Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.


# Supporting Information for

# Influence of axial fluorination of SubPc on photoresponse performances of organic small-molecule photodiodes

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**This file includes:**

Figures S1 to S5

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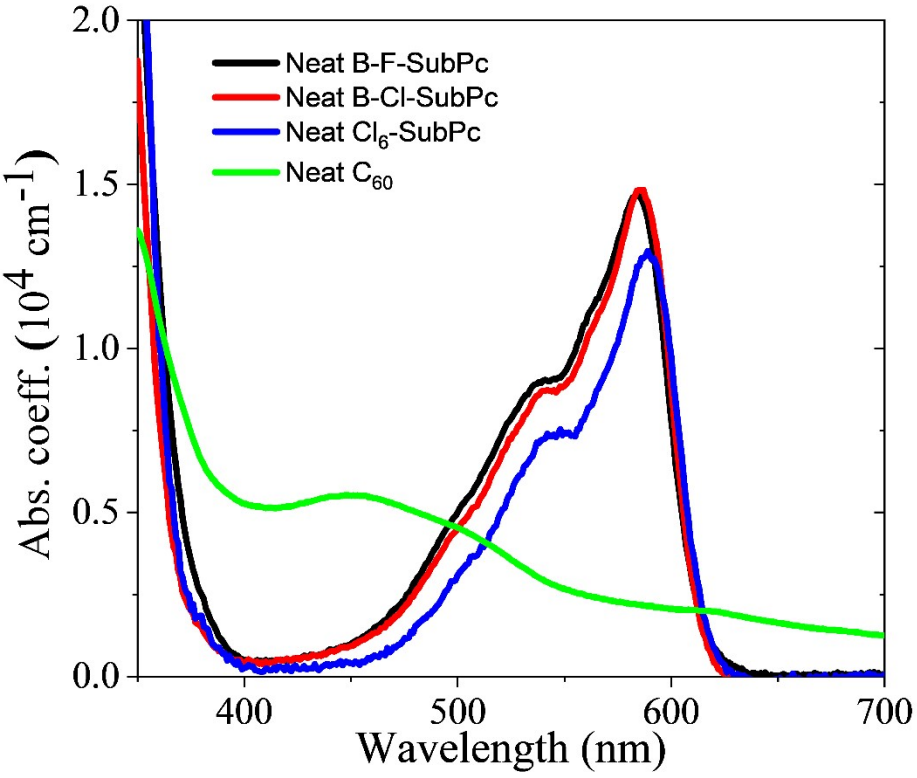


