Electronic Supplementary Information (ESI)

Aggregation-induced emission (AIE) active iridium(III) complex toward highly efficient single-layer non-doped electroluminescent device

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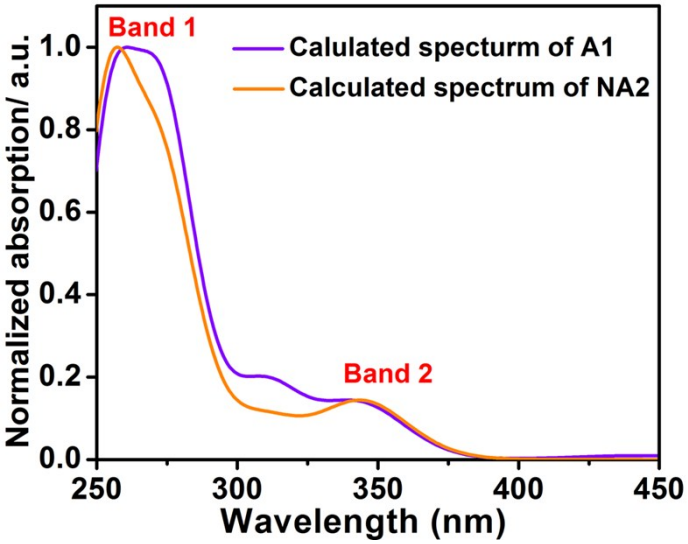

Fig. S1.TD-DFT simulated absorption spectra of **A1** and **NA2** in CH_3CN.

Table S1. Calculated excited energies, dominant orbital excitations, and oscillator strengths (*f*) of **A1** in CH_3CN solution obtained from TD-DFT calculation.

A1	Excited state	eV/nm	*f*	Major contributions[a]	Character[b]
Band 1	S35	4.86/255	0.38	H-6→L+3 (17%)	IL
				H-5→L+2 (15%)	IL
				H-3→L+3 (19%)	IL
	S26	4.56/272	0.21	H-9→L (38%)	IL
				H-6→L+1 (30%)	IL/MLCT/LLCT
				H-5→L+1 (15%)	IL/MLCT/LLCT
Band 2	S6	3.61/344	0.08	H-6→L (92%)	MLCT/LLCT

[a] H and L denote HOMO and LUMO, respectively. [b] MLCT, LLCT and IL denote metal-to-ligand charge transfer, ligand-to-ligand and ligand centered charge transfer, respectively.

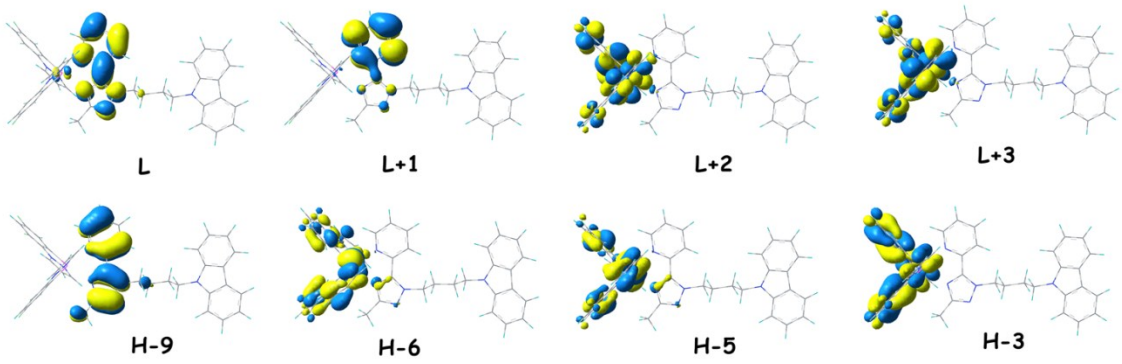

Fig. S2. Selected frontier molecular orbitals involved in crucial electronic excitations of **A1**. H and L denote HOMO and LUMO, respectively.

Table S2. Calculated excited energies, dominant orbital excitations, and oscillator strength (*f*) of **NA2** in CH_3CN solution obtained from TD-DFT calculation.

NA2	Excited state	eV/nm	*f*	Major contributions[a]	Character[b]
Band 1	S30	4.86/255	0.37	H-6→L+3 (16%)	IL
				H-5→L+2 (16%)	IL
				H-3→L+3 (18%)	IL/MLCT/LLCT
	S21	4.52/274	0.05	H-8→L (38%)	LLCT
				H-6→L+1 (31%)	IL
Band 2	S5	3.59/345	0.07	H-6→L (52%)	MLCT/LLCT
				H-2→L (44%)	MLCT/LLCT

[a] H and L denote HOMO and LUMO, respectively. [b] MLCT, LLCT and IL denote metal-to-ligand charge transfer, ligand-to-ligand and ligand centered charge transfer, respectively.

