Supporting Imformation

Dramatic improvement in stability of high-performance inverted polymer solar cells featuring solution-processed buffer layer

Yun-Ming Sung,[1,2] *Cheng-Hsun-Tony Chang,*[3] *Cheng-Si Tsao,**[1] *Hua-Kai Lin,*[1] *Hou-Chin Cha,*[1] *Pei-Cheng Jiang,*[3] *Tian-Cheng Liu,*[1] *Kang-Wei Chang,*[4] *Yu-Ching Huang,**[4] *Jyh-Shen Tsay,**[5]

[1]Institute of Nuclear Energy Research, Longtan, Taoyuan 32546, Taiwan.

[2]Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei 10617, Taiwan.

[3]Department of Electronic Engineering, Minghsin University of Science and Technology, Hsinchu 30401, Taiwan

[4]Department of Materials Engineering, Ming-Chi University of Technology, New Taipei City 24301, Taiwan.

[5]Department of Physics, National Taiwan Normal University. Taipei 116, Taiwan.

*Corresponding author:

E-mail: cstsao@iner.gov.tw (Cheng-Si Tsao); huangyc@mail.mcut.edu.tw (Yu-Ching Huang)
jstsay@phy.ntnu.edu.tw (Jyh-Shen Tsay)

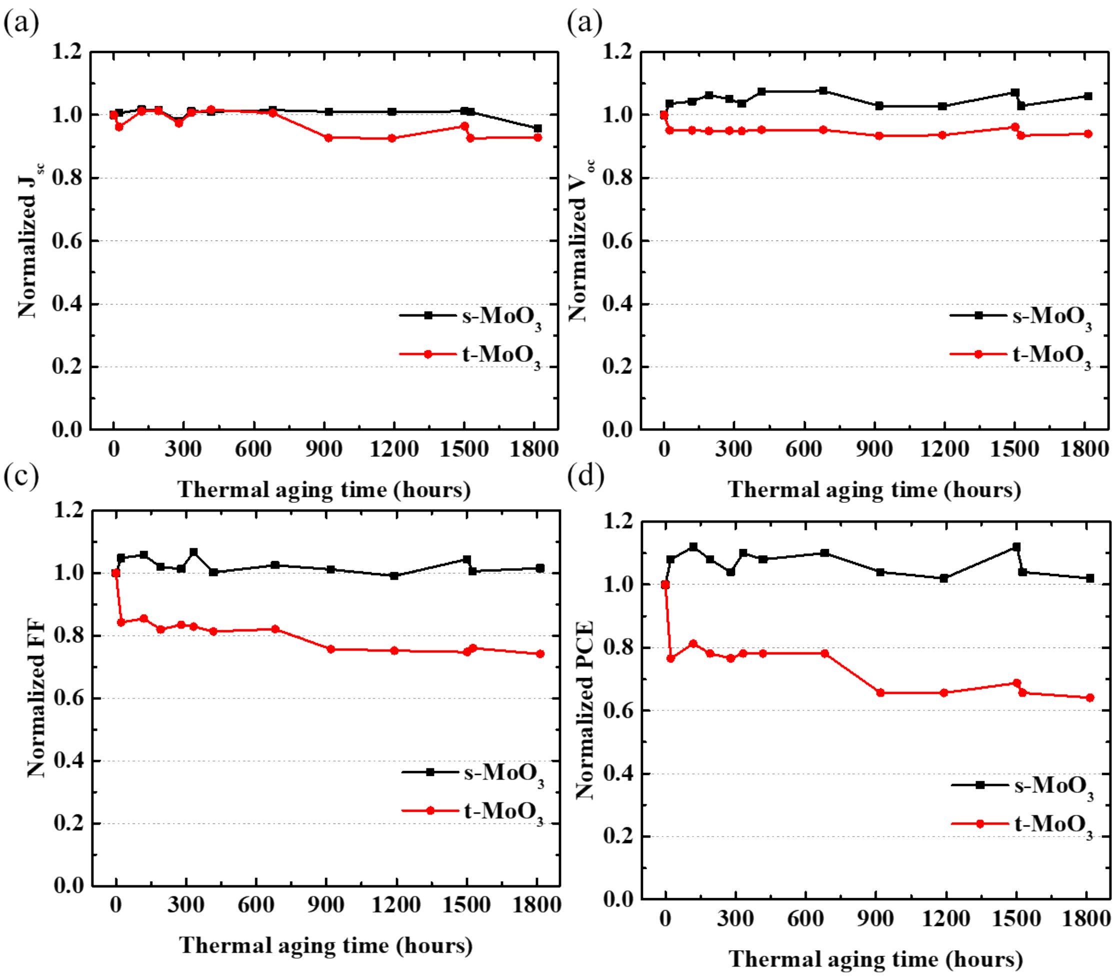

Fig. S1. The variation of photovoltaic characteristics with thermally aging time for the inverted PTB7:$PC_{71}BM$ devices with t-MoO_3 HTL and s-MoO_3 HTL, respectively. All the devices are thermally aged at 65°C in the dark nitrogen glove box.