**Figure S1.** Absorption profiles of neat B-F-SubPc, B-Cl-SubPc, $C_{60}$, and $Cl_6$-SubPc films.

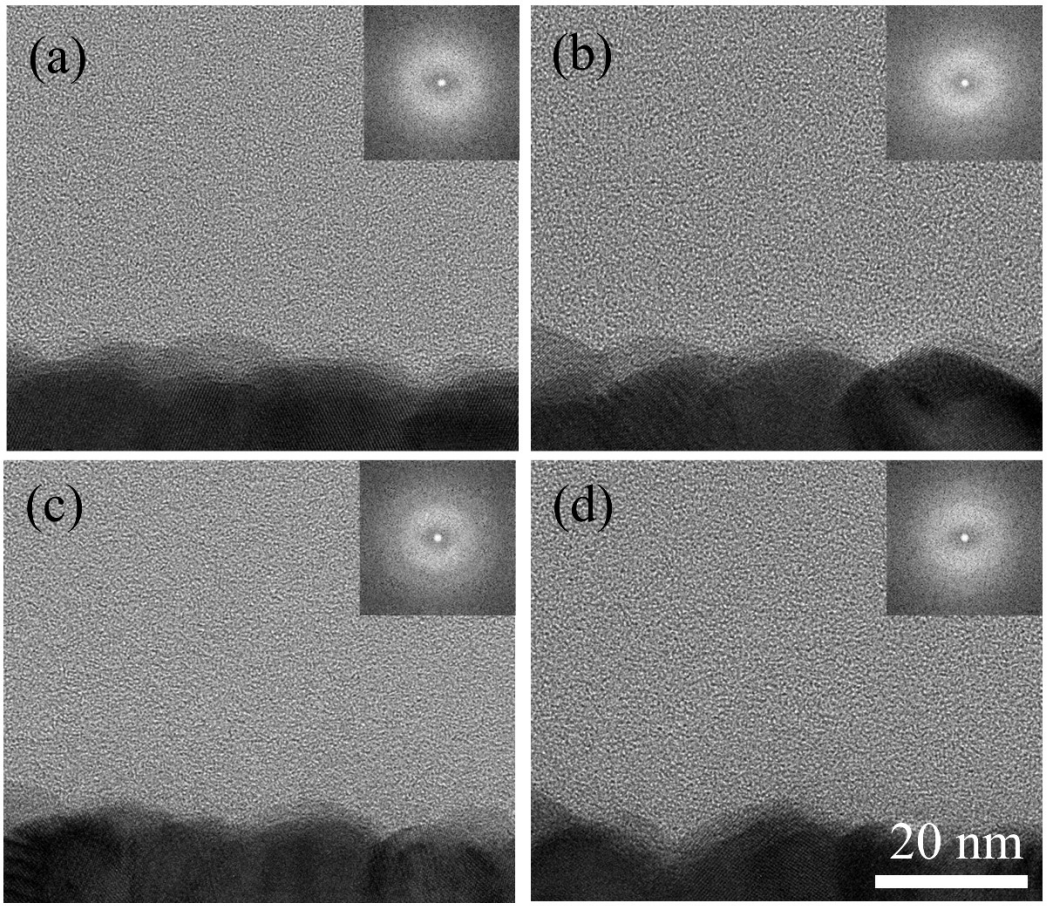


**Figure S2.** High resolution transmission electron microscopy (HR-TEM) images of sectional cross view of active layers for (a) B-Cl-SubPc+$C_{60}$, (b) B-F-SubPc+$C_{60}$, (c) B-Cl-SubPc+$Cl_6$-SubPc, and (d) B-F-SubPc+$Cl_6$-SubPc blends. The insets indicate Fast-Fourier transforms of selected region of the corresponding image.

