ADVANCED FUNCTIONAL MATERIALS

Supporting Information

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The neglected influence of zinc oxide light-soaking on stability measurements of inverted organic solar cells

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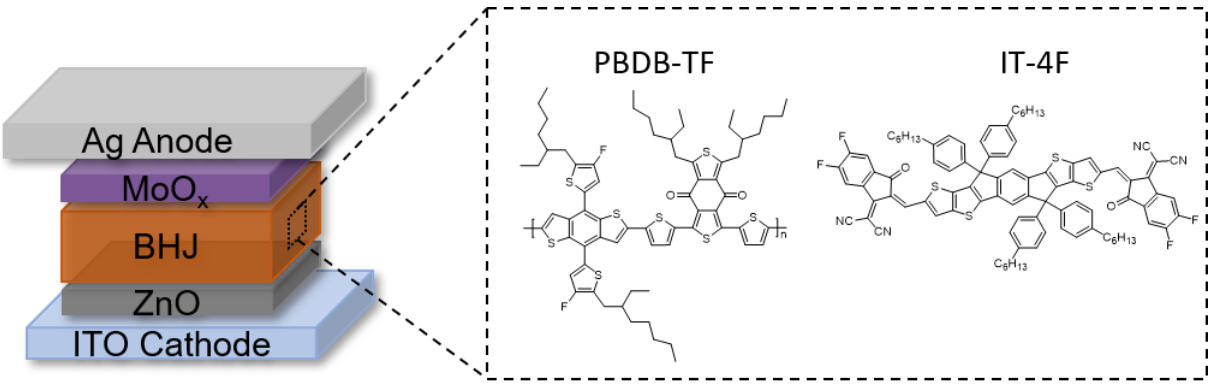

Figure S1: Schematic architecture of the inverted organic solar cells and molecular structures of the used absorbing materials PBDB-TF and IT-4F.

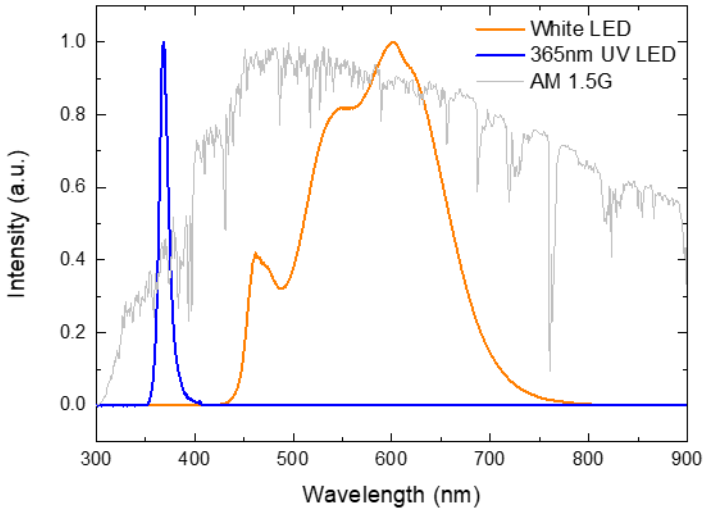

Figure S2: Normalized spectra of the used white LED and UV LED compared to the normalized AM 1.5G spectrum.

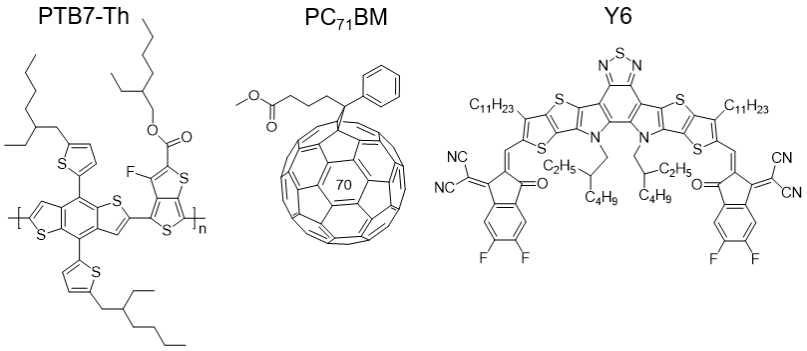

Figure S3: Chemical structures of the molecules used for the alternative blends PBDB-TF:Y6 and PTB7-Th:$PC_{71}BM$.

