

Supporting Information

Polymer/Polymer Blend Solar Cells Using Tetraazabenzodifluoranthene Diimide Conjugated Polymers as Electron Acceptors

Haiyan Li,[†] Ye-Jin Hwang,[†] Taeshik Earmme,[†] Rachel C. Huber,[‡] Brett A. E. Courtright,[†] Conor O'Brien,[†] Sarah H. Tolbert^{‡,§} and Samson A. Jenekhe^{*,†}

[†] Department of Chemical Engineering and Department of Chemistry, University of Washington, Seattle, WA 98195-1750, USA.

[‡] Department of Chemistry and Biochemistry and the California NanoSystems Institute, UCLA, , Los Angeles, California 90095-1569, USA.

[§] Department of Materials Science and Engineering, UCLA, Los Angeles, CA 90095, USA

1. Supporting Figures

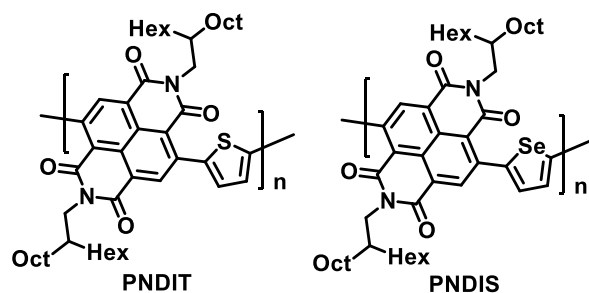


Figure S1. Molecular structures of PNDIT and PNDIS.

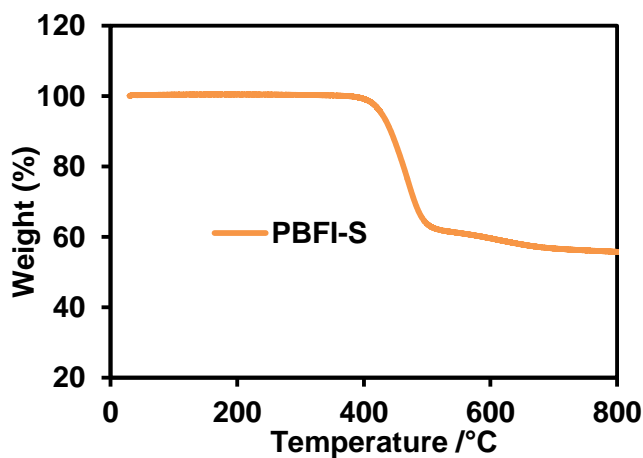


Figure S2. The TGA trace of PBFI-S (heating at 10 °C/min under N₂).

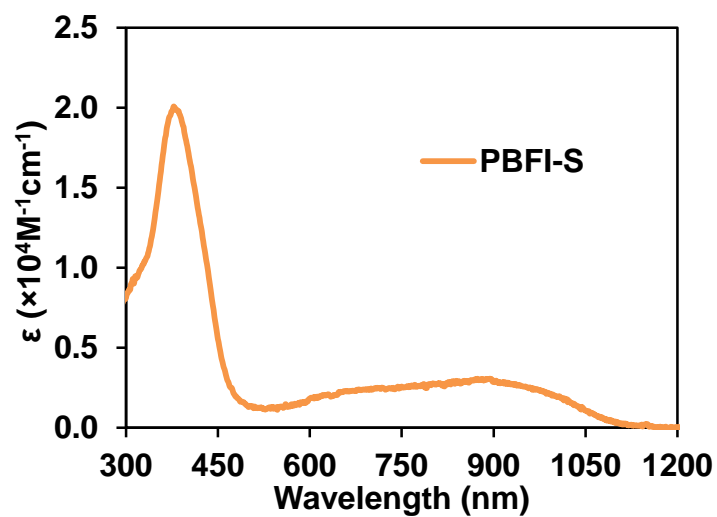


Figure S3. Optical absorption spectra of PBFI-S in CHCl_3 .

