Supporting information

Highly Efficient Indoor Organic Solar Cells by Voltage Losses Minimization through Fine-tuning of Polymer Structures

Ranbir Singh,[†] Christos L. Chochos,[*,§,∥] Vasilis G. Gregoriou,[⊥] Alkmini D. Nega,[⊥] Min Kim,[#] Manish Kumar,[∇] Sang-Chul Shin,[‡] Sang Hyeon Kim,[‡] Jae Won Shim,[‡,Ψ] and Jae-Joon Lee[*,†]

[†] Department of Energy & Materials Engineering, Research Center for Photoenergy Harvesting & Conversion Technology (*phct*) and [‡] Division of Electronics and Electrical Engineering, Dongguk University, Seoul 04620, Republic of Korea

[§] Advent Technologies SA, Stadiou Street, Platani, Rio, Patras 26504, Greece

[∥] Institute of Chemical Biology, National Hellenic Research Foundation, 48 Vassileos Constantinou Avenue, Athens 11635, Greece

[⊥] National Hellenic Research Foundation, 48 Vassileos Constantinou Avenue, Athens 11635, Greece

[#] Center for Nano Science and Technology@Polimi, Istituto Italiano di Tecnologia, via Giovanni Pascoli 70/3, Milan 20133, Italy

[∇] Pohang Accelerator Laboratory, Pohang University of Science and Technology, Pohang 37673, Republic of Korea

[Ψ] School of Electrical Engineering, Korea University, Seoul 02841, Republic of Korea

*Corresponding authors: jjlee@dongguk.edu, cchochos@advent-energy.com, chochos@eie.gr

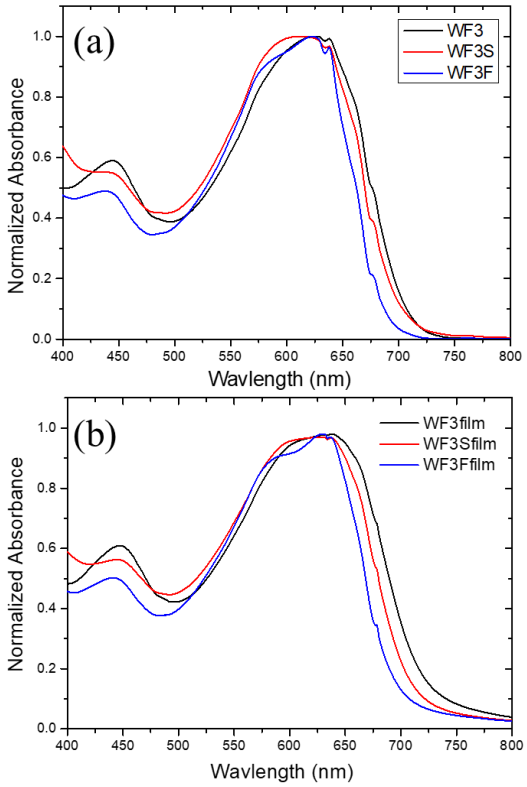

Figure S1. Absorption spectra of WF3, WF3S and WF3F in (a) solution, and (b) as thin films.