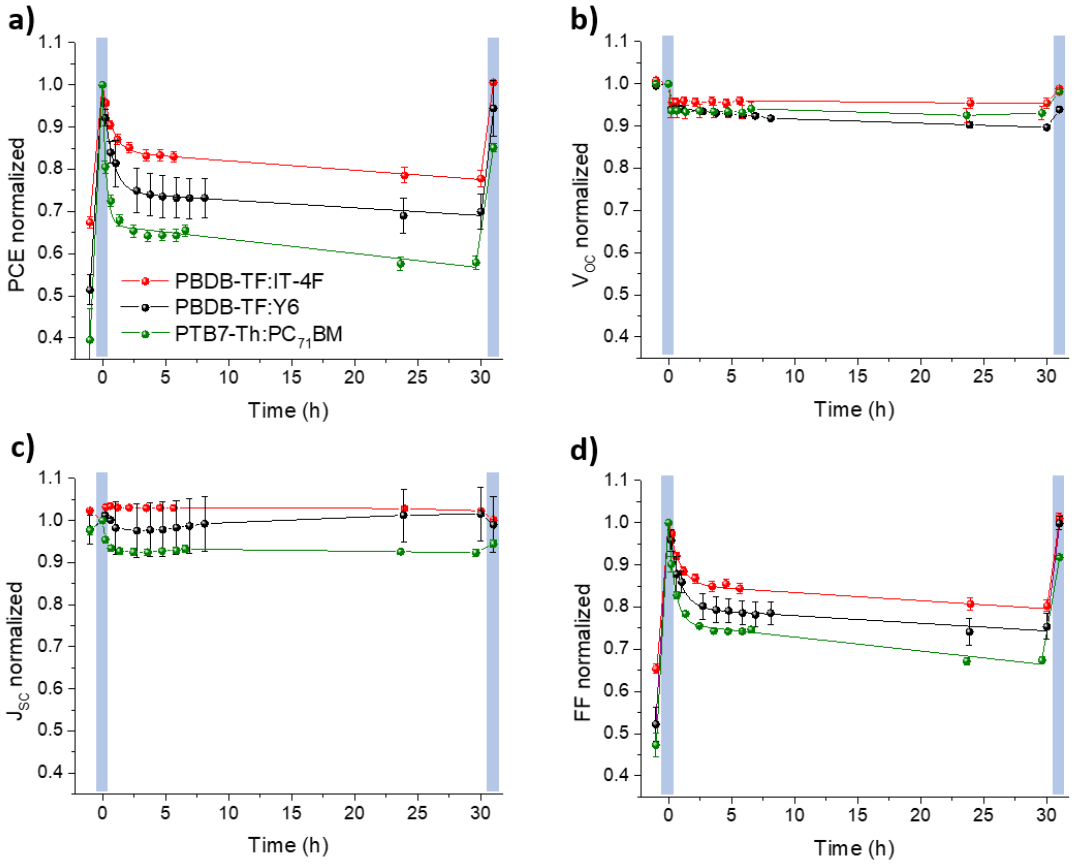

Figure S4: Normalized **a)** PCE, **b)** V_{OC}, **c)** J_{SC}, and **d)** FF as a function of time for the three different active layers PBDB-TF:IT-4F (red), PBDB-TF:Y6 (black), and PTB7-Th:$PC_{71}BM$ (green). The measurements were run according to the procedure described in FIG 2a of the main text, with the first data point being the pristine cells, the second data point (blue marking) being the UV-soaked cells, followed by a thermal aging at 85 °C, and the last data point representing the cells that were UV-soaked again (blue marking). All data points are averaged over 6 independently measured cells.