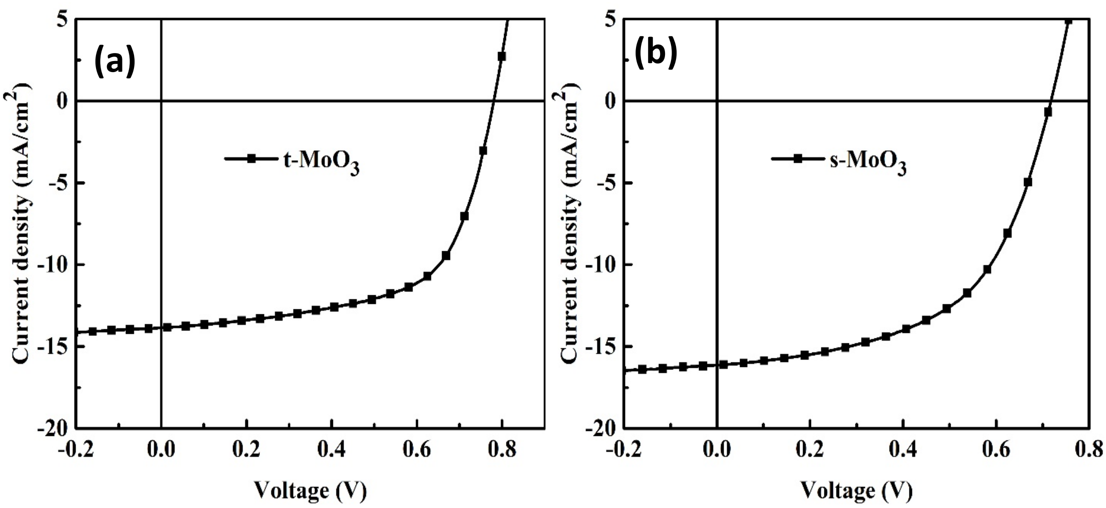

Fig. S2 (a) The current density-voltage curve of the PTB7:$PC_{71}BM$ device with t-MoO_3 without thermal aging (b) The current density-voltage curve of the PTB7:$PC_{71}BM$ device with s-MoO_3 without thermal aging.

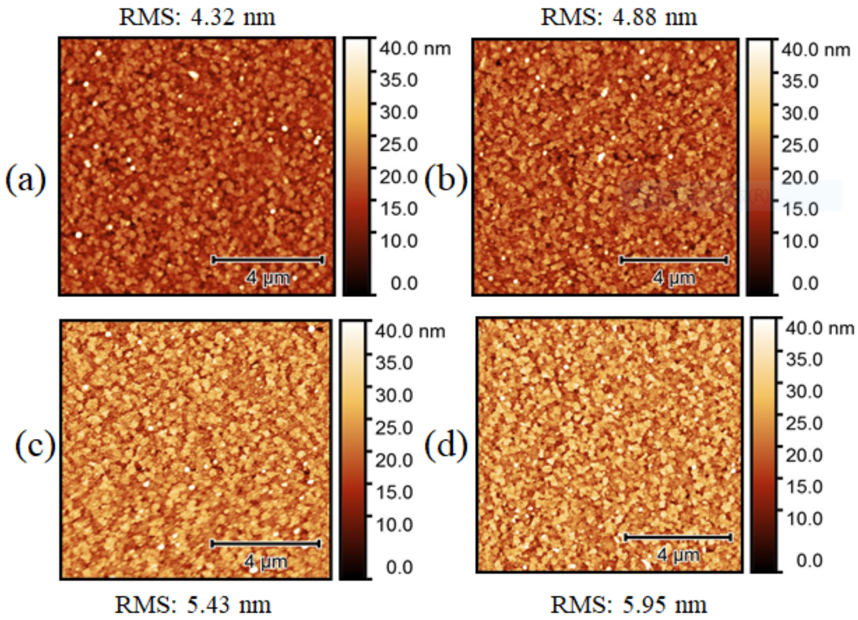

Fig. S3. Topographies of ITO/8 nm t-MoO_3 (a) without and (b) with aging and ITO/15 nm s-MoO_3 (c) without and (d) with aging. The thermal aging is at 85 °C for 100 h. The scale bar is 4 μm. The RMS of ITO is 3.00 nm.