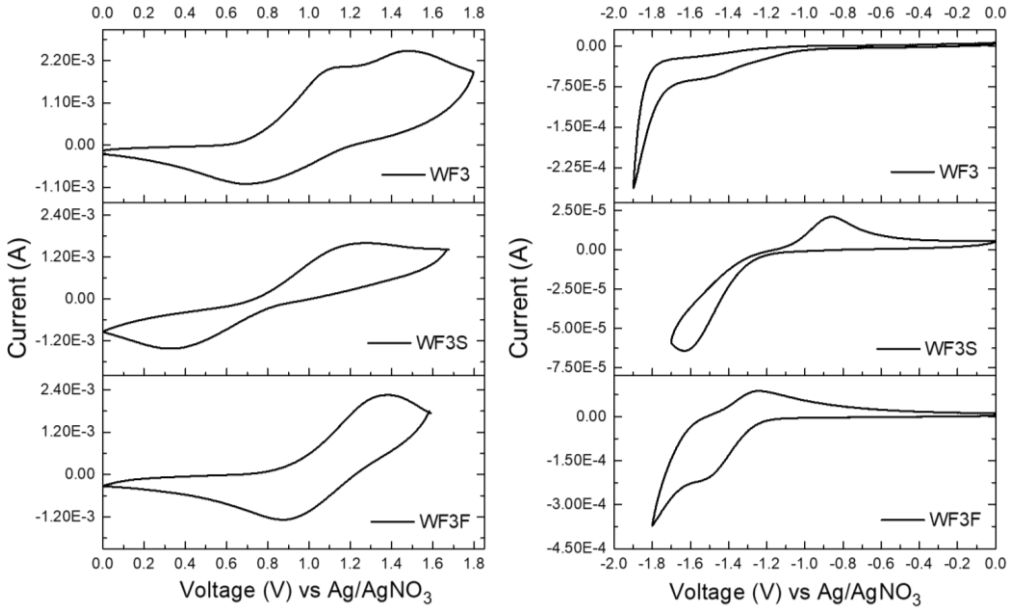

Figure S2. Oxidation (left) and reduction (right) processes of WF3, WF3S and WF3F as thin f ilms.

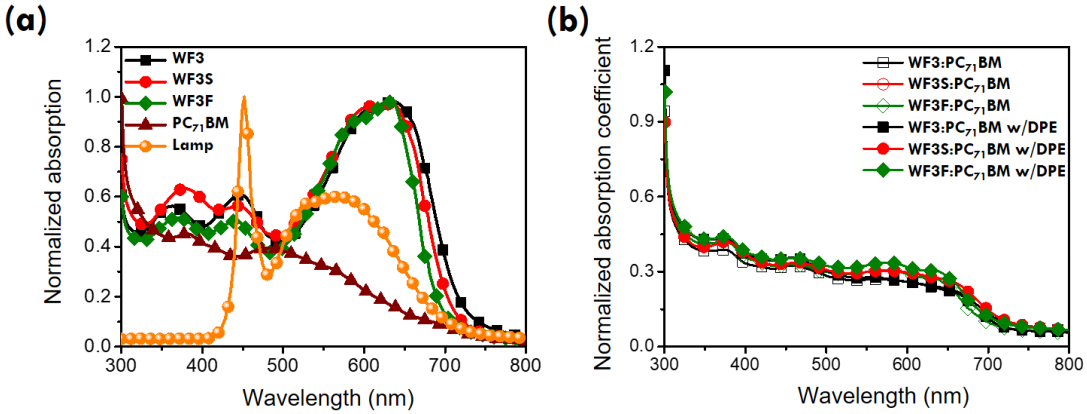

Figure S3. (a) Normalized absorption spectra for the polymers, $PC_{71}BM$ films and LED lamp spectrum (b) normalized absorption coefficient for blend films with (w/) and without (w/o) D PE.