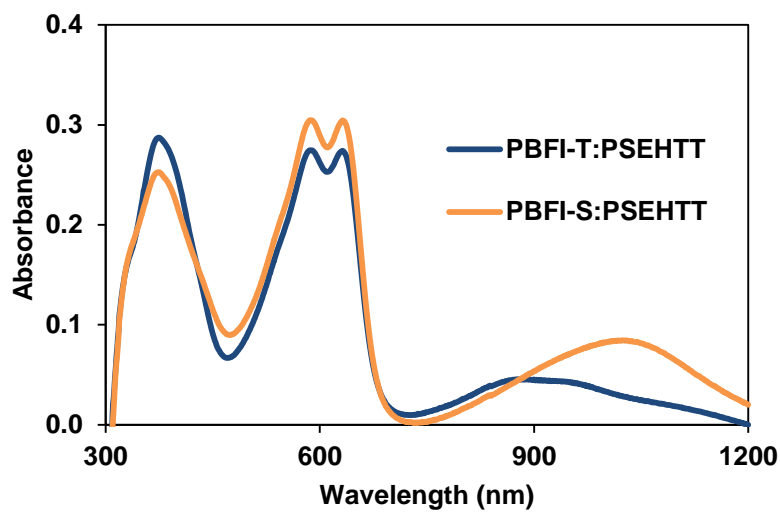


Figure S4. Optical absorption spectra of PBFI-T:PSEHTT and PBFI-S:PSEHTT blend active layers.

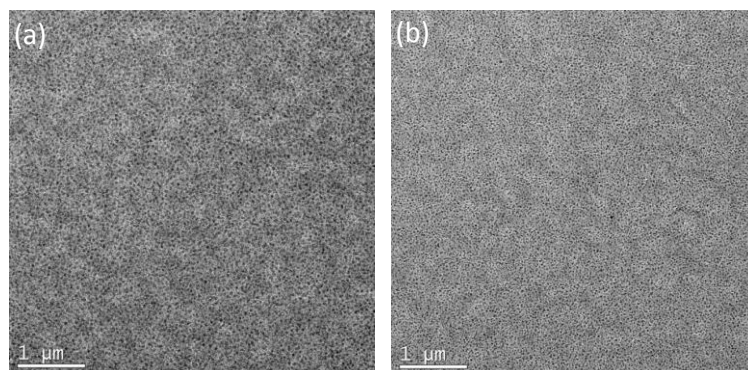


Figure S5. Bright-field TEM images of the PBFI-S:PSEHTT (a) and PBFI-T:PSEHTT (b) blends.

