Supporting Information

Efficient and Stable Operation of Nonfullerene Organic Solar Cells: Retaining a High Built-in Potential

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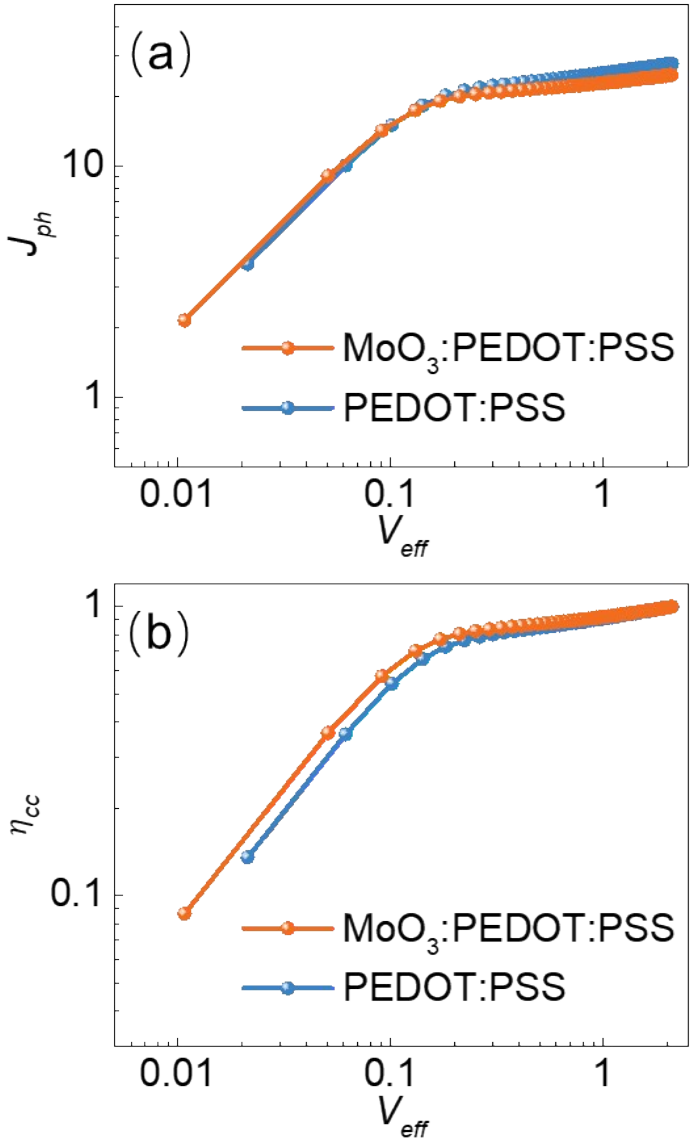

Figure S1. (a) J_{ph}–V_{eff} characteristics measured for the as-prepared PBDB-T-2F:IT-4F-based OSCs with a MoO_3:PEDOT:PSS HTL and a control OSC with a pristine PEDOT:PSS HTL, and (b) the charge collection efficiency (η_{cc}) measured for the PBDB-T-2F:IT-4F-based OSCs with a MoO_3-PEDOT:PSS HTL and a control OSC with a pristine PEDOT:PSS HTL.