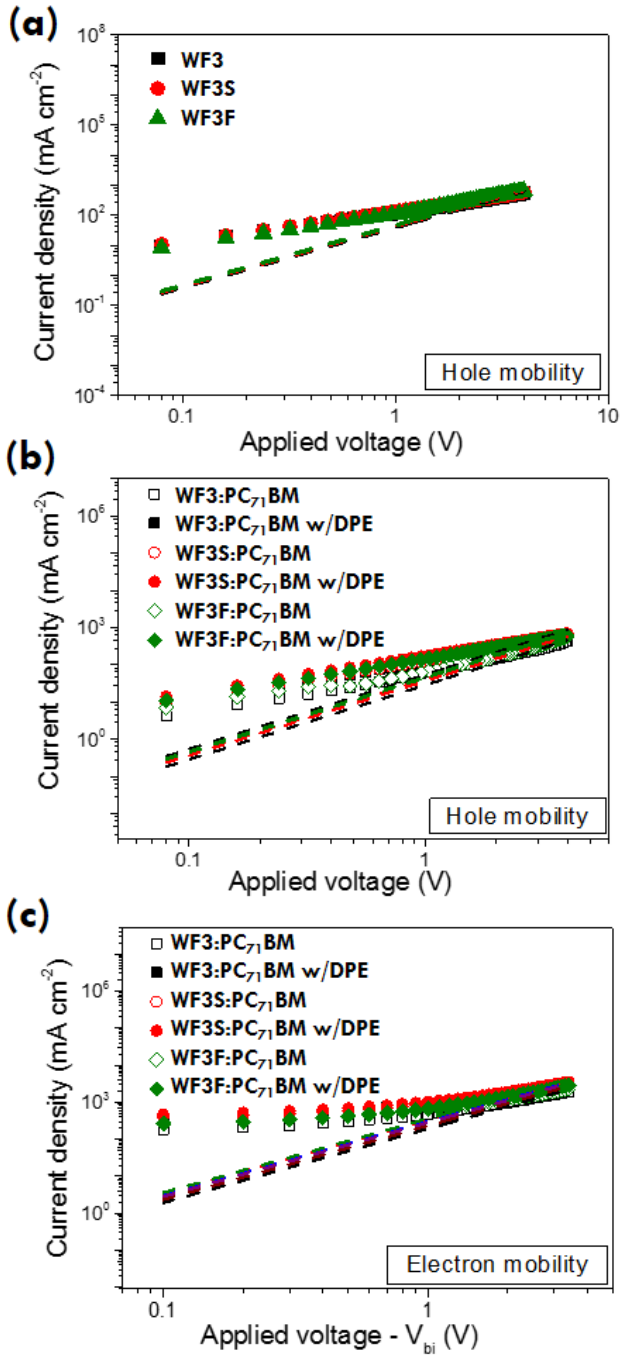

Figure S4. Dark J-V characteristics for the (a) hole only devices for the pure polymers (WF3, WF3S and WF3F). J-V characteristics for the (b) hole only and (c) electron only devices of the WF3:PC_{71}BM, WF3S:PC_{71}BM and WF3F:PC_{71}BM blend system. Experimental data fitted with Mott-Gurney equation to extract chare carrier mobility values.[1]

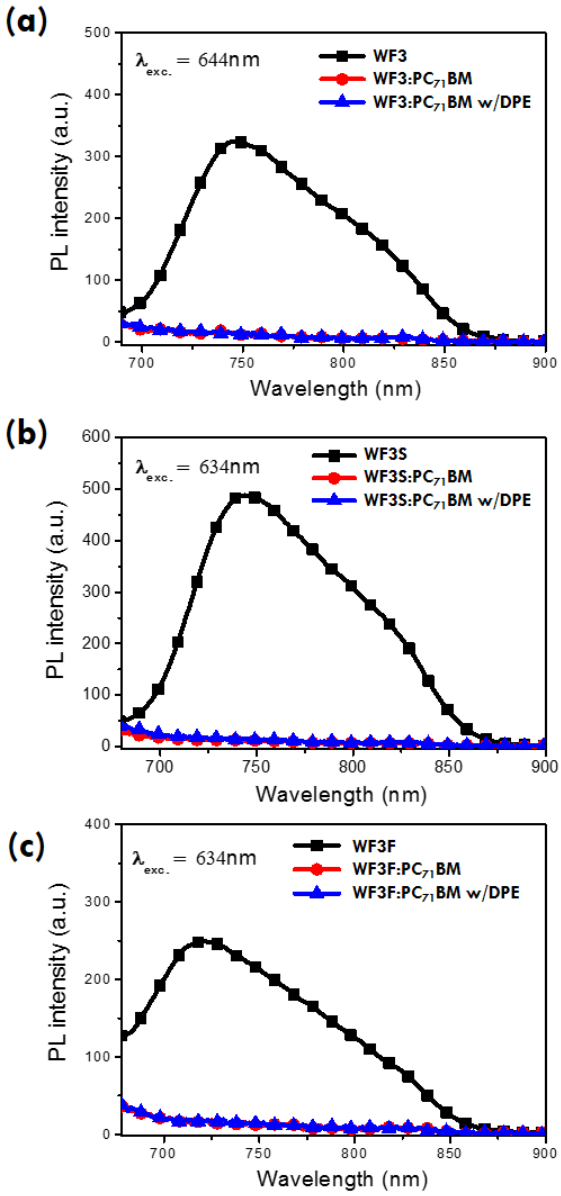

Figure S5. PL spectra of the pristine and blend films (a) WF3, WF3:$PC_{71}BM$, WF3:$PC_{71}BM$ w/DPE (b) WF3S, WF3S:$PC_{71}BM$, WF3S:$PC_{71}BM$ w/DPE and (c) WF3F, WF3F:$PC_{71}BM$, WF3F:$PC_{71}BM$ w/DPE.

