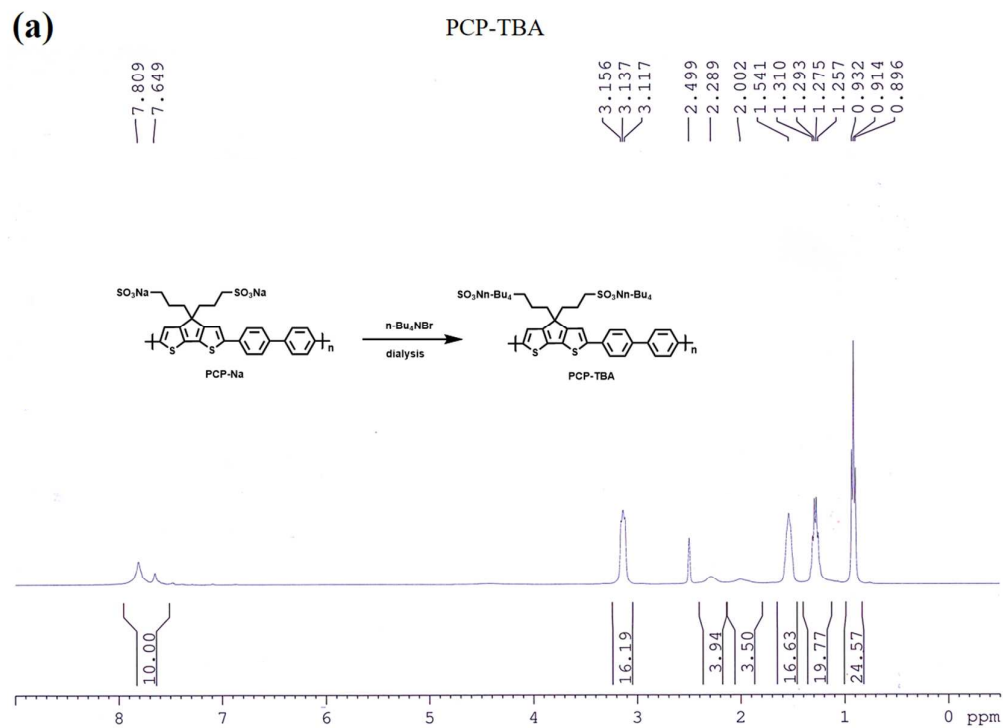


A Novel pH Neutral Self-doped Polymer for Anode Interfacial Layer in Efficient Polymer Solar Cells

