

Supporting Information

Tuning the Buried Interface with D-Sorbitol-Modified Mixed SAMs for High-Efficiency

Inverted Perovskite Solar Cells

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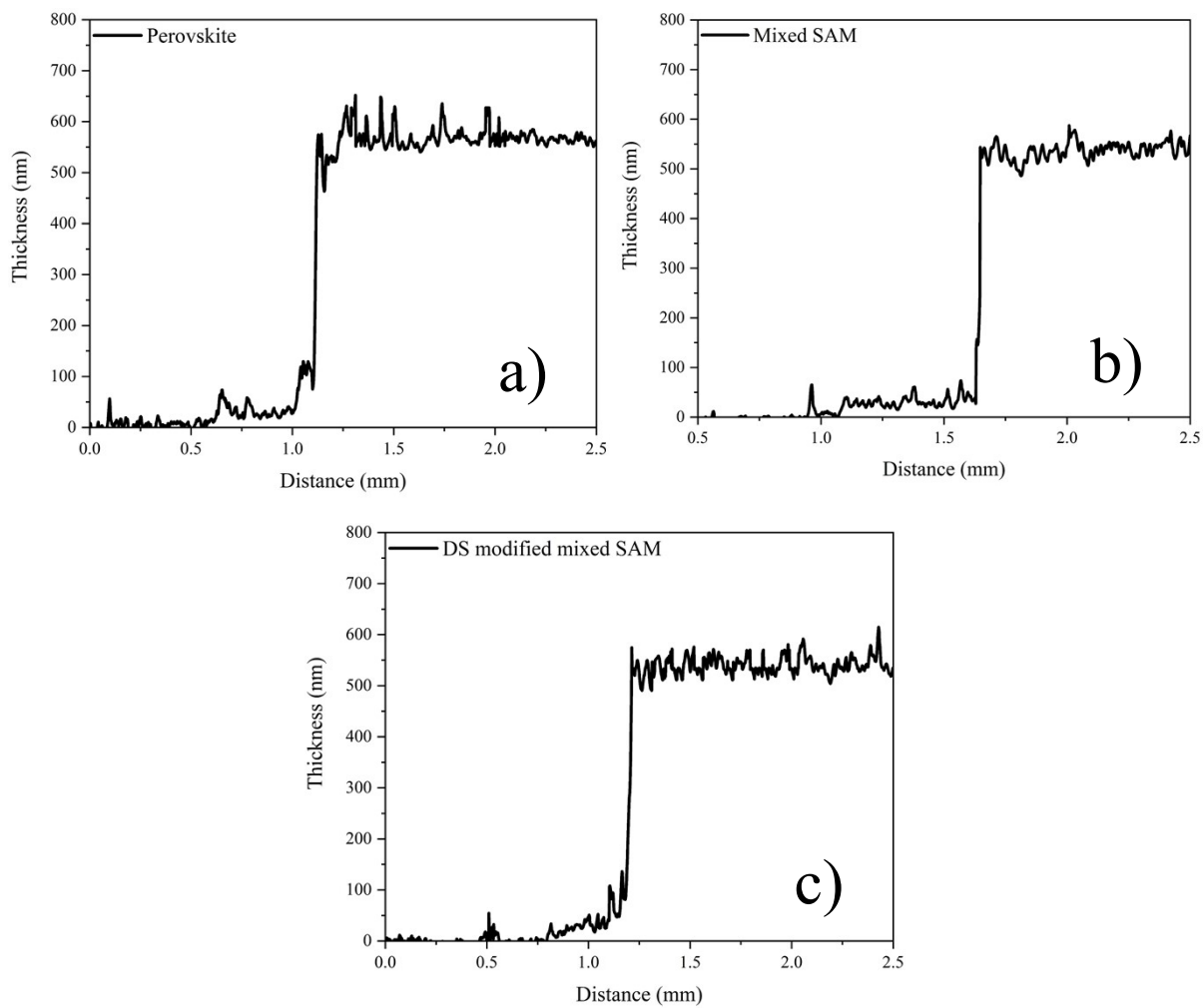


Figure S1. Stylus profilometry thickness profiles of perovskite films deposited on different buried-contact configurations: (a) FTO/perovskite, (b) FTO/Mixed-SAM/perovskite, and (c) FTO/DS-modified Mixed-SAM/perovskite.