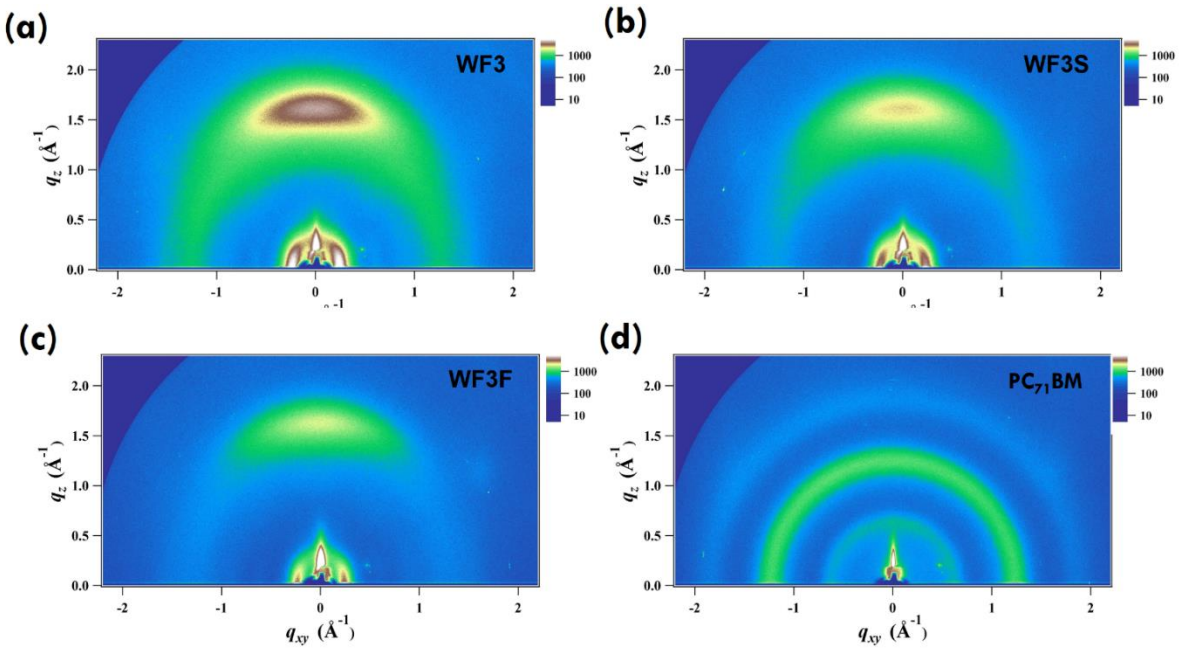

Figure S6. GIWAXS images for the polymers (a) WF3, (b) WF3S and (c) WF3F and (d) $PC_{71}BM$ film, where all the polymer films were spin-coated on the Si-wafer substrates.

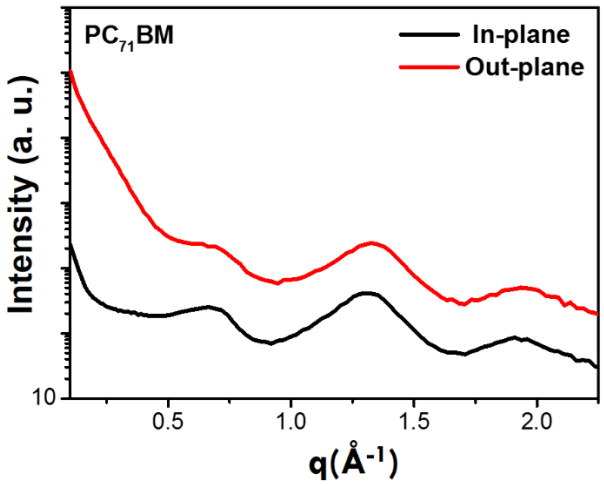

Figure S7. In-plane and out-of-plane GIWAXS scans for the $PC_{71}BM$ film.