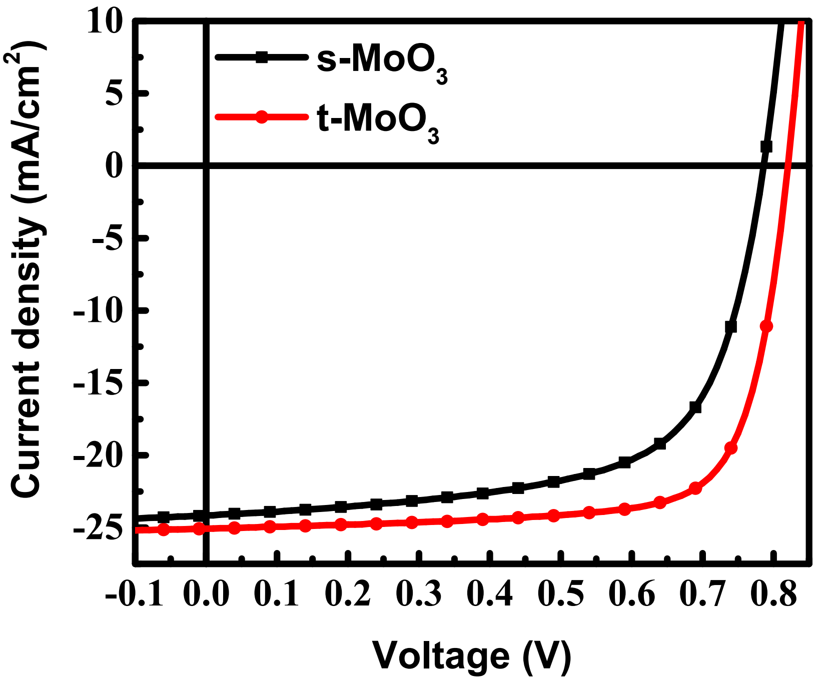

Fig. S4 Current density-voltage curves of t-MoO_3- and s-MoO_3 –based PM6:Y6 PSCs.