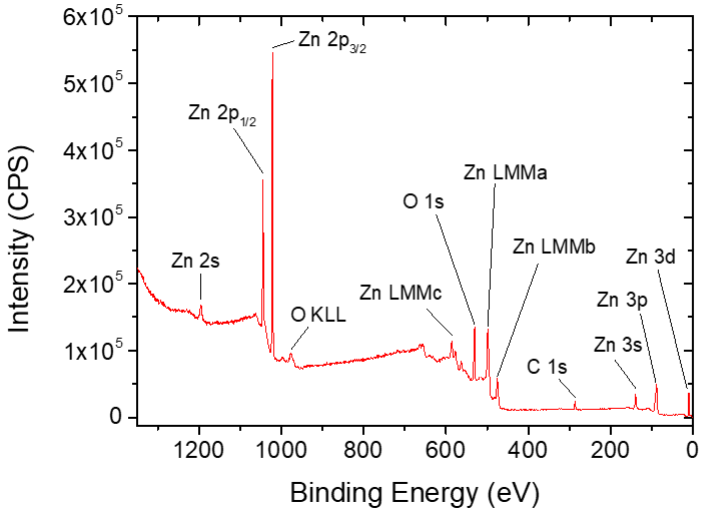

Figure S5: XPS survey scan of the ZnO layer, showing emissions from the elements Zn, O, and C.