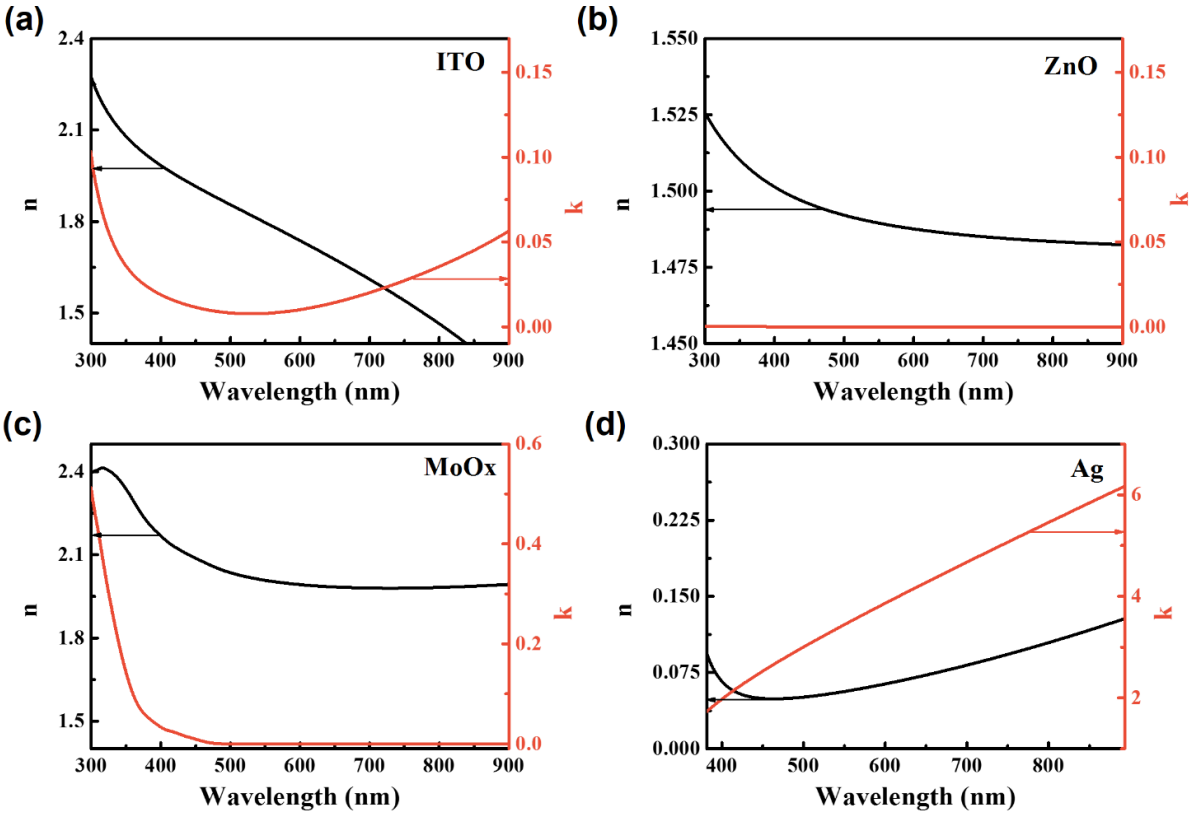

Figure S8. n(λ) and k(λ) values for the thin films (a) ITO, (b) Ag, (c) MoOx and (d) Ag meas ured with the Spectroscopic Ellipsometer (Woollam, M2000D).