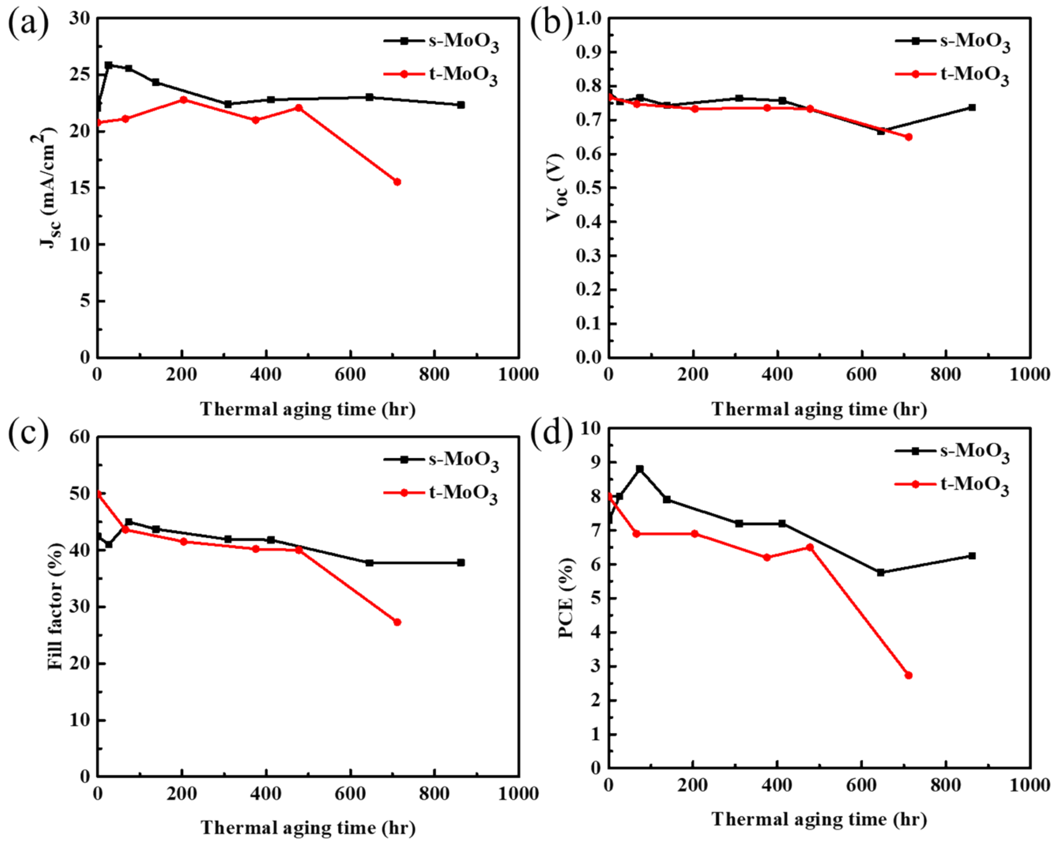

Fig. S5 Variation in the photovoltaic characteristics with respect to the thermal aging time for inverted PM6:Y6 devices incorporating t-MoO_3 and s-MoO_3 HTLs, respectively.

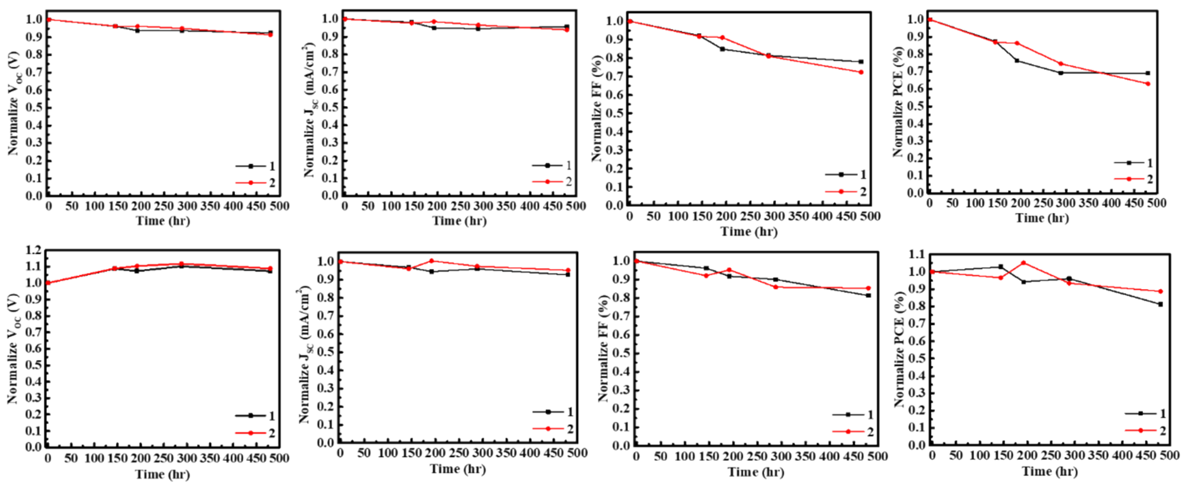

Fig. S6 Variation in the normalized photovoltaic characteristics with respect to the thermal aging time for inverted t-MoO_3-based and s-MoO_3-based PM6:Y6 devices.

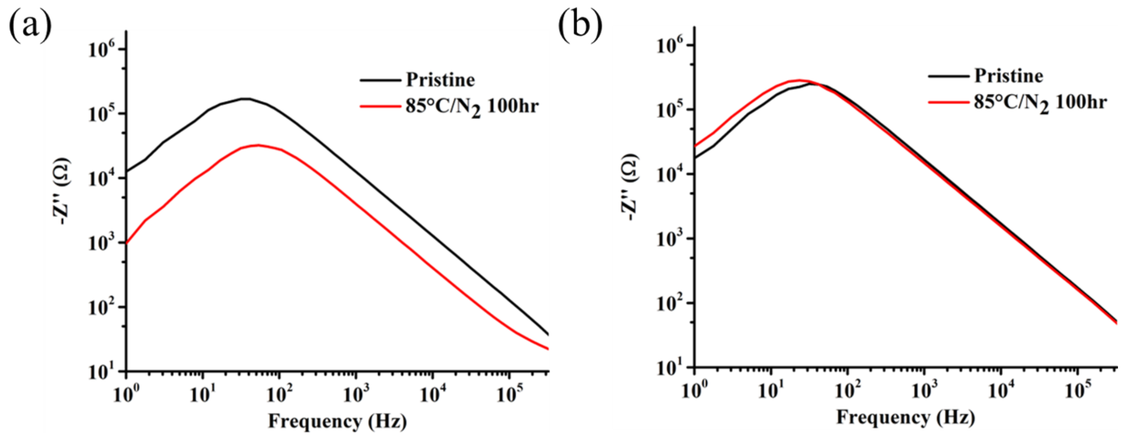

Fig. S7 (a) and (b) are the imaginary component (-Z”)-frequency plots corresponding to Fig. 2(c) and (d), respectively.