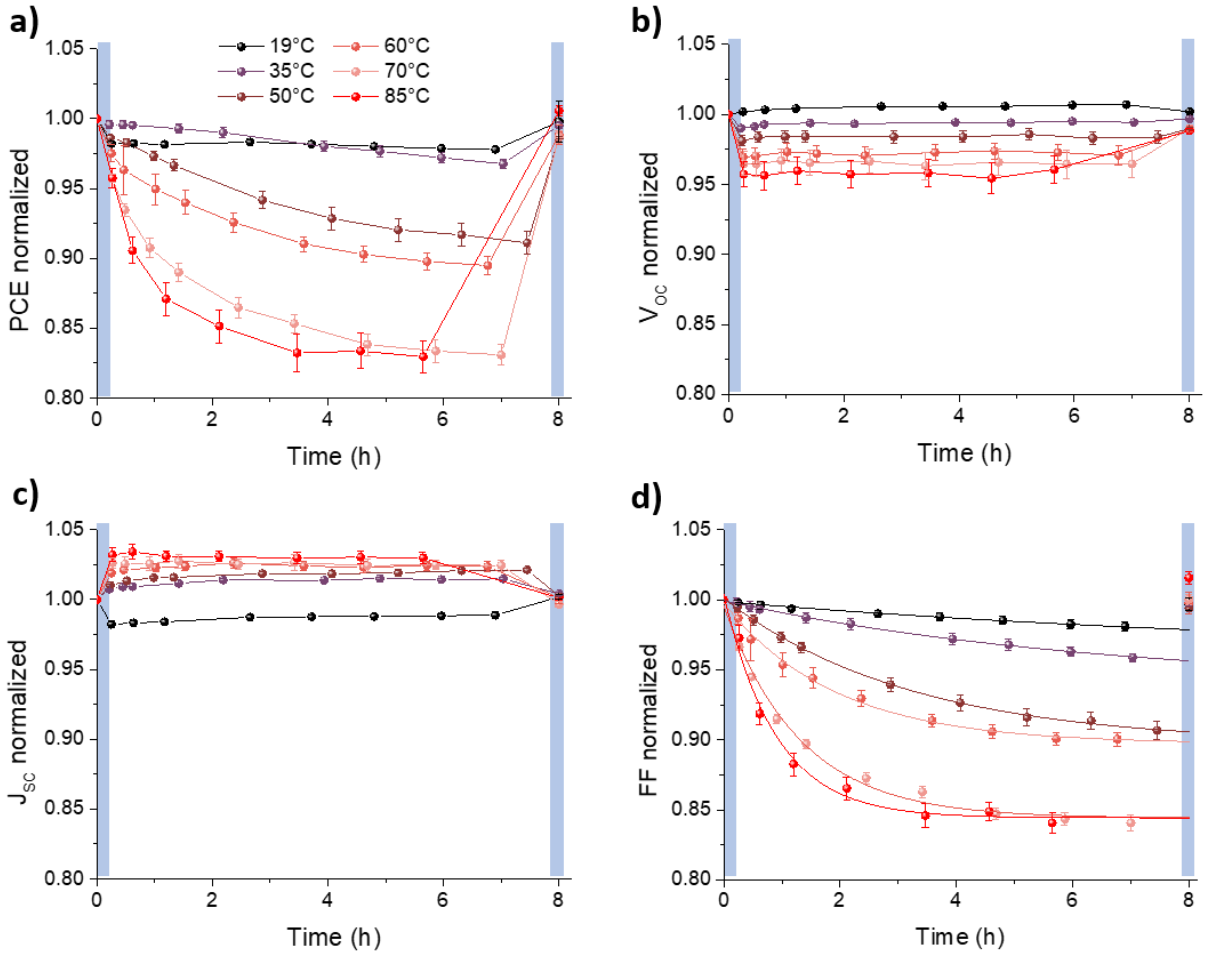

Figure S6: Development of the normalized **a)** PCE, **b)** V_{OC}, **c)** J_{SC}, and **d)** FF as a function of time for PBDB-TF:IT-4F devices heated at different temperatures between 19 °C and 85 °C, with the data points being the average of five separately aged solar cells. All values are normalized to the initial performance after 5s of UV illumination (time = 0, blue marking) and after 8 hours of thermal degradation the devices were exposed to a second UV illumination of 5 s (blue marking).

Table S1: Fitting parameters for the exponential fit of the fill factor decay over time for different temperatures and adjusted R-square for each fit.

Temperature (°C)	**τ (s^{-1})**	**A**	**y_0**	**Adjusted R-square**
85	0.9007	0.1595	0.8443	0.988
70	1.3202	0.1513	0.8442	0.992
60	1.9213	0.1005	0.8973	0.995
50	3.2166	0.1039	0.89771	0.999
35	6.5698	0.0611	0.9385	0.999
19	11.0092	0.0388	0.96	0.990