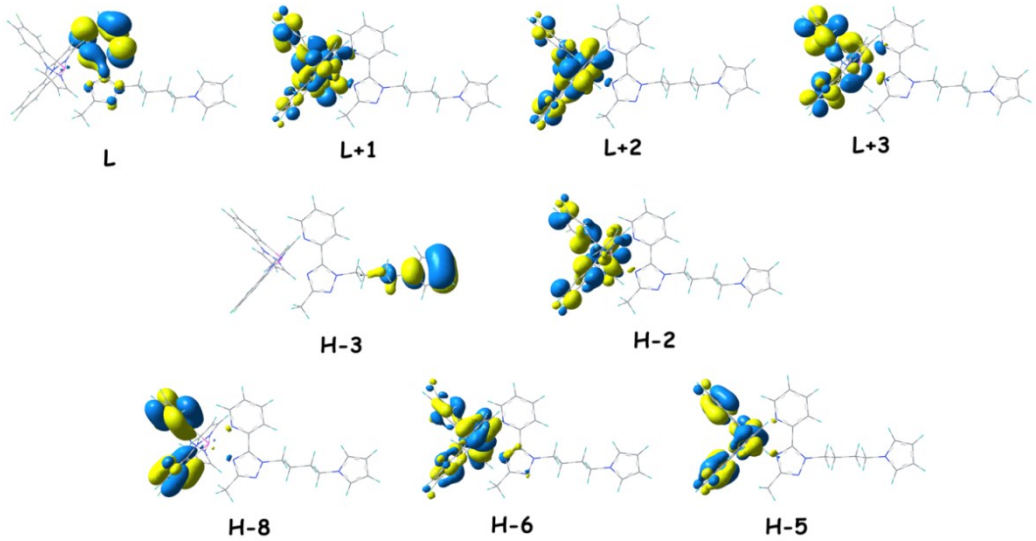

Fig. S3. Selected frontier molecular orbitals involved in crucial electronic excitations of **NA2**. H and L denote HOMO and LUMO, respectively.

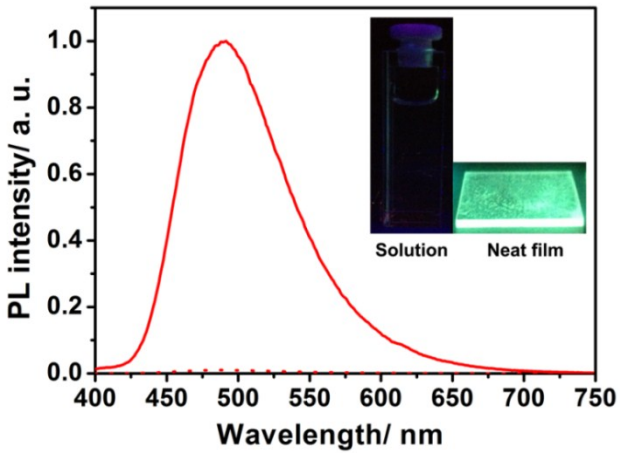

Fig. S4. Emission spectra of **A2** in CH_3CN solution and in neat film.

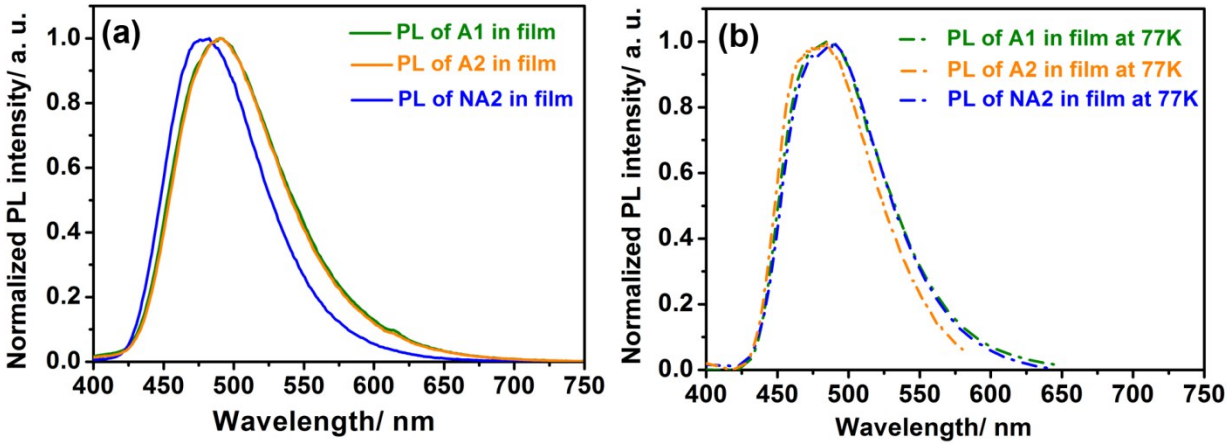

Fig. S5. Emission spectra of complexes **A1**, **A2** and **NA2** in neat film at room temperatures (a) and 77 K (b).