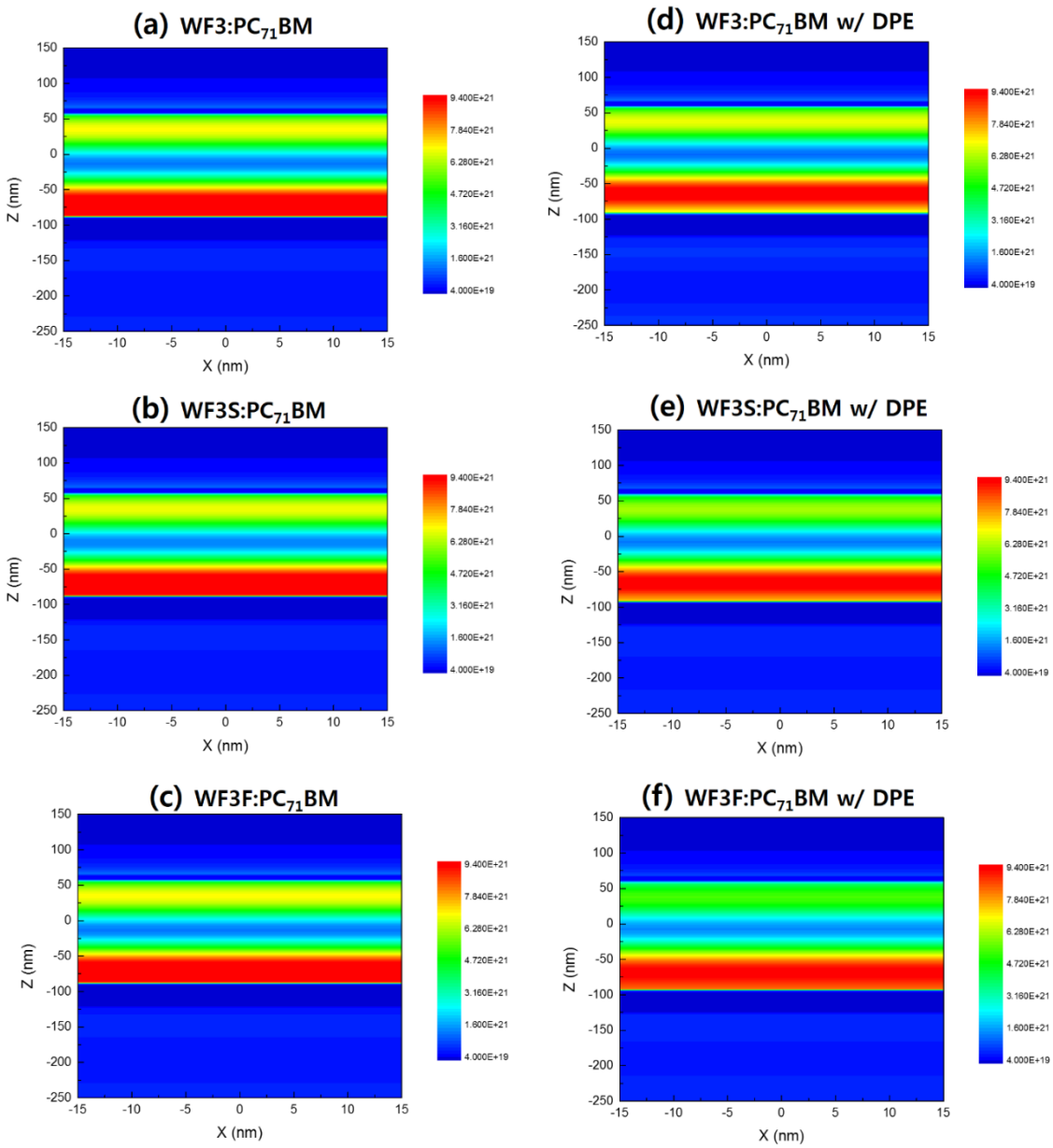

Figure S9. Power absorption profile in the devices with different photoactive layers (a) WF3:$PC_{71}BM$, (b) WF3S:$PC_{71}BM$, (c) WF3F:$PC_{71}BM$, (d) WF3:$PC_{71}BM$, (e) WF3S:$PC_{71}BM$ and (f) WF3F:$PC_{71}BM$, which is measured at wavelength ~ 450nm.

Table S1. Photovoltaic properties of the WF3:$PC_{71}BM$, WF3S:$PC_{71}BM$ and WF3F:$PC_{71}BM$ OPVs with varied composition of donor and acceptor measured under a standard indoor LED lamp system (500lx) and one-sun conditions. The values indicate averages over eight devices.

System	V_{OC} (V)	J_{SC} (mA cm^{-2})	FF (%)	PCE_{ave} (%)	PCE_{max} (%)	PCE_{max} (%)
	Under an indoor light condition					Under a one-sun condition
WF3:$PC_{71}BM$ (1:1)	0.56 ± 0.005	38.67 ± 1.31	46.34 ± 1.12	5.81 ± 0.26	6.07	4.57
WF3:$PC_{71}BM$ (1:1.5)	0.57 ± 0.01	51.46 ± 2.02	58.86 ± 1.32	9.85 ± 0.48	10.33	6.77
WF3:$PC_{71}BM$ (1:2)	0.57 ± 0.01	48.97 ± 0.89	54.63 ± 1.18	8.63 ± 0.32	8.95	6.45
WF3S:$PC_{71}BM$ (1:1)	0.61 ± 0.002	46.16 ± 1.29	49.1 ± 1.06	8.13 ± 0.33	8.46	4.74
WF3S$PC_{71}BM$ (1:1.5)	0.61 ± 0.006	52.73 ± 1.75	59.47 ± 1.75	11.37 ± 0.41	11.88	7.01
WF3S:$PC_{71}BM$ (1:2)	0.59 ± 0.002	51.27 ± 1.07	52.46 ± 1.12	9.33 ± 0.84	8.68	6.65
WF3F:$PC_{71}BM$ (1:1)	0.66 ± 0.005	48.63 ± 1.29	50.1 ± 1.08	9.45 ± 0.43	9.88	5.58
WF3F:$PC_{71}BM$ (1:1.5)	0.69 ± 0.004	55.42 ± 1.35	62.23 ± 1.35	13.89 ± 0.47	14.36	8.41
WF3F:$PC_{71}BM$ (1:2)	0.68 ± 0.01	51.34 ± 1.27	58.6 ± 0.66	12.04 ± 0.37	12.41	8.09

Table S2. Photovoltaic properties of the WF3:$PC_{71}BM$, WF3S:$PC_{71}BM$ and WF3F:$PC_{71}BM$ OPVs with additive DPE measured under a standard indoor LED lamp system (500lx) and one-sun conditions. The values indicate averages over eight devices.