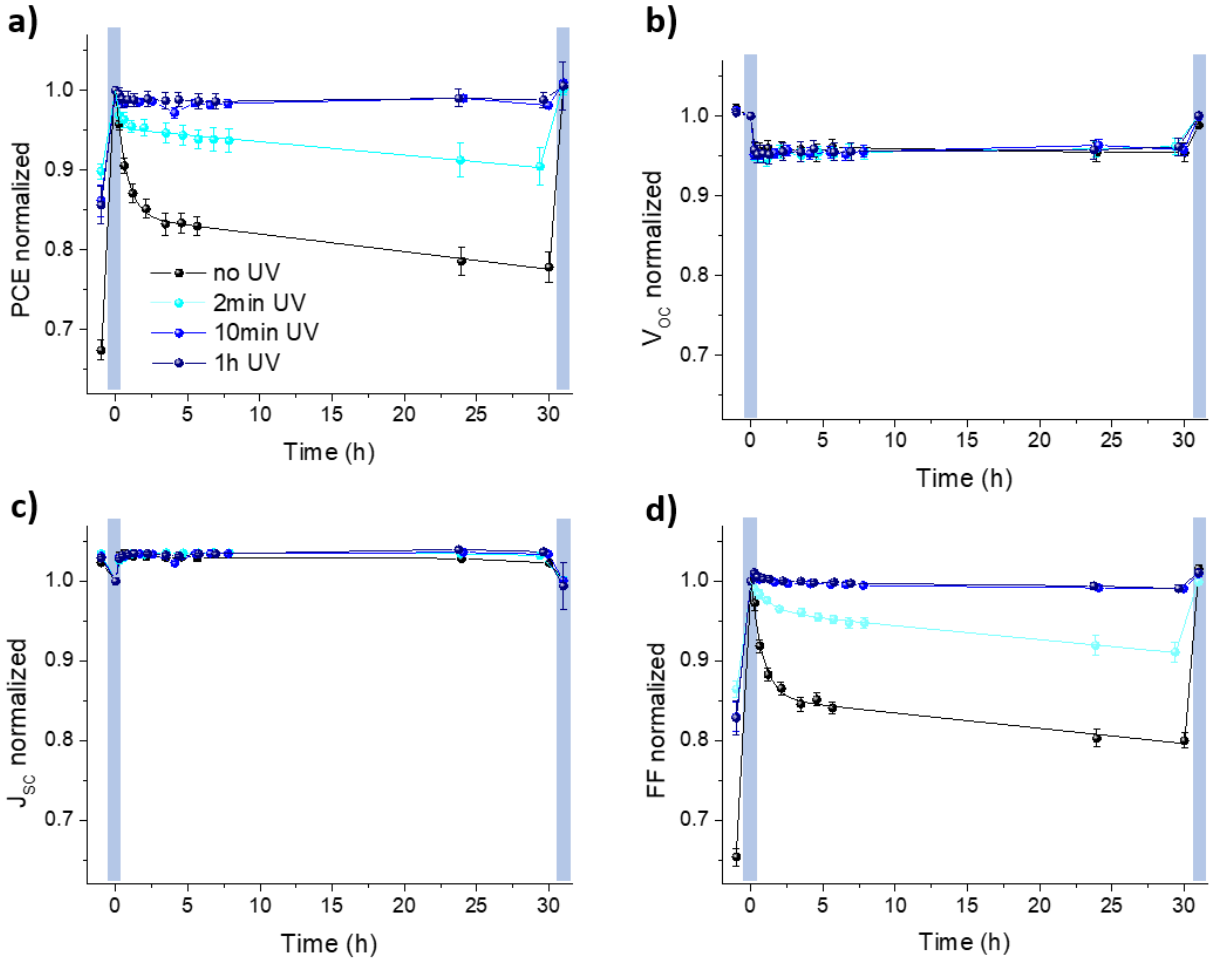

Figure S7: Normalized **a)** PCE, **b)** V_{OC}, **c)** J_{SC}, and **d)** FF as a function of time for PBDB-TF:IT-4F cells, for which the ZnO was illuminated with UV light for different times as a pretreatment. The measurements were run according to the procedure described in FIG 2a in the main text, with the first data point being the pristine cells, the second data point being the UV-soaked cells (blue marking), followed by a thermal aging at 85 °C, and the last data point representing the cells that were UV-soaked again (blue marking).

Table S2: Integrals of the different XPS fitting components (main text Figure 6c) for stochiometric oxygen (O_{st}), the oxygen in oxygen deficient regions (O_{def}), and adsorbed oxygen species (O_{ads}), and their respective percentage of the total O 1s integral.

Condition	Component	Integral	Percentage of O 1s integral (%)
Before UV-illumination	O_{st}	8208	51
	O_{def}	3611	22
	O_{ads}	4288	27
	O 1s	16107	100
After UV-illumination	O_{st}	8677	55
	O_{def}	3711	23
	O_{ads}	3451	22
	O 1s	15839	100

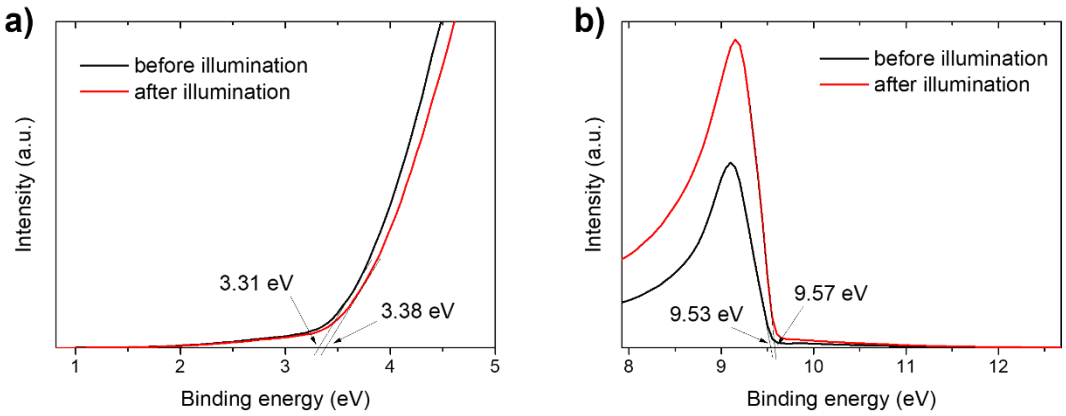

Figure S8: Ultraviolet photoelectron spectra of a ZnO layer before and after illumination with UV light. a) Valence band region with indicated low binding energy onsets which correspond to the energetic difference between valence band and Fermi level. b) Secondary-electron cut-off region (measured at a bias of 8 eV) with indicated cut-off energies, from which the work functions can be calculated.