Yong Cui, Bowei Xu*, Bei Yang, Huifeng Yao, Sunsun Li, and Jianhui Hou*



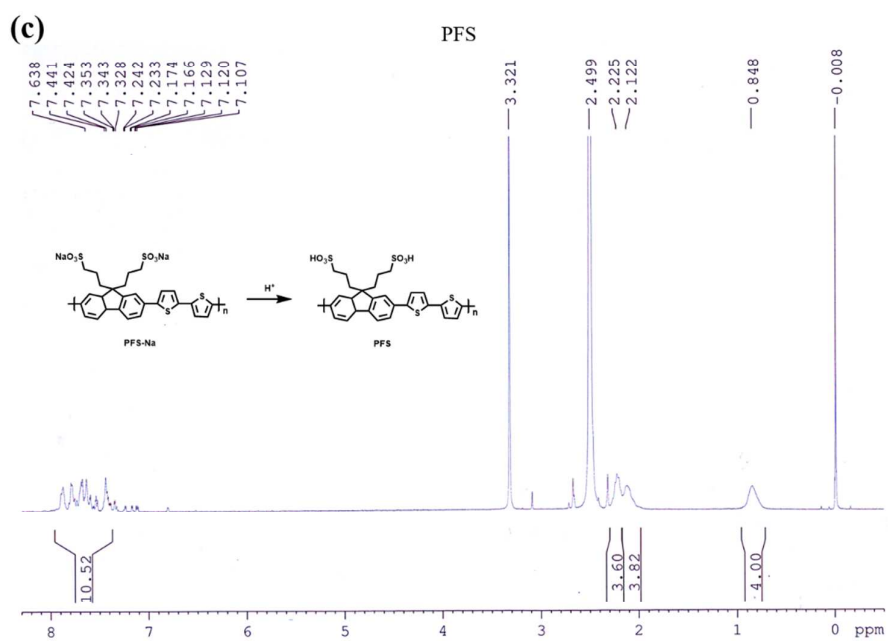
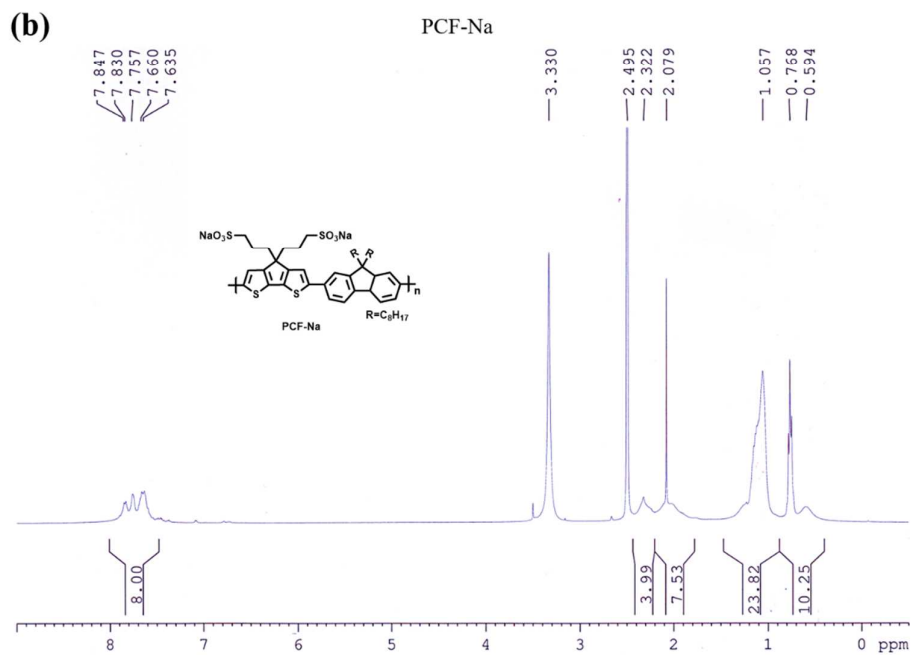


Figure S1. The ¹H NMR spectra of (a) PCP-TBA, (b) PCF-Na and (c) PFS in DMSO-d₆.

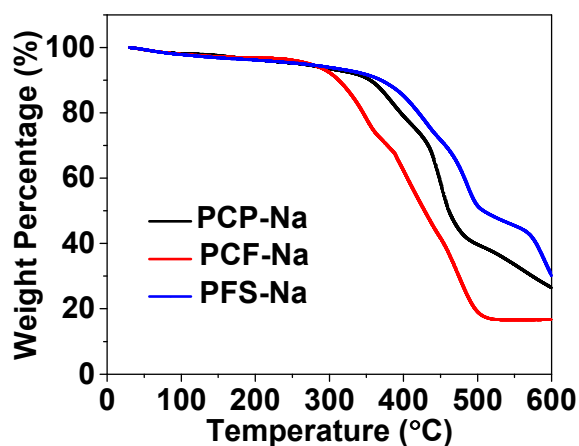


Figure S2. TGA curves of three anode interface layer materials at scan rate of 6 °C/min under N₂ atmosphere.

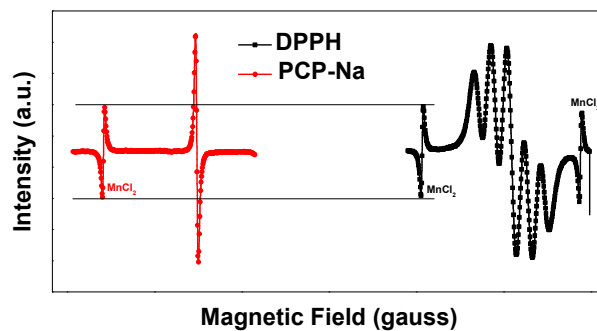


Figure S3. EPR curves of PCP-Na and DPPH.