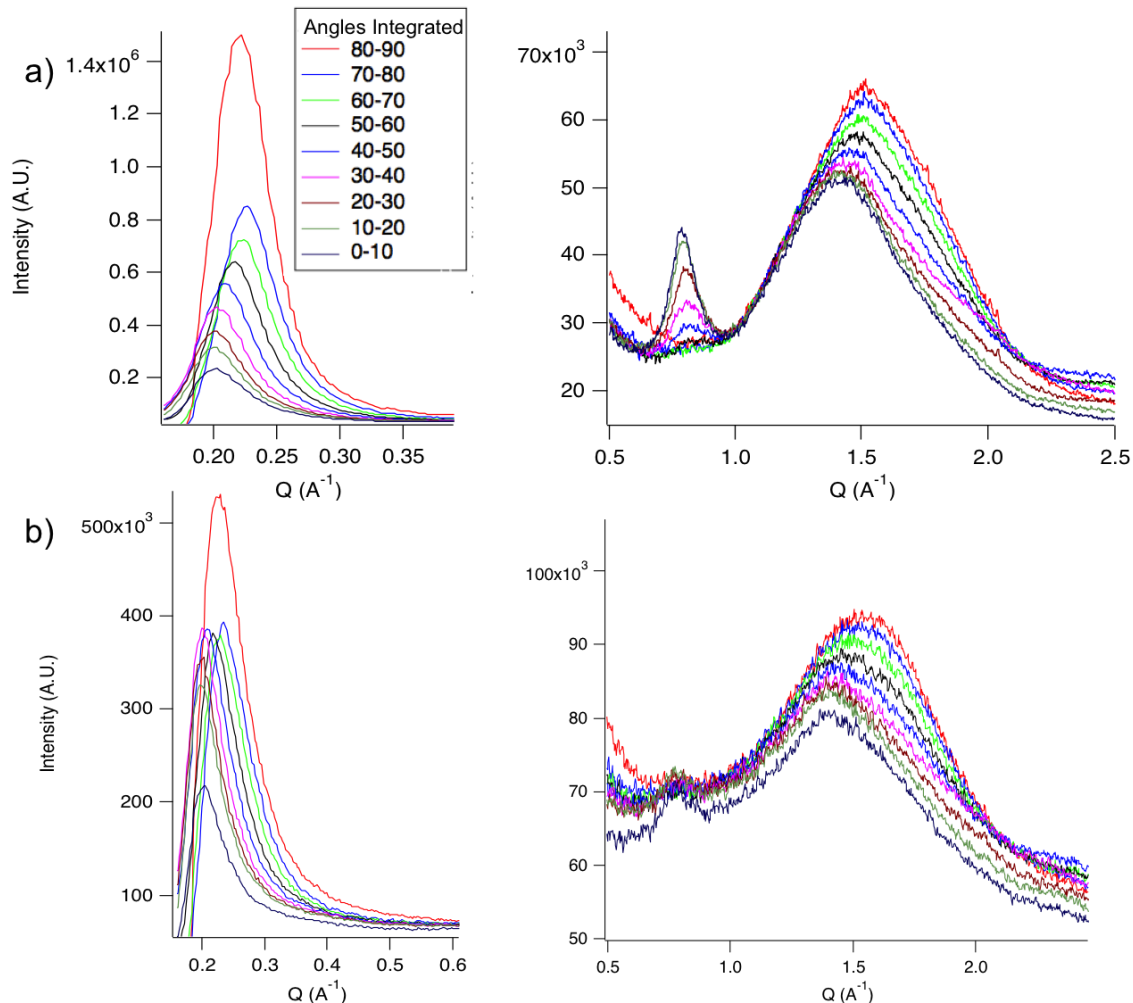


Figure S6: X-ray diffraction patterns as a function of diffractometer angle χ . Pure PBFI-T (a) and pure PBFI-S (b) integrations of 2D diffraction pattern in 10° slices from 0 - 90° . The 0 - 10° integration corresponds to the in-plane diffraction and the 80 - 90° integration is the out-of-plane diffraction. The shift between in and out-of-plane is significant for both the (100) and (010) peaks. Because a gradual peak shift is observed going from in- to out-of-plane diffraction, this shift is likely indicative of a real change in lattice constant caused by packing differences between edge-on and face-on oriented polymer chains. It is unlikely to be caused by interference from specular reflectance, which should only affect angle near 90° .