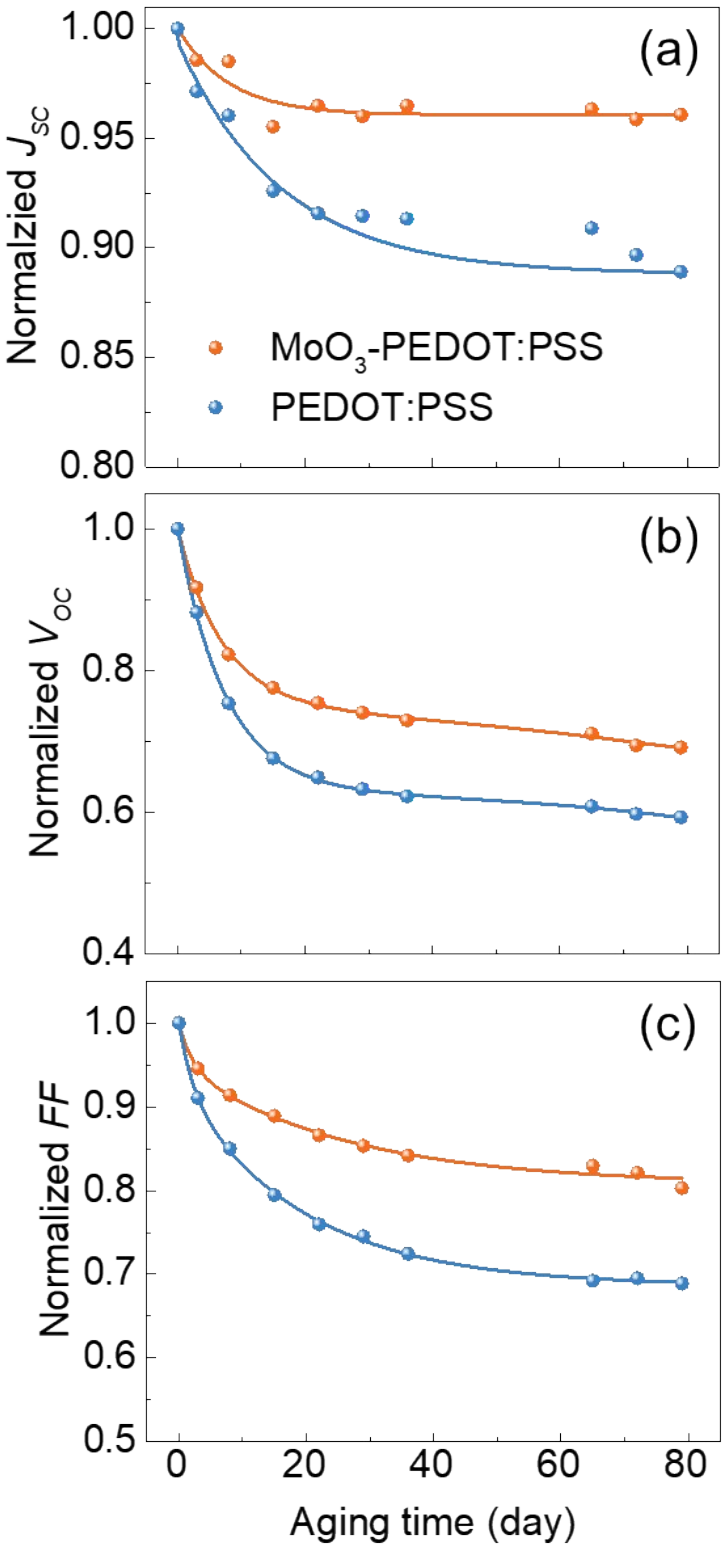

Figure S2. Normalized (a) J_{SC} (b) V_{OC} and (c) *FF* measured for the PBDB-T-2F:IT-4F based OSCs with a hybrid MoO_3-PEDOT:PSS HTL and a pristine PEDOT:PSS HTL.