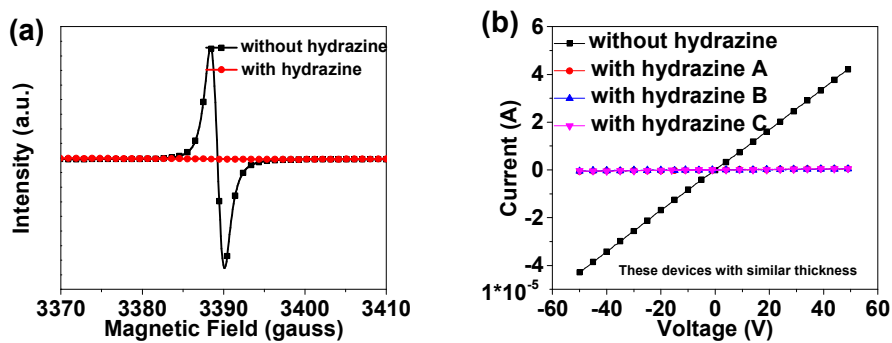


Figure S4. (a) EPR curves of PCP-Na with and without hydrazine. (b) I - V characteristics of thin films with and without hydrazine. A: in the nitrogen; B:

annealing for 15min in the air; C: Stand for 24 hours in the air.

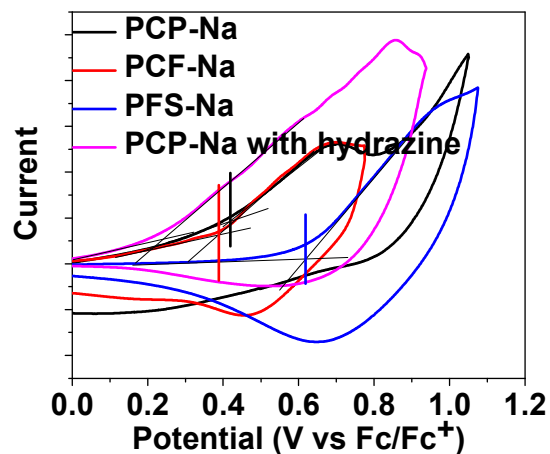


Figure S5. CV curves of PCP-Na, PCF-Na, PFS-Na and PCP-Na with hydrazine. The cyclic voltammetry (CV) experiments were performed in anhydrous acetonitrile solution with 0.1 mol/L Bu₄NPF₆ at scan rate 50 mV/s.

The HOMO level of PCP-Na was obtained according to the following equation: $E_{HOMO} = (h\nu - E_{onset}) + E_{cutoff}$, Where $h\nu$ is the incident photon energy ($h\nu = 21.22$ eV) for He; E_{onset} is the onset value of HOMO energy region as shown in the right panel; E_{cutoff} is defined as the inelastic secondary electron edge obtained from the left panel. Thus, the HOMO level of PEDOT:PSS and PCP-Na is -5.11 eV and -5.25 eV, respectively.