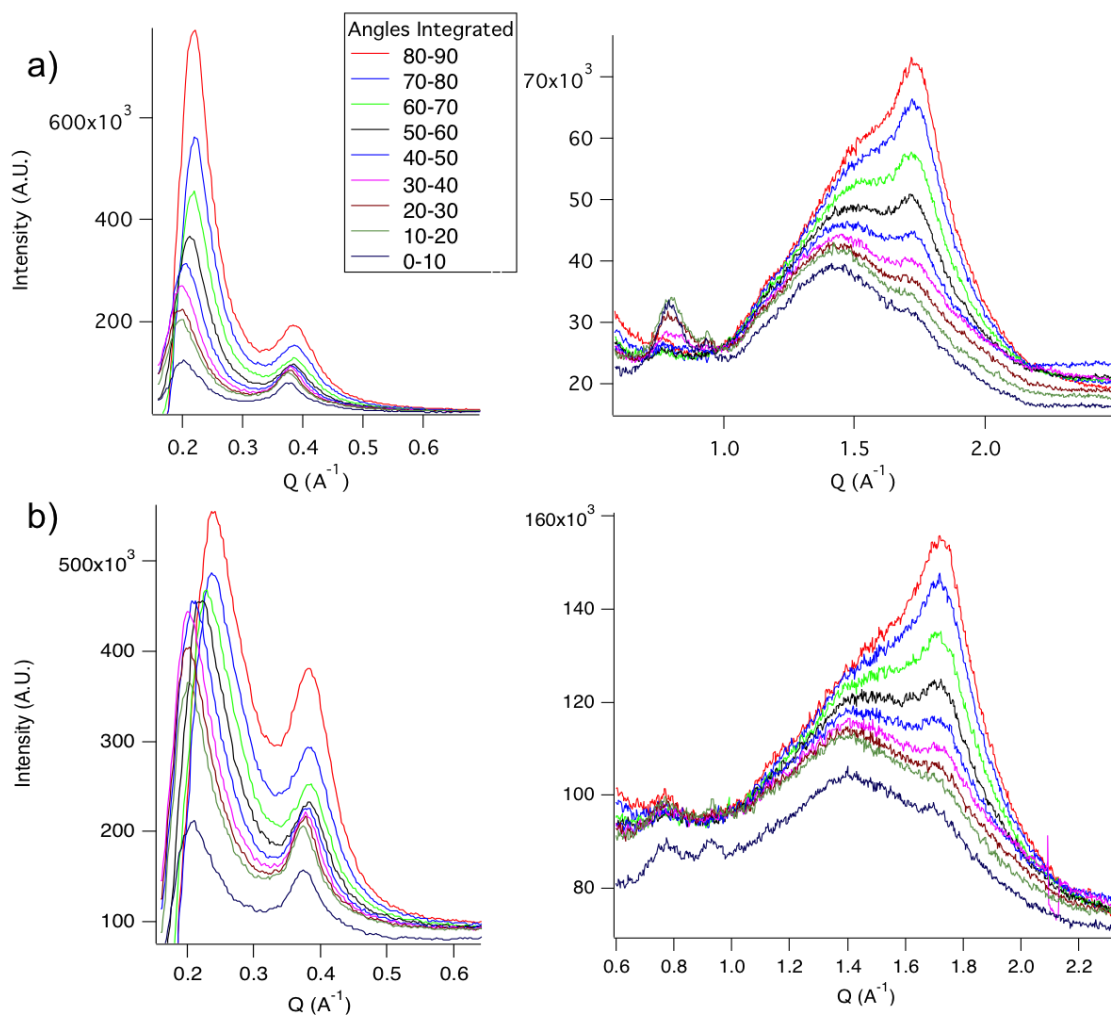


Figure S7: a) X-ray diffraction patterns as a function of diffractometer angle χ . PSEHTT:PBFI-T BHI blend (a) and PSEHTT:PBFI-S blend (b) integrations of 2D diffraction pattern in 10° slices from $0-90^\circ$. The $0-10^\circ$ integration corresponds to the in-plane diffraction and the $80-90^\circ$ integration is the out-of-plane diffraction. Significant shifts are again observed for the PBFI-T and PBFI-S peaks, but the PSEHTT peaks show almost no shifts, indicating less conformational freedom for the PSEHTT.