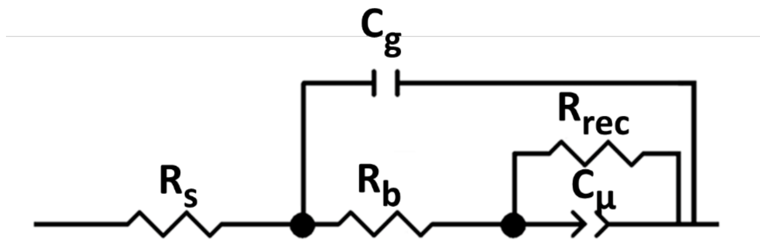

Fig. S8 Equivalent circuit of bulk heterojunction PSC for model analysis.

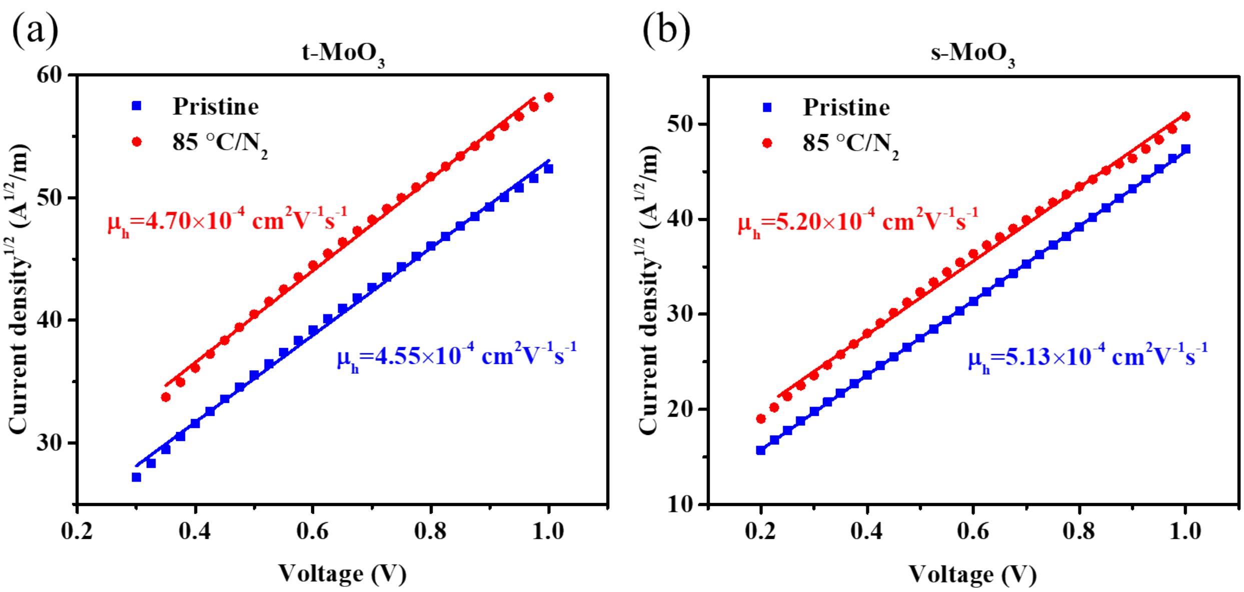

Fig. S9 Current density-voltage curves and hole mobility values of the hole only devices based on (a) t-MoO_3 and (b) s-MoO_3 as HTL before and after thermal aging at 85 °C in nitrogen for 100 hours.