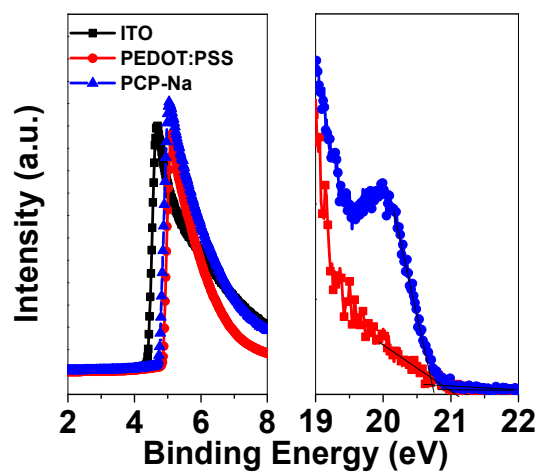


Figure S6. Ultraviolet photoelectron spectra (UPS) of PEDOT:PSS and PCP-Na

Thickness data of PCP-Na, PCF-Na and PFS-Na film

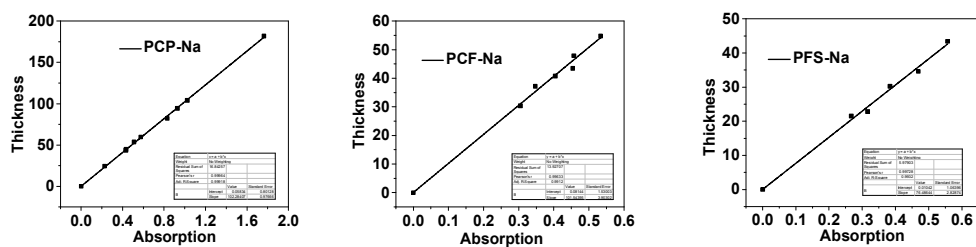
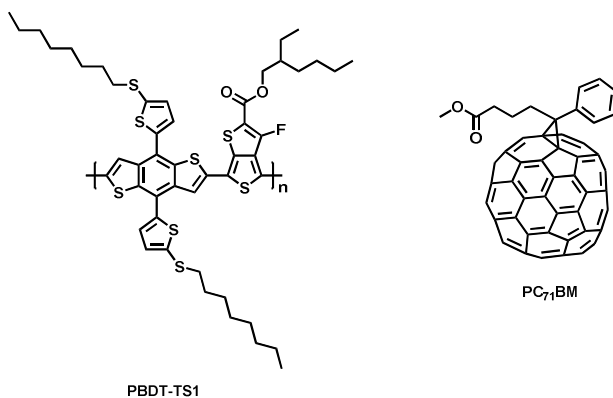


Figure S7. A linear relationship of absorption versus thickness.



Scheme S1. The chemical structures of PBDT-TS1 and PC₇₁BM

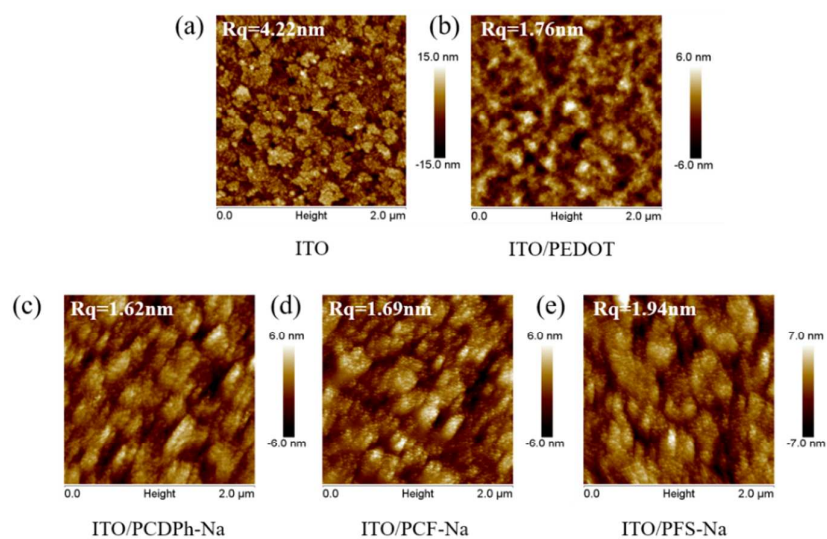


Figure S8. AFM height images of (a) the bare ITO and the ITO modified by (b) PEDOT, (c) PCP-Na, (d) PCF-Na, (e) PFS-Na.