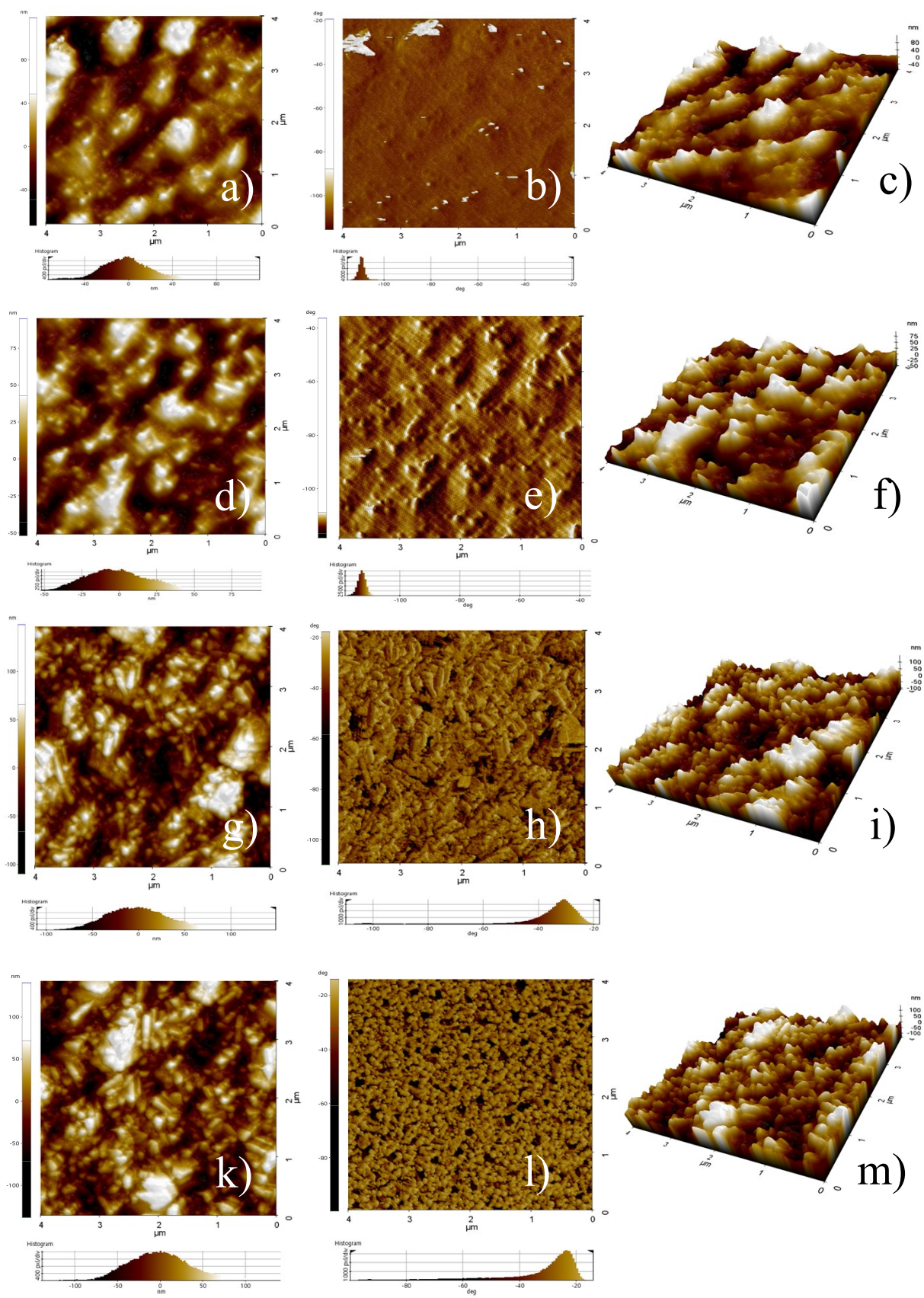


Figure S2. High-haze FTO: AFM topography, phase and 3D images of (a-c) bare FTO, (d-f) FTO/Mixed SAM (no rinse), (g-i) FTO/Mixed SAM (IPA rinsed), and (l-m) FTO/DS modified mixed SAM (DS in IPA) thin films.

