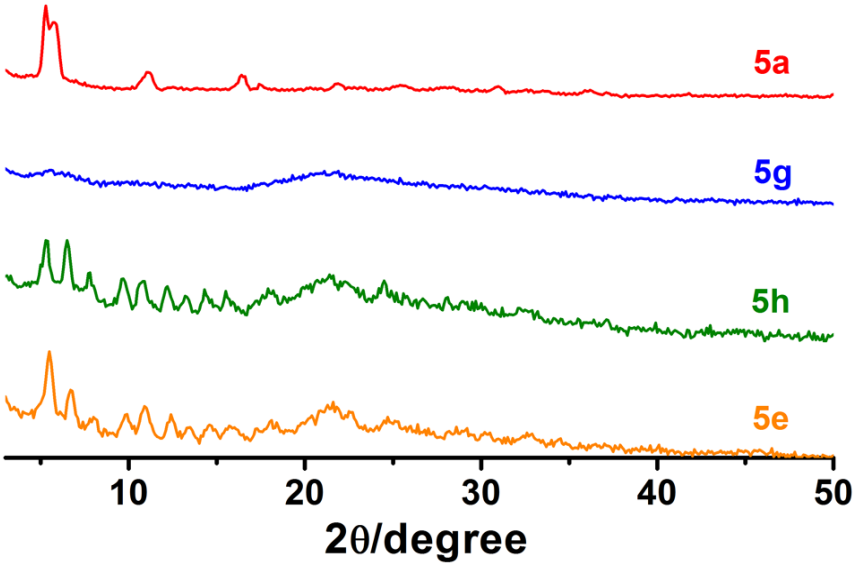

Fig. S14 PXRD curves of complex **5** in different states.