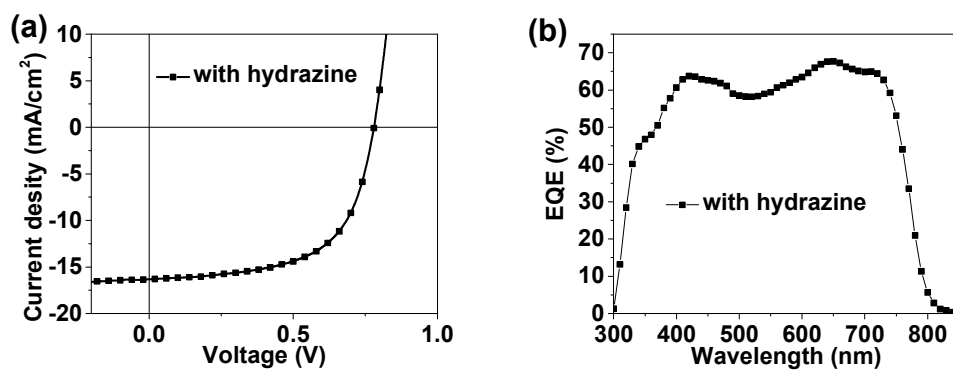


Figure S9. (a) $J-V$ curves and (b) EQE of solar cells based on PCP-Na with hydrazine.

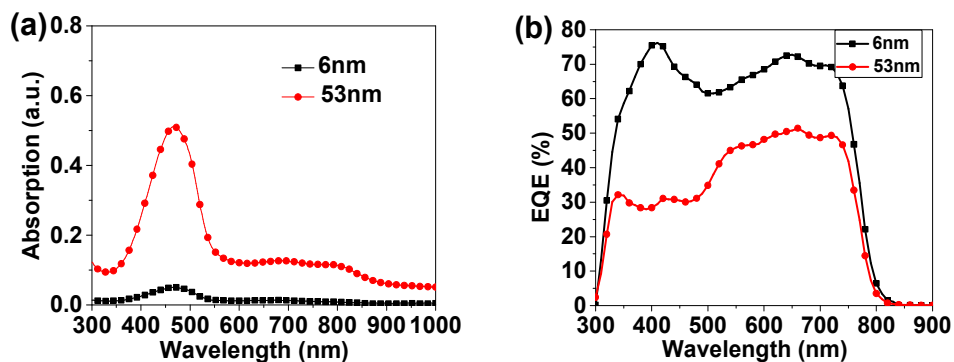


Figure S10. (a) Absorption spectra and (b) EQE spectra of the devices with different PCP-Na thicknesses.

Table S1. Devices parameters using different anode interfacial layer with different thickness. The device structure is ITO/interfacial layer/PBDT-TS1:PC₇₁BM/Mg/Al.

Interfacial layer	V_{oc} [V]	J_{sc} [mA·cm ⁻²]	FF[%]	PCE[%]	Thickness(nm) ^a
PCP-Na	0.799	16.18	68.77	8.89	1.59
	0.798	17.36	69.35	9.61	4.05
	0.803	17.46	70.57	9.89	6.23
	0.800	17.25	70.42	9.72	9.14
	0.798	16.27	70.87	9.20	19.8
	0.795	15.19	70.15	8.47	29.8
	0.793	13.8	70.34	7.70	37.1
	0.786	11.83	70.11	6.52	52.9
	0.782	10.48	70.69	5.80	73.9
	0.774	9.43	70.66	5.16	95.0
	0.777	8.4	70.14	4.57	105
	0.774	7.76	70.04	4.21	180
	0.767	6.92	70.39	3.74	308
	0.775	16.96	66.18	8.7	2.11
PCF-Na	0.793	17.01	69.13	9.33	3.02
	0.797	17.47	67.9	9.45	4.95
	0.800	17.29	67.93	9.40	9.36
	0.796	15.8	59.27	7.45	26.5

	0.797	15.26	42.57	5.18	35.3
	0.791	12.53	26.12	2.59	48.9
PFS-Na	0.690	16.44	62.81	7.12	2.22
	0.791	16.45	62.69	8.16	4.82
	0.793	15.89	55.23	6.96	9.21
	0.796	15.23	40.50	4.91	15.4
PEDOT	0.795	16.81	66.94	8.95	6.83
	0.784	13.91	67.33	7.35	334
