

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

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Electronic Supporting Information.

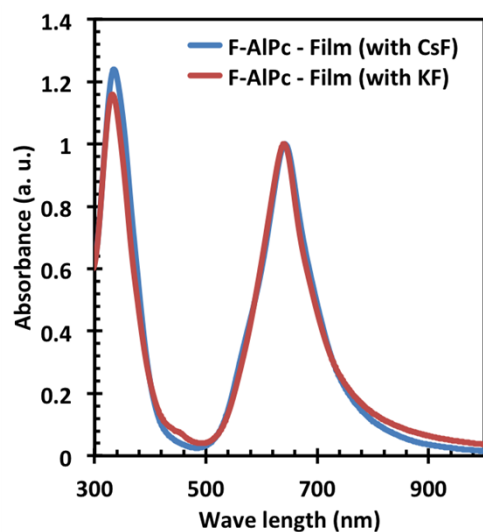


Figure S1. Normalized absorbance spectra of films of F-AlPc synthesized using CsF or KF.

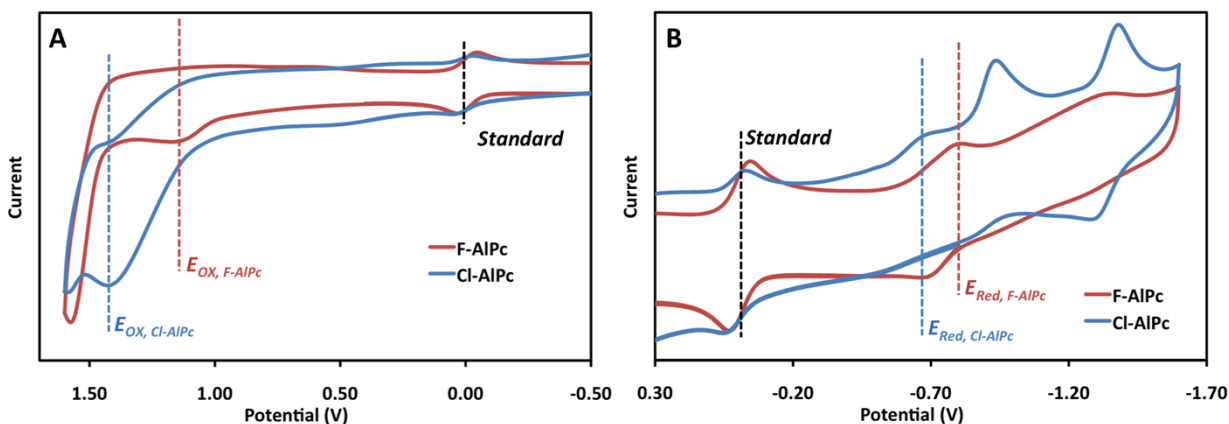


Figure S2. Characteristic electrochemical spectra for the A) oxidative scanning and B) reductive scanning of Cl-AlPc & F-AlPc. Electrochemistry was performed at 100mV/s scan rate (3 cycles) using a reference electrode of Ag/AgCl and internal standard of decamethyl ferrocene.

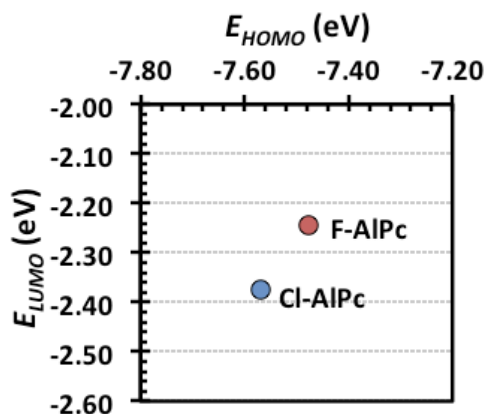


Figure S3. Highest occupied molecular orbital (E_{HOMO}) and lowest unoccupied molecular orbital (E_{LUMO}) estimated using preliminary modeling with semi-empirical level using the PM3 parameter for both F-AlPc and Cl-AlPc.

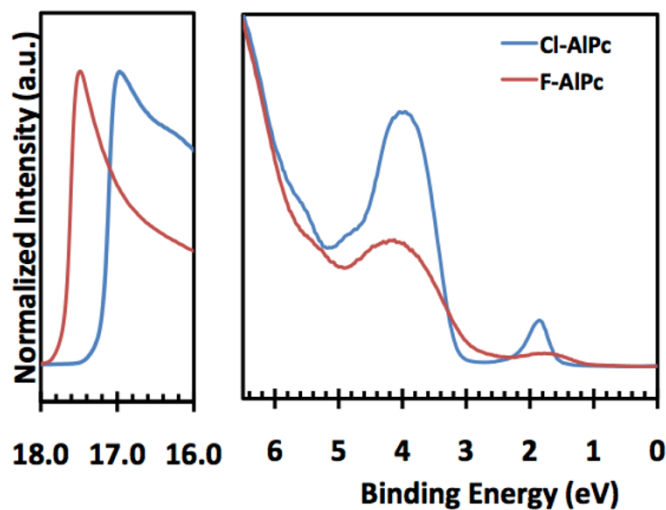


Figure S4 - Ultraviolet photoelectron spectroscopy (UPS) spectra of both the Cl-AlPc (blue line) and the F-AlPc (red line). The energy levels are aligned to its vacuum level work function, of highly ordered pyrolytic graphite, at 4.45 eV.

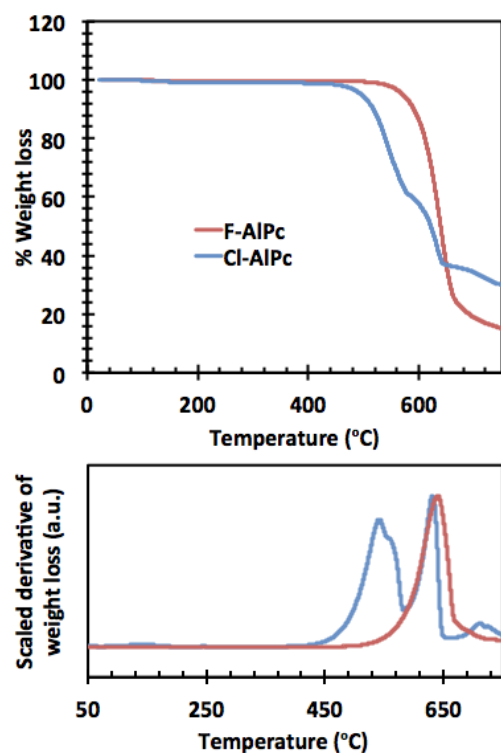


Figure S5. Characteristic thermo gravimetric analysis (TGA) spectra, where top figure is the %mass loss relative to temperature (°C) and the bottom figure corresponds to the scaled derivative of the mass loss relative to temperature (°C) for the Cl-AlPc and F-AlPc.

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

Sample	DMSO		Chloroform		Toluene		Films	
	λ_{max} (nm)	E _{gap} (eV)	λ_{max} (nm)	E _{gap} (eV)	λ_{max} (nm)	E _{gap} (eV)	λ_{max} (nm)	E _{gap} (eV)
AlPc-Cl	680	1.78	681	1.77	688	1.77	771	1.48
AlPc-F	671	1.81	688	1.77	690	1.76	647	1.61