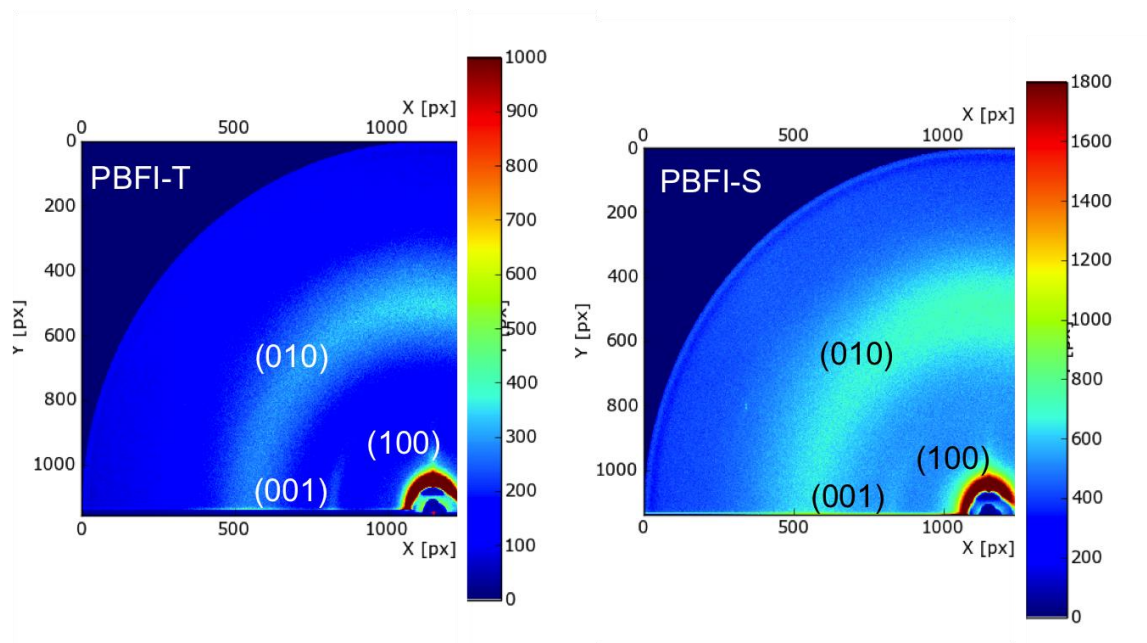


Figure S8: Raw 2D grazing incidence diffraction patterns for pure PBFI-T and PBFI-S films. The vertical axis corresponds to out-of-plane diffraction and the horizontal axis corresponds to in-plane diffraction. Peaks are indexed on the image.

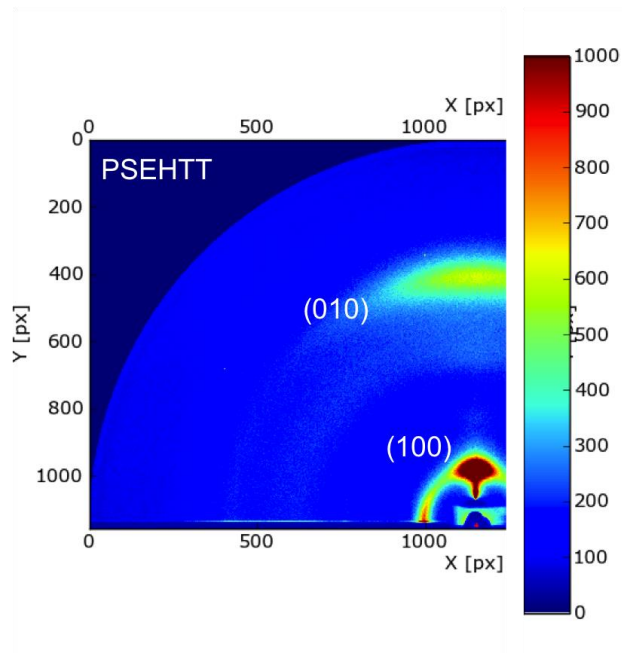


Figure S9: Raw 2D grazing incidence diffraction patterns for a pure PSEHTT film. The vertical axis corresponds to out-of-plane diffraction and the horizontal axis corresponds to in-plane diffraction. Peaks are indexed on the image.