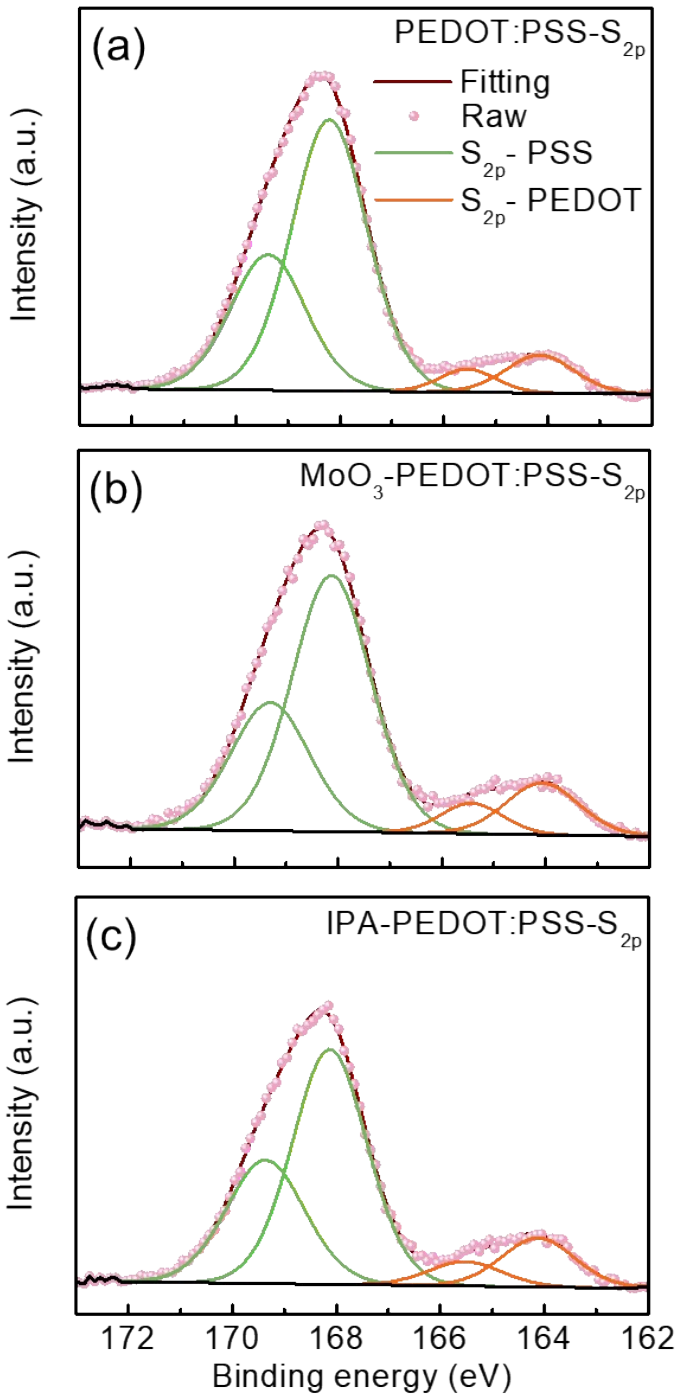

Figure S3. S_{2p} XPS spectra measured for (a) a PEDOT:PSS layer, (b) a hybrid MoO_3-PEDOT:PSS layer, and (c) an IPA:PEDOT:PSS layer.