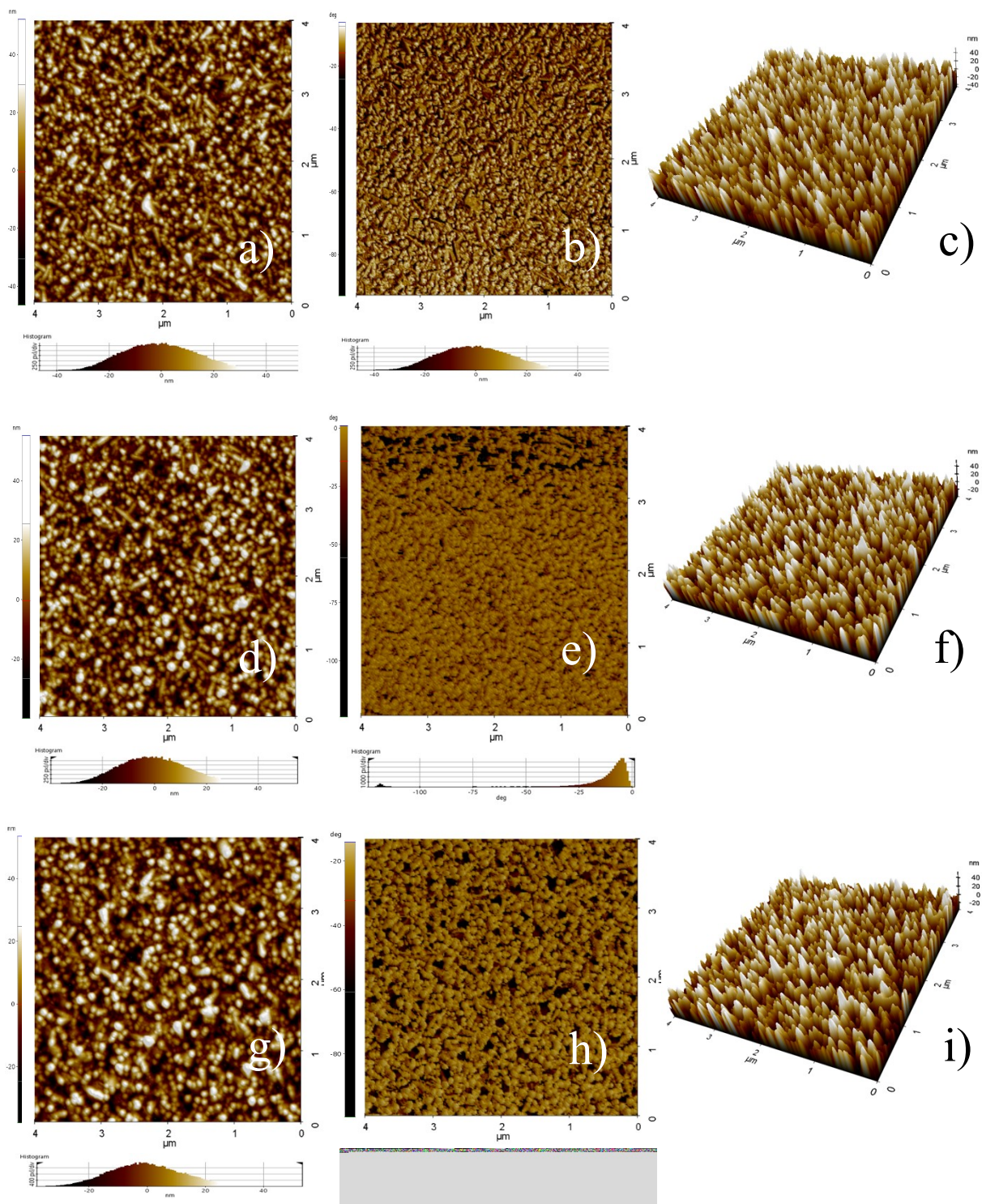


Figure S3. Low-haze FTO: AFM topography, phase and 3D images of (a-c) bare FTO, (d-f) FTO/Mixed SAM (IPA rinsed) and (g-i) FTO/DS modified mixed SAM (DS in IPA) thin films.