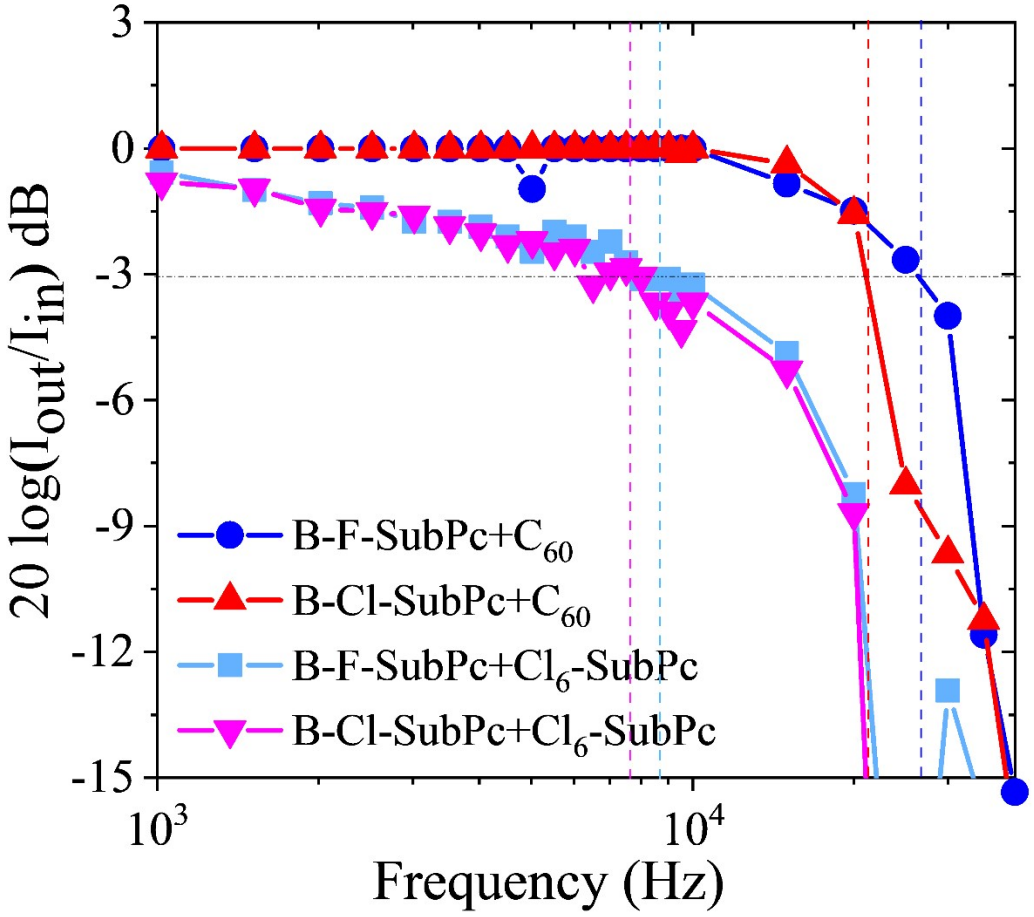


**Fig S3** Frequency-dependent photoresponse curves under zero bias (light intensity = 1 mW/cm$^2$, wavelength = 553 nm)

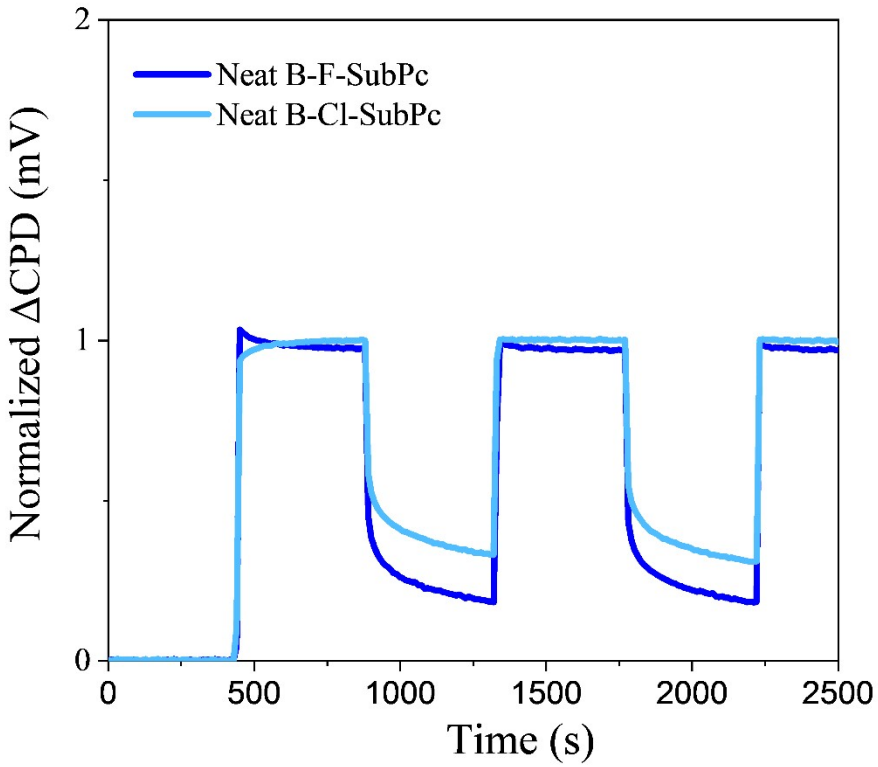


**Figure S4.** Normalized surface photovoltage plot as a function of time for isolated B-F-SubPc and B-Cl-SubPc films deposited on an EBL/Ag substrate (light: 545 nm, duration of dark/illuminated conditions: 400 s).