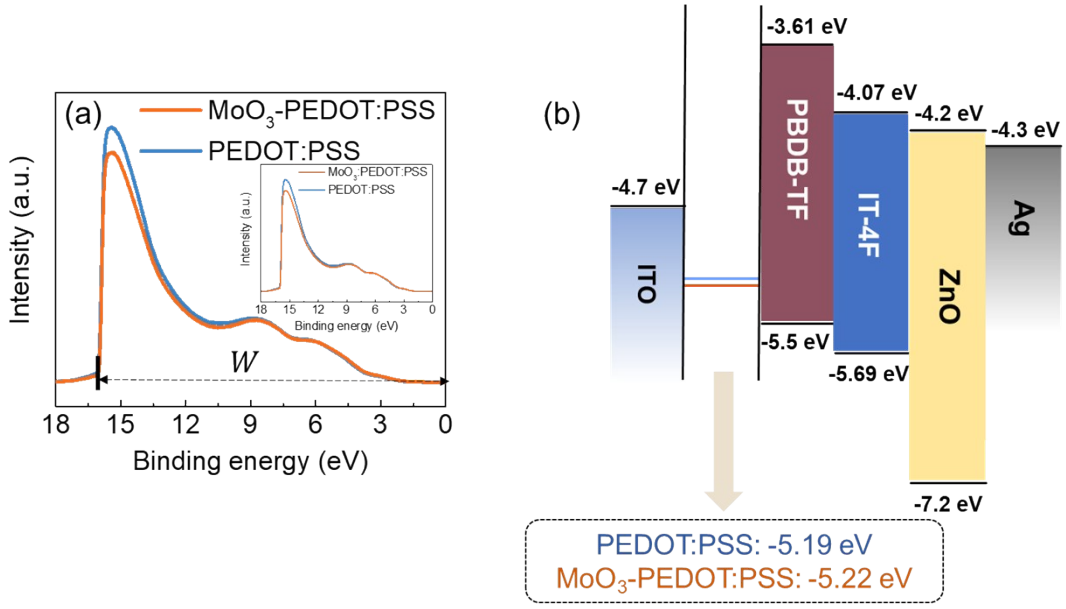

Figure S4. (a) The UPS spectra measured for the PEDOT:PSS and MoO_3-PEDOT:PSS layers. (b) The schematic diagram illustrating the energy levels of the functional materials use in the PBDB-T-2F:IT-4F-based OSCs made with different HTLs.

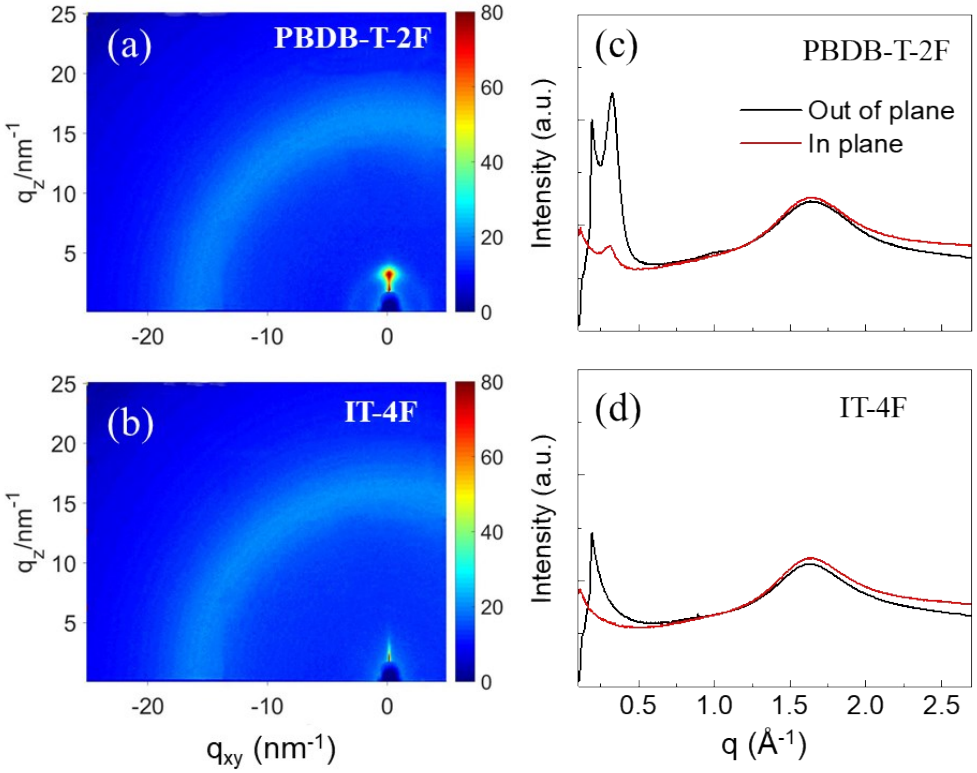

Figure S5. 2D GIWAXS images measured for (a) a PBDB-T-2F film, (b) an IT-4F film. The corresponding integrated profiles along the q_{xy} (in-plane) and q_z (out of plane) directions for (c) the PBDB-T-2F and (d) IT-4F films.