Table S1. AFM topography and phase metrics for mixed-SAM and DS-modified mixed-SAM on low and high-haze FTO (scan area: $4 \times 4 \mu\text{m}^2$).

Substrate / treatment	Topography R_q (nm)	Topography R_{pv} (nm)	Phase mean (deg)	Phase R_q (deg)
High-haze FTO (bare)	24.905	191.776	-108.084	10.324
High-haze FTO/mixed-SAM (no IPA rinse)	21.796	146.621	-112.745	2.056
High-haze FTO/mixed-SAM (IPA-rinsed)	33.623	258.636	-34.849	12.018
High-haze FTO/DS-modified mixed-SAM (DS in IPA rinse)	36.559	279.325	-52.100	20.848
Low-haze FTO (bare)	14.092	98.633	-15.836	4.311
Low-haze FTO /mixed-SAM (IPA-rinsed)	13.200	95.180	-14.154	21.218
Low-haze FTO /DS-modified mixed-SAM (DS in IPA rinse)	12.591	91.322	-32.348	14.473

R_q : RMS roughness; R_{pv} : peak-to-valley height range. Phase values are extracted from NCM phase backward images.

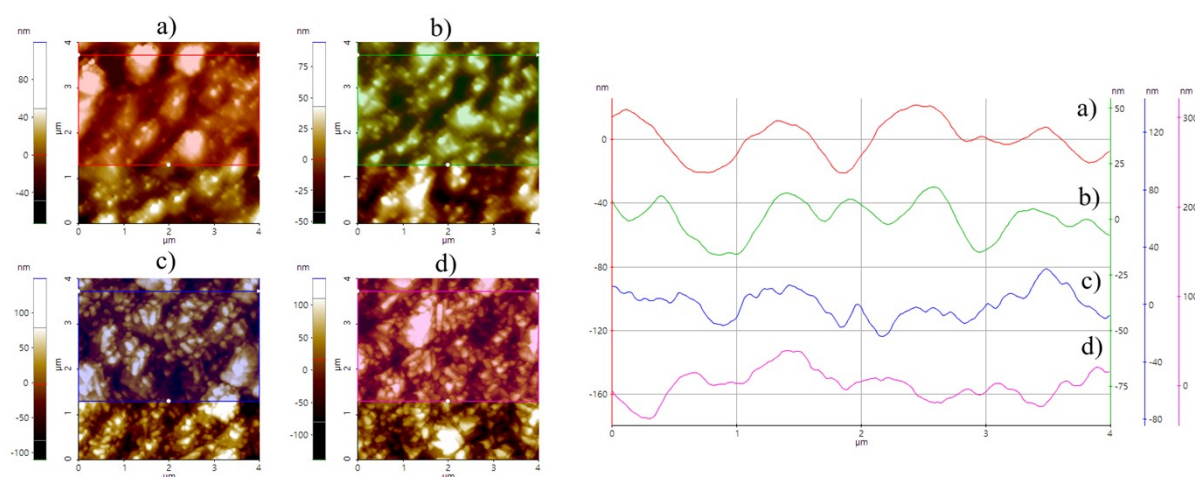


Figure S4. Representative AFM height maps ($4 \times 4 \mu\text{m}^2$) and corresponding line profiles extracted along the same horizontal scan line (colored line) for high-haze FTO before and after mixed-SAM processing: (a) bare high-haze FTO, (b) FTO/mixed-SAM (non-rinsed), (c)

FTO/mixed-SAM after rinsing with IPA, and (d) FTO/DS-modified mixed-SAM after rinsing with DS-containing IPA.