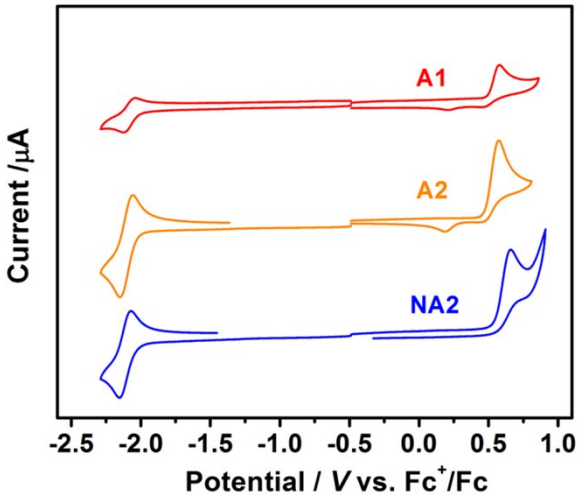

Fig. S6. CV curves of **A1**, **A2** and **NA2.**

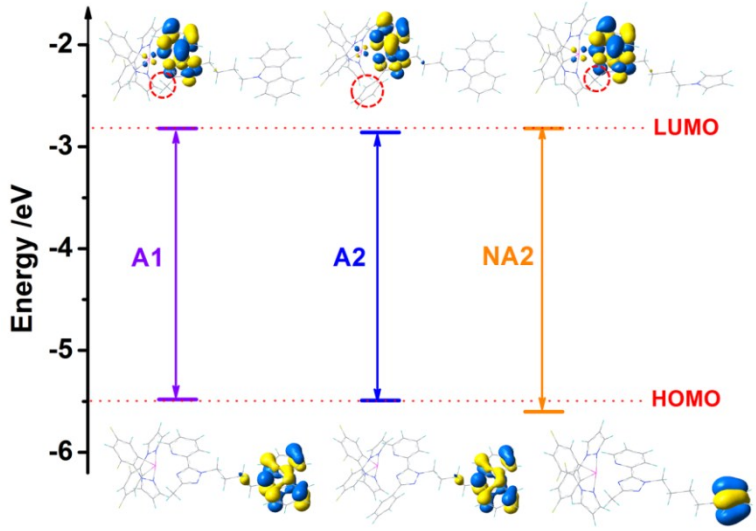

Fig. S7. HOMOs and LUMOs of **A1**, **A2** and **NA2** calculated by DFT method.

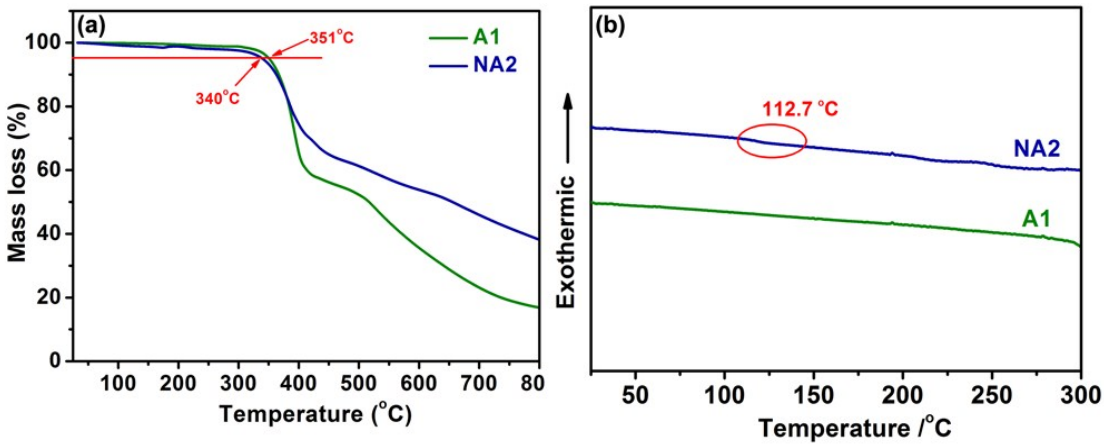

Fig. S8. TGA (a) and DSC (b) curves of the iridium(III) complexes of **A1** and **NA2**.