System	DPE additive (v/v %)	V_{OC} (V)	J_{SC} (mA cm^{-2})	FF (%)	PCE_{ave} (%)	PCE_{max} (%)	PCE_{max} (%)
		Under an indoor light condition					Under a one-sun condition
WF3:$PC_{71}BM$ (1:2)	3%	0.57 ± 0.01	53.38 ± 1.02	58.86 ± 1.32	10.53 ± 0.51	11.04	7.28
	4%	0.57 ± 0.01	57.12 ± 0.71	61.93 ± 1.04	11.86 ± 0.41	12.27	7.63
	5%	0.57 ± 0.01	58.32 ± 1.53	64.16 ± 1.53	12.37 ± 0.46	12.83	7.94
	6%	0.57 ± 0.01	56.12 ± 1.09	61.53 ± 1.18	11.57 ± 0.31	11.88	7.67
WF3S:$PC_{71}BM$ (1:1.5)	3%	0.61 ± 0.006	56.73 ± 1.21	60.37 ± 1.18	12.46 ± 0.41	12.87	7.87
	4%	0.61 ± 0.02	59.27 ±1.13	63.6 ±0.75	13.74 ±0.21	13.95	8.09
	5%	0.61 ± 0.02	60.36 ± 1.21	65.72 ±1.21	14.05 ±0.27	14.31	8.19
	6%	0.60 ± 0.005	60.02 ± 0.89	61.6 ± 1.12	13.26 ±0.32	13.58	8.04
WF3F:PC71BM (1:2)	3%	0.69 ± 0.004	57.61 ± 1.05	63.23 ± 1.35	14.78 ± 0.47	15.25	8.68
	4%	0.69 ± 0.003	59.71 ± 9.71	65.62 ± 0.75	15.39 ± 0.19	15.58	9.12
	5%	0.69 ± 0.01	63.57 ± 1.86	67.39 ± 1.86	17.12 ± 0.22	17.34	9.44
	6%	0.69 ± 0.006	63.12 ±1.11	65.28 ± 1.15	16.74 ± 0.32	17.06	9.06

Table S3. The hole mobility (μ_h) values of the polymers (WF3, WF3S and WF3F) extracted from the dark J-V characteristics in Figure S6a.

Polymer	μ_h **(cm^2 V^{-1} s^{-1})**
WF3	1.56×10^{-4}
WF3S	1.74×10^{-4}
WF3F	1.82×10^{-4}

Table S4. The electron mobility (μ_e) and hole mobility (μ_h) values of the WF3:$PC_{71}BM$, WF3S:$PC_{71}BM$ and WF3F:$PC_{71}BM$ blend systems extracted from the dark J-V characteristics in Figure S6b and c.

System	μ_e (cm^2 V^{-1} s^{-1})	μ_h (cm^2 V^{-1} s^{-1})	μ_e/μ_h
WF3:$PC_{71}BM$	7.45×10^{-4}	1.11×10^{-4}	6.71
WF3S:$PC_{71}BM$	1.19×10^{-3}	1.68×10^{-4}	7.08
WF3F:$PC_{71}BM$	9.56×10^{-4}	1.41×10^{-4}	6.78
WF3:$PC_{71}BM$ w/DPE	1.32×10^{-3}	1.58×10^{-4}	8.35
WF3S:$PC_{71}BM$ w/DPE	1.40×10^{-3}	2.10×10^{-4}	6.66
WF3F:$PC_{71}BM$ w/DPE	1.10×10^{-3}	1.83×10^{-4}	6.01

Table S5. Crystalline properties obtained from X-ray diffraction profile.