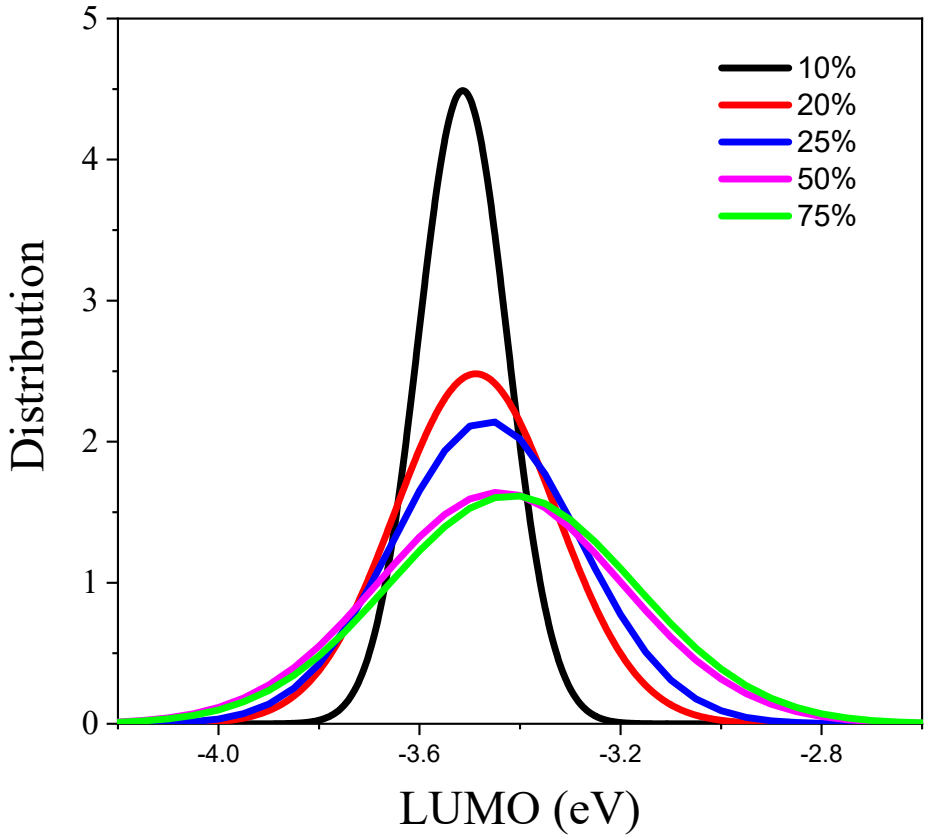


**Figure S5.** Simulated energy distribution of the LUMO for $C_{60}$ in a blend with different mixing ratios of B-Cl-SubPc.

**Table S1.**

Optoelectronic properties of fabricated BHJ blend films

| Blend film (Donor+Acceptor) | $\lambda_{max}$ (nm) | FWHM (nm) | Absorption coefficient ($\alpha$, $10^4$ $cm^{-1}$) |
|---|---|---|---|
| B-F-SubPc+$C_{60}$ | 577 | 88 | 7.0 |
| B-Cl-SubPc+$C_{60}$ | 581 | 82 | 6.9 |
| B-F-SubPc+$Cl_6$-SubPc | 578 | 110 | 11.37 |
| B-Cl-SubPc+ $Cl_6$-SubPc | 581 | 106 | 12.72 |

**Table S2.**

Average electron hopping rates ($k_{nn}$) for dimers of donor-donor molecules and percentages of molecular pairs with a low hopping rate (defined as $\log(k_{nn}) < 6$) in morphologies of BHJ layers obtained by DFT calculations.

| Donor | Acceptor | $k_{nn}$ / $10^{13}$ | Low-hopping-rate pairs [%] |
|---|---|---|---|
| B-F-SubPc | $Cl_6$-SubPc | 0.23 | 15.5 |
| B-Cl-SubPc | $Cl_6$-SubPc | 0.60 | 14.5 |
| B-F-SubPc | $C_{60}$ | 1.3 | 5.0 |
| B-Cl-SubPc | $C_{60}$ | 1.1 | 10.0 |