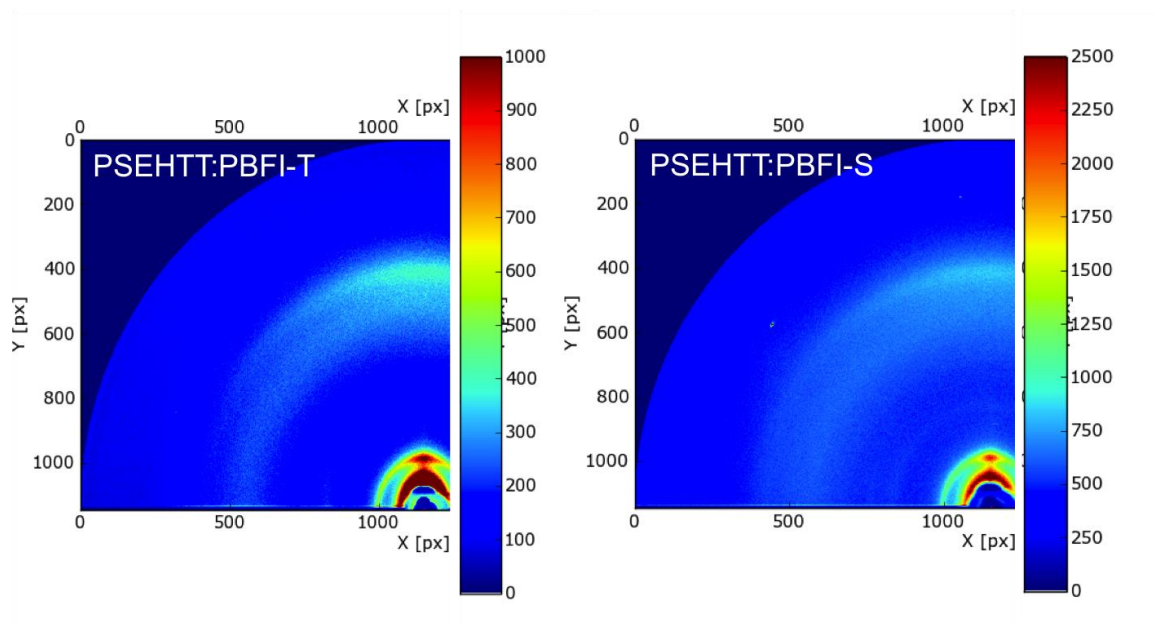


Figure S10: Raw 2D grazing incidence diffraction patterns for PSEHTT:PBFI-T and PSEHTT:PBFI-S blend films. The vertical axis corresponds to out-of-plane diffraction and the horizontal axis corresponds to in-plane diffraction.

Table S1. Summary of photovoltaic properties of PBFI-T:PSEHTT and PBFI-S:PSEHTT blends^a

Blend	Blend Ratio (wt:wt)	J_{sc} (mA/cm ²)	V_{oc} (V)	FF	PCE (%)
PBFI-T: PSEHTT	3:1	3.86 (3.78±0.07)	0.67 (0.67±0.00)	0.50 (0.49±0.01)	1.30 (1.23±0.6)
PBFI-T: PSEHTT	1:1	5.18 (5.15±0.03)	0.68 (0.68±0.00)	0.53 (0.52±0.01)	1.87 (1.82±0.05)
PBFI-S: PSEHTT	3:1	2.52 (2.47±0.05)	0.51 (0.51±0.00)	0.36 (0.36±0.01)	0.46 (0.46±0.01)
PBFI-S: PSEHTT	1:1	2.83 (2.73±0.09)	0.51 (0.51±0.00)	0.43 (0.44±0.01)	0.62 (0.62±0.01)

^aActive layers were deposited from the PBFI-X (X = T or S):PSEHTT (1:1 or 3:1 wt/wt) blend solutions in chlorobenzene, respectively, followed by annealing at 175 °C for 10 min.

Table S2: In- and out-of-plane peak positions of pure polymers, blends and fits for Figures 6 and 7.

	Out-of-Plane Peak Position (Å ⁻¹)				In-Plane Peak Position (Å ⁻¹)			
	(100)	(001)	(010)		(100)	(001)	(010)	
PBFI-T	0.22	0.80	1.52		0.20	0.80	1.44	
PBFI-S	0.23	0.80	1.57		0.20	0.80	1.39	
PSEHTT	0.38	---	1.31	1.72	0.37	0.93	1.31	1.72
PBFI-T:PSEHTT	PBFI-T	0.22	---	1.52	0.2	0.80	1.41	
	PSEHTT	0.39	---	1.73	0.38	0.93	1.70	
PBFI-S:PSEHTT	PBFI-S	0.24	---	1.56	0.21	0.80	1.39	
	PSEHTT	0.38		1.72	0.37	0.93	1.70	
PBFI-T:PSEHTT Fits	PBFI-T	0.22	---	1.51	0.20	0.80	1.43	
	PSEHTT	0.41	---	1.73	0.37	0.93	---	
PBFI-S:PSEHTT Fits	PBFI-S	0.23	---	1.55	0.20	0.80	1.37	
	PSEHTT	0.40	---	1.73	0.37	0.93	1.70	