	In-plane diffraction			Out-of-plane diffraction		
Sample	**Diffraction peaks**	**q ($Å^{-1}$)**	**d-spacing (Å)**	**Diffraction peaks**	**q ($Å^{-1}$)**	**d-spacing (Å)**
Pristine WF3	(100)	0.264	23.84	(010)	1.684	3.73
	(002)	0.665	9.45	-		
Pristine WF3S	(100)	0.255	24.68	(010)	1.696	3.70
	(002)	0.665	9.45	-		
Pristine WF3F	(100)	0.259	24.23	(010)	1.711	3.67
	(002)	0.665	9.45	-		
Pristine $PC_{71}BM$	I	0.661	9.51	I	0.692	9.08
	II	1.303	4.82	II	1.321	4.76
	III	1.923	3.27	III	1.945	3.23
WF3:$PC_{71}BM$	(100)	0.294	21.36	-		
	$PC_{71}BM$	0.672	9.35	$PC_{71}BM$	0.700	8.98
	$PC_{71}BM$	1.313	4.79	$PC_{71}BM$	1.345	4.67
	$PC_{71}BM$	1.922	3.27	$PC_{71}BM$	1.905	3.30
WF3S:$PC_{71}BM$	(100)	0.287	21.88	-		
	$PC_{71}BM$	0.672	9.35	$PC_{71}BM$	0.700	8.98
	$PC_{71}BM$	1.313	4.79	$PC_{71}BM$	1.345	4.67
	$PC_{71}BM$	1.922	3.27	$PC_{71}BM$	1.905	3.30
WF3F:$PC_{71}BM$	(100)	0.285	27.66	-		
	$PC_{71}BM$	0.672	9.35	$PC_{71}BM$	0.700	8.98
	$PC_{71}BM$	1.313	4.79	$PC_{71}BM$	1.345	4.67
	$PC_{71}BM$	1.922	3.27	$PC_{71}BM$	1.905	3.30
WF3:$PC_{71}BM$ w/DPE	(100)	0.287	21.88	-		
	$PC_{71}BM$	0.672	9.35	$PC_{71}BM$	0.700	8.98
	$PC_{71}BM$	1.313	4.79	$PC_{71}BM$	1.345	4.67
	$PC_{71}BM$	1.922	3.27	$PC_{71}BM$	1.905	3.30
WF3S:$PC_{71}BM$ w/DPE	(100)	0.284	22.11	-		
	$PC_{71}BM$	0.672	9.35	$PC_{71}BM$	0.700	8.98
	$PC_{71}BM$	1.313	4.79	$PC_{71}BM$	1.345	4.67
	$PC_{71}BM$	1.922	3.27	$PC_{71}BM$	1.905	3.30
WF3F:$PC_{71}BM$ w/DPE	(100)	0.282	22.26	-		
	$PC_{71}BM$	0.672	9.35	$PC_{71}BM$	0.700	8.98
	$PC_{71}BM$	1.313	4.79	$PC_{71}BM$	1.345	4.67
	$PC_{71}BM$	1.922	3.27	$PC_{71}BM$	1.905	3.30

Table S6. Crystalline properties obtained from X-ray diffraction profile.

Sample	In-plane (100) diffraction peak, q (Å^{-1})	FWHM (Å^{-1})	Coherence length (nm)
Pristine WF3	0.264	0.100	5.65
Pristine WF3S	0.255	0.091	6.22
Pristine WF3F	0.259	0.091	6.23
WF3:PC$_{71}$BM	0.310	0.126	4.49
WF3S:PC$_{71}$BM	0.302	0.104	5.44
WF3F:PC$_{71}$BM	0.298	0.107	5.29
WF3:PC$_{71}$BM w/ DPE	0.297	0.105	5.39
WF3S:PC$_{71}$BM w/ DPE	0.295	0.096	5.89
WF3F:PC$_{71}$BM w/ DPE	0.289	0.101	5.59

Table S7. R_{Sh} and Rs values of the WF3:PC$_{71}$BM, WF3S:PC$_{71}$BM and WF3F:PC$_{71}$BM devices extracted from the J-V characteristics in Figure 1a and 1b.

System	R_S (Ohm cm^2)	R_{Sh} (Ohm cm^2)
Under indoor light condition		
WF3:PC$_{71}$BM	12.9×10^2	7.61×10^4
WF3S:PC$_{71}$BM	12.0×10^2	10.35×10^4
WF3F:PC$_{71}$BM	11.1×10^2	11.56×10^4
WF3:PC$_{71}$BM w/DPE	10.9×10^2	12.31×10^4
WF3S:PC$_{71}$BM w/DPE	8.4×10^2	12.37×10^4
WF3F:PC$_{71}$BM w/DPE	7.8×10^2	17.42×10^4
Under 1-sun condition		
WF3:PC$_{71}$BM	9.13	45.2
WF3S:PC$_{71}$BM	8.47	49.5
WF3F:PC$_{71}$BM	6.85	65.7
WF3:PC$_{71}$BM w/DPE	5.88	60.7
WF3S:PC$_{71}$BM w/DPE	5.37	67.6
WF3F:PC$_{71}$BM w/DPE	5.26	88.4

References.

[1] T. Ye, R. Singh, H. -J. Butt, G. Floudas, P. E. Keivanidis, Effect of Local and Global Structural Order on the Performance of Perylene Diimide Excimeric Solar Cells, *ACS Appl. Mater. Interfaces* **2013**, *5*, 11844.