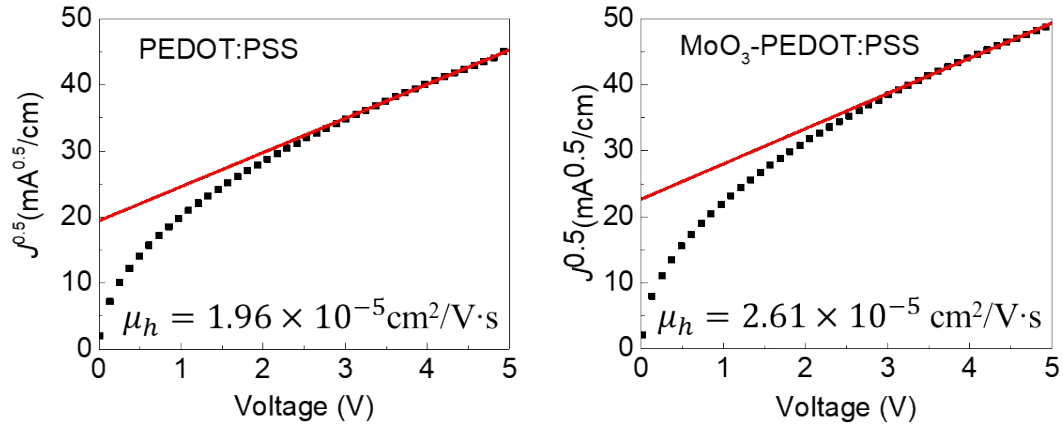

Figure S6. $J^{0.5}$–V characteristics obtained for the ITO/PEDOT:PSS/Au and ITO/MoO_3-PEDOT:PSS/Au devices.

Table S1. Performance summary of the PBDB-T-2F:IT-4F OSCs with different HTLs of PEDOT:PSS and MoO_3-PEDOT:PSS.

HTL	J_{SC} (mA/cm^2)	V_{OC} (V)	*FF* (%)	*PCE* (%) (best cell)
PEDOT:PSS	23.91 ± 0.31	0.86 ± 0.00	65.30 ± 0.56	13.41 ± 0.09 (13.48)
MoO_3-PEDOT:PSS (1:4)	21.98 ± 0.20	0.86 ± 0.00	67.83 ± 1.64	12.87 ± 0.28 (13.10)
MoO_3-PEDOT:PSS (1:3)	21.97 ± 0.44	0.86 ± 0.00	68.32 ± 1.04	12.91 ± 0.24 (13.28)
MoO_3-PEDOT:PSS (1:2)	21.97 ± 0.08	0.86 ± 0.00	69.01 ± 0.04	13.01 ± 0.06 (13.07)
MoO_3-PEDOT:PSS (1:1)	21.71 ± 0.16	0.86 ± 0.00	70.56 ± 0.06	13.19 ± 0.14 (13.34)
MoO_3-PEDOT:PSS (2:1)	20.96 ± 0.17	0.86 ± 0.00	71.58 ± 0.32	12.88 ± 0.11 (13.04)
MoO_3-PEDOT:PSS (3:1)	21.80 ± 0.18	0.85 ± 0.00	67.26 ± 0.66	12.53 ± 0.03 (12.56)

Table S2. The area ratios of N_{1S} XPS peak to S_{2P} XPS peak, measured for the top surfaces of the binary PBDB-T:NFA blend layers having INCN groups in NFA, e.g., ITIC, formed on different substrates.

Substrate	N_{1S}/S_{2P}
Si	0.090
PEDOT:PSS	0.110
MoO_3	0.087
ZnO	0.108

Table S3. GIWAXS results measured for the PBDB-T-2F:IT-4F blend layer formed on (a) a hybrid MoO_3-PEDOT:PSS HTL and (b) a pristine PEDOT:PSS HTL aged over different time periods.

(a)

Aging period	Peak position (A^{-1})		FWHM (nm^{-1})	π-π stacking (Å)	Coherence length (Å)
	100	010	010		
As-prepared	0.33	1.61	6.210	3.90	9.40
14-day	0.33	1.62	6.314	3.87	9.31
19-day	0.33	1.61	6.207	3.90	9.44

(b)

Aging period	Peak position (A^{-1})		FWHM (nm^{-1})	π-π stacking (Å)	Coherence length (Å)
	100	010	010		
As-prepared	0.33	1.61	6.288	3.89	9.31
14-day	0.33	1.61	6.360	3.89	9.18
19-day	0.33	1.63	6.317	3.84	9.22