

# **From Chloro to Fluoro, Expanding the Role of Aluminium Phthalocyanine in Organic Photovoltaic Devices.**

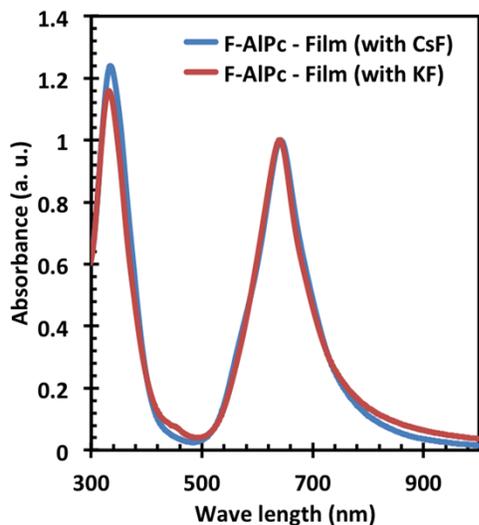
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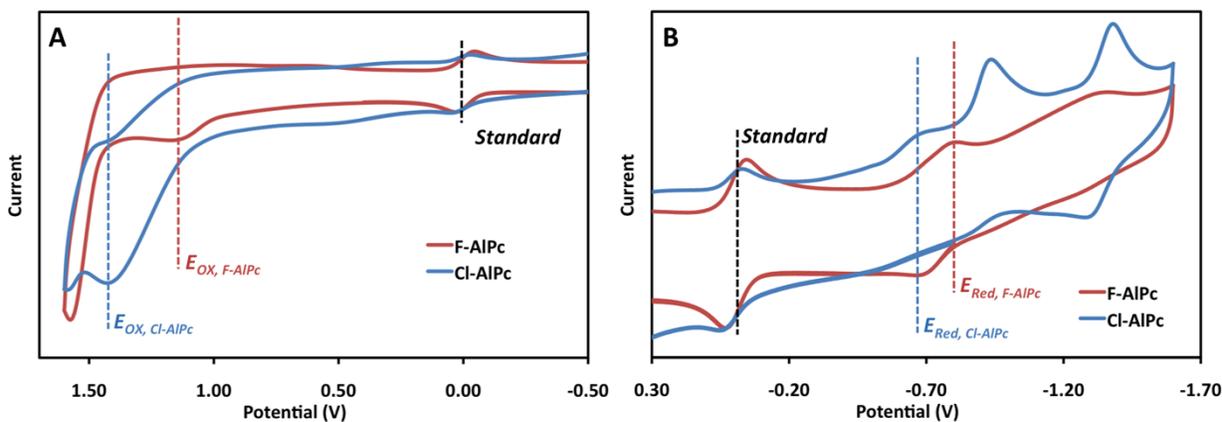
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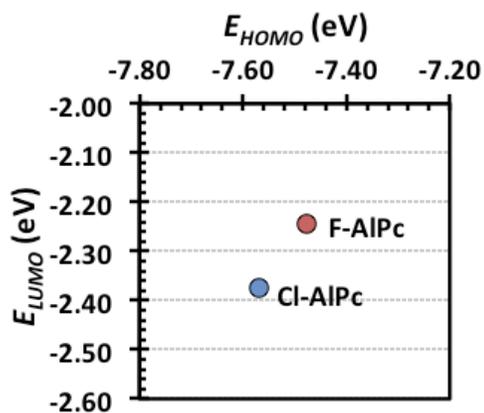
**Electronic Supporting Information.**



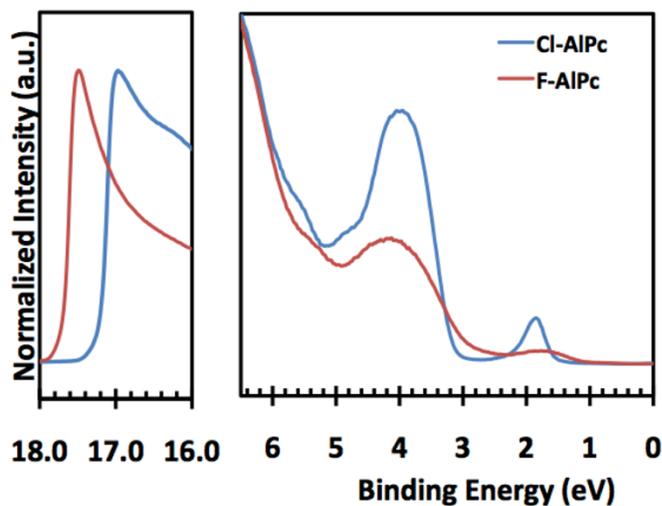
**Figure S1.** Normalized absorbance spectra of films of F-AIPc synthesized using CsF or KF.



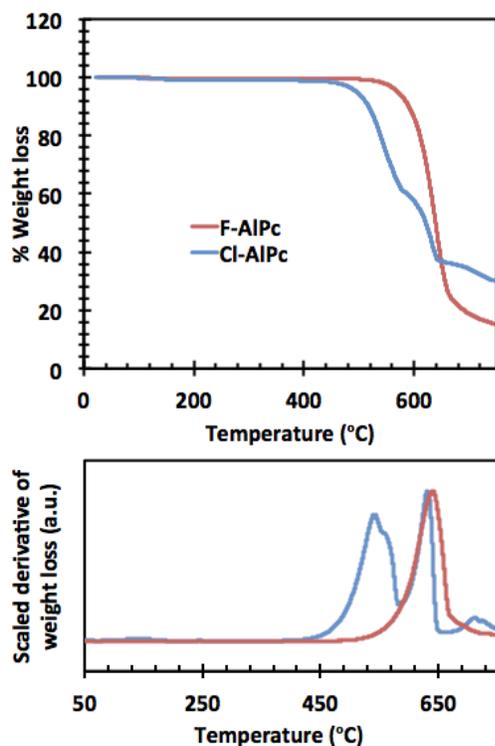
**Figure S2.** Characteristic electrochemical spectra for the A) oxidative scanning and B) reductive scanning of Cl-AIPc & F-AIPc. Electrochemistry was performed at 100mV/s scan rate (3 cycles) using a reference electrode of Ag/AgCl and internal standard of decamethyl ferrocene.



**Figure S3.** Highest occupied molecular orbital ( $E_{HOMO}$ ) and lowest unoccupied molecular orbital ( $E_{LUMO}$ ) estimated using preliminary modeling with semi-empirical level using the PM3 parameter for both F-AIPc and Cl-AIPc.



**Figure S4** - Ultraviolet photoelectron spectroscopy (UPS) spectra of both the Cl-AIPc (blue line) and the F-AIPc (red line). The energy levels are aligned to its vacuum level work function, of highly ordered pyrolytic graphite, at 4.45 eV.



**Figure S5.** Characteristic thermo gravimetric analysis (TGA) spectra, where top figure is the %mass loss relative to temperature (°C) and the bottom figure corresponds to the scaled derivative of the mass loss relative to temperature (°C) for the Cl-AlPc and F-AlPc.

**Table S1.** UV-Vis absorbances spectroscopy results for chloro and fluoro aluminum phthalocyanine .

Sample	DMSO		Chloroform		Toluene		Films	
	$\lambda_{\max}$ (nm)	E <sub>gap</sub> (eV)						
<b>AlPc-Cl</b>	680	1.78	681	1.77	688	1.77	771	1.48
<b>AlPc-F</b>	671	1.81	688	1.77	690	1.76	647	1.61