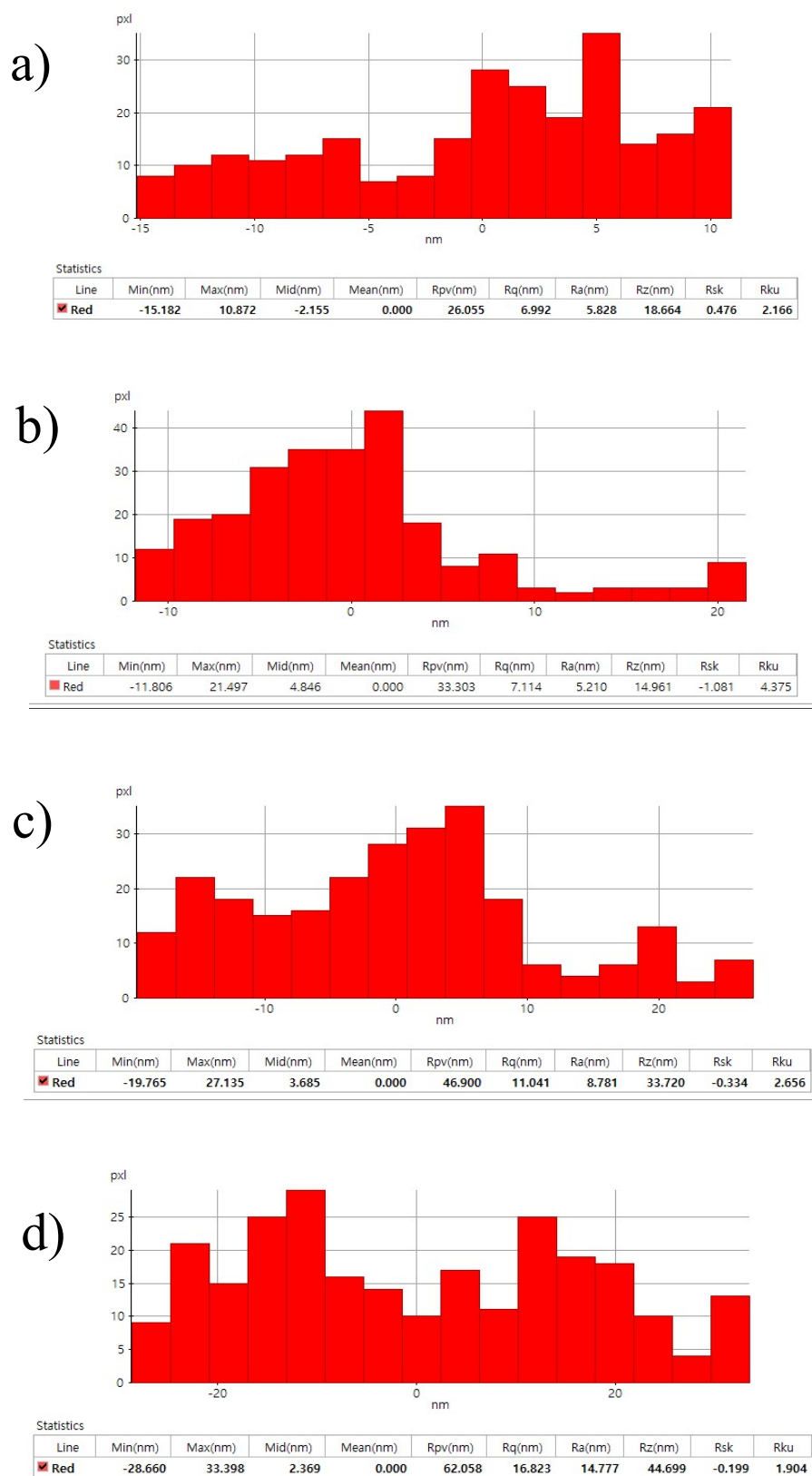


Figure S5. Scan-wide height-distribution (histogram) analysis derived from the $4 \times 4 \mu\text{m}^2$ AFM height maps for high-haze FTO surfaces: (a) bare high-haze FTO, (b) FTO/mixed-SAM (non-

rinsed), (c) FTO/mixed-SAM after rinsing with IPA, and (d) FTO/DS-modified mixed-SAM after rinsing with DS-containing IPA.