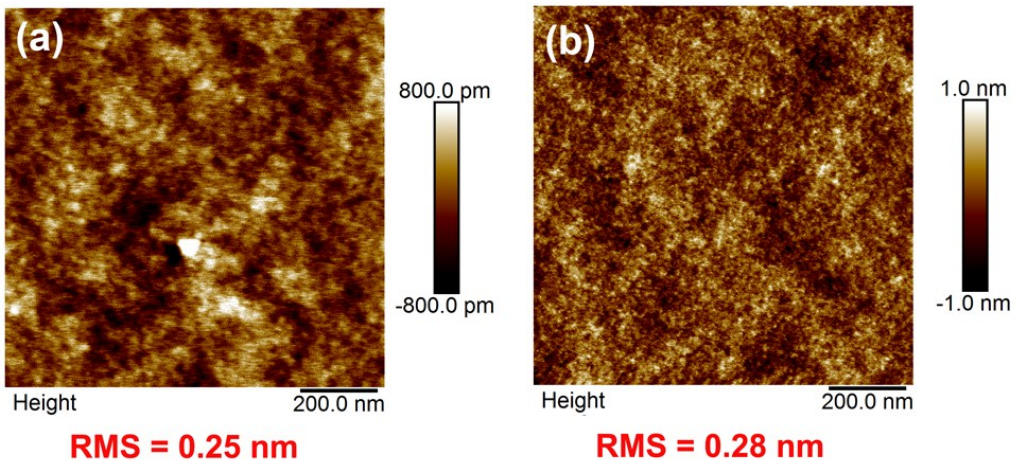

Fig. S9. AFM topographic images of the solution-processed films of **A1** (a) and N**A2** (b).

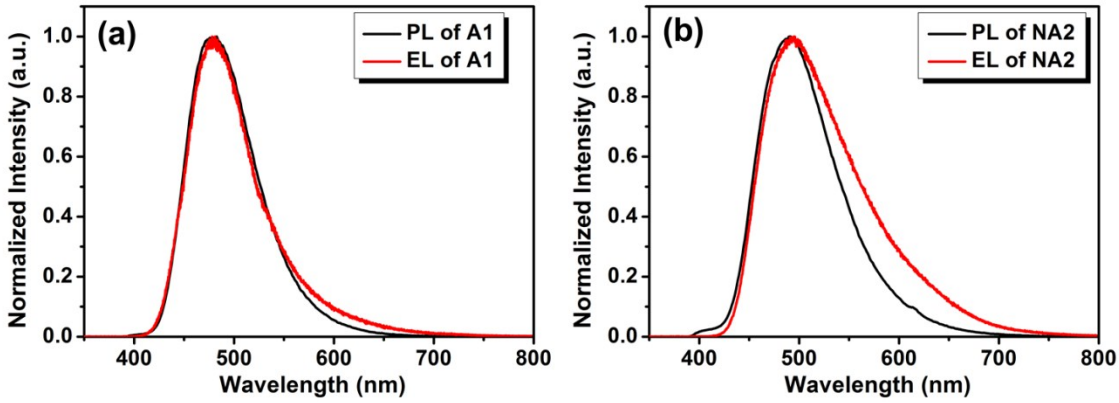

Fig.S10. PL spectra in neat films and EL spectra of **A1** (a) and **NA2** (b)

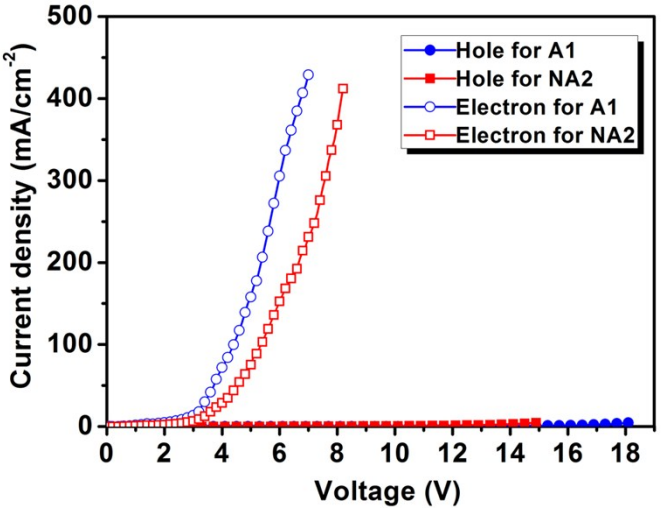

Fig. S11. Current density-Voltage (J-V) of the hole-only and electron-only devices based complexes **A1** and **NA2**.

Table S3 Vertical ionization potential (IP), vertical electron affinity (EA), extraction potential (HEP and EEP) and intramolecular reorganization energy (λ_{hole} and $\lambda_{electron}$).

	IP (v)	HEP (v)	EA (v)	EEP (v)	λ_{hole}	$\lambda_{electron}$
A1	8.47	8.30	4.24	3.77	0.17	0.47
NA2	8.92	8.68	4.24	3.78	0.24	0.46