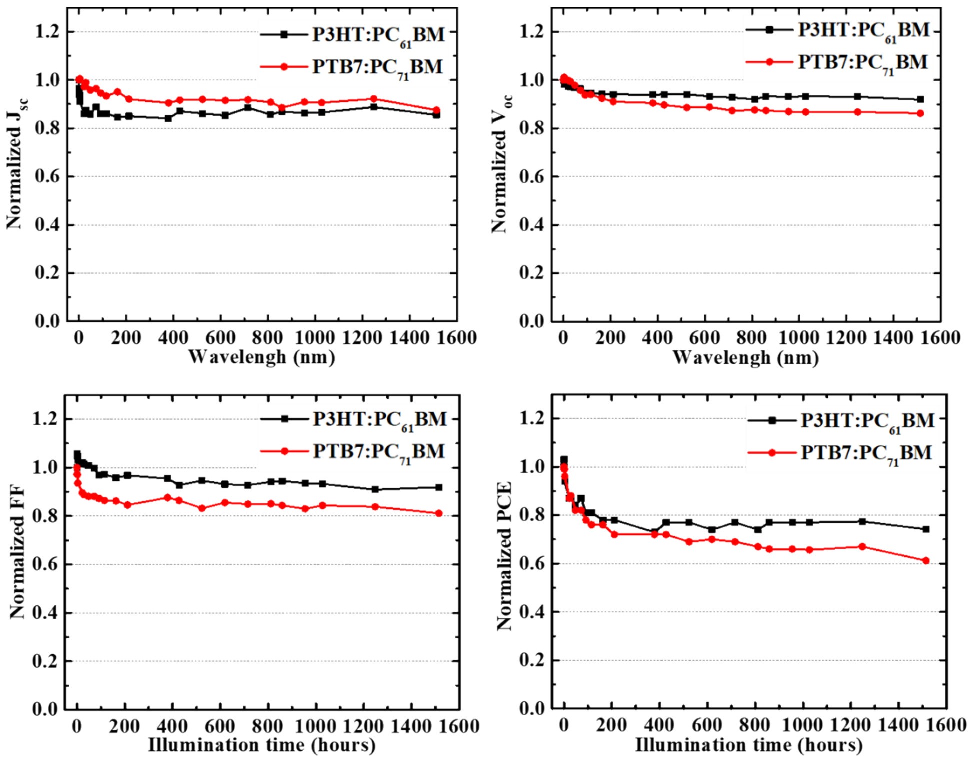

Fig. S10 Variation of photovoltaic parameters for the encapsulated inverted PTB7:$PC_{71}BM$ and P3HT:$PC_{61}BM$ devices with s-MoO_3 HTLs with aging time under the continuous AM 1.5G solar illumination with UV filter.

Table S1 Performance characteristics of t-MoO_3- and s-MoO_3-based PM6:Y6 PSCs. Values are for the highest-PCE device, and the average data are obtained from 10 devices in the brackets.

HTL	Voc (V)	Jsc (mA/cm^2)	FF (%)	PCE (%)
t-MoO_3	0.81 (0.81±0.01)	26.02 (25.16±0.67)	72.93 (70.61±3.58)	15.35 (14.33±1.18)
s-MoO_3	0.79 (0.78±0.00)	24.14 (23.46±0.48)	64.80 (64.11±1.23)	12.28 (11.80±0.36)

Table S2. Photovoltaic characteristics of inverted t-MoO_3- and s-MoO_3-based PM6:Y6 devices with PCE > 11%.

HTL	Device	V_{OC} (V)	J_{SC} (mA/cm^2)	FF (%)	PCE (%)
Evaporation MoO_3	1	0.81	25.14	72.13	14.60
		0.79 ±0.02	25.02 ±0.42	63.31 ±6.33	12.54 ±1.62
	2	0.81	26.02	72.93	15.35
		0.81 ±0.01	25.16 ±0.67	70.61 ±3.58	14.33 ±1.18
H-MoO_3	1	0.70	26.70	67.17	12.59
		0.69 ±0.02	26.04 ±0.51	63.86 ±3.51	11.56 ±1.04
	2	0.68	26.06	66.49	11.78
		0.69 ±0.02	25.58 ±0.55	61.91 ±6.74	10.85 ±1.17

Table S3 Electric parameters determined by model fitting for the t-MoO_3- and s-MoO_3-based PTB7:$PC_{71}BM$/8 PSCs before and after annealing at 85 °C for 100 h

HTL	Condition	R_s (Ω)	R_b (Ω)	C_g (10^{-8} F)	C_μ (10^{-8} F)	R_{rec} (kΩ)	τ_{avg} (ms)
t-MoO_3	Pristine	13.56	318.7	1.29	9.71	39.9	2.89
	85°C/N_2 100 hr	69.82	50.2	3.87	6.20	17.2	0.74
s-MoO_3	Pristine	11.04	396.3	0.82	0.96	109.4	0.73
	85°C/N_2 100 hr	10.51	126.5	1.04	0.22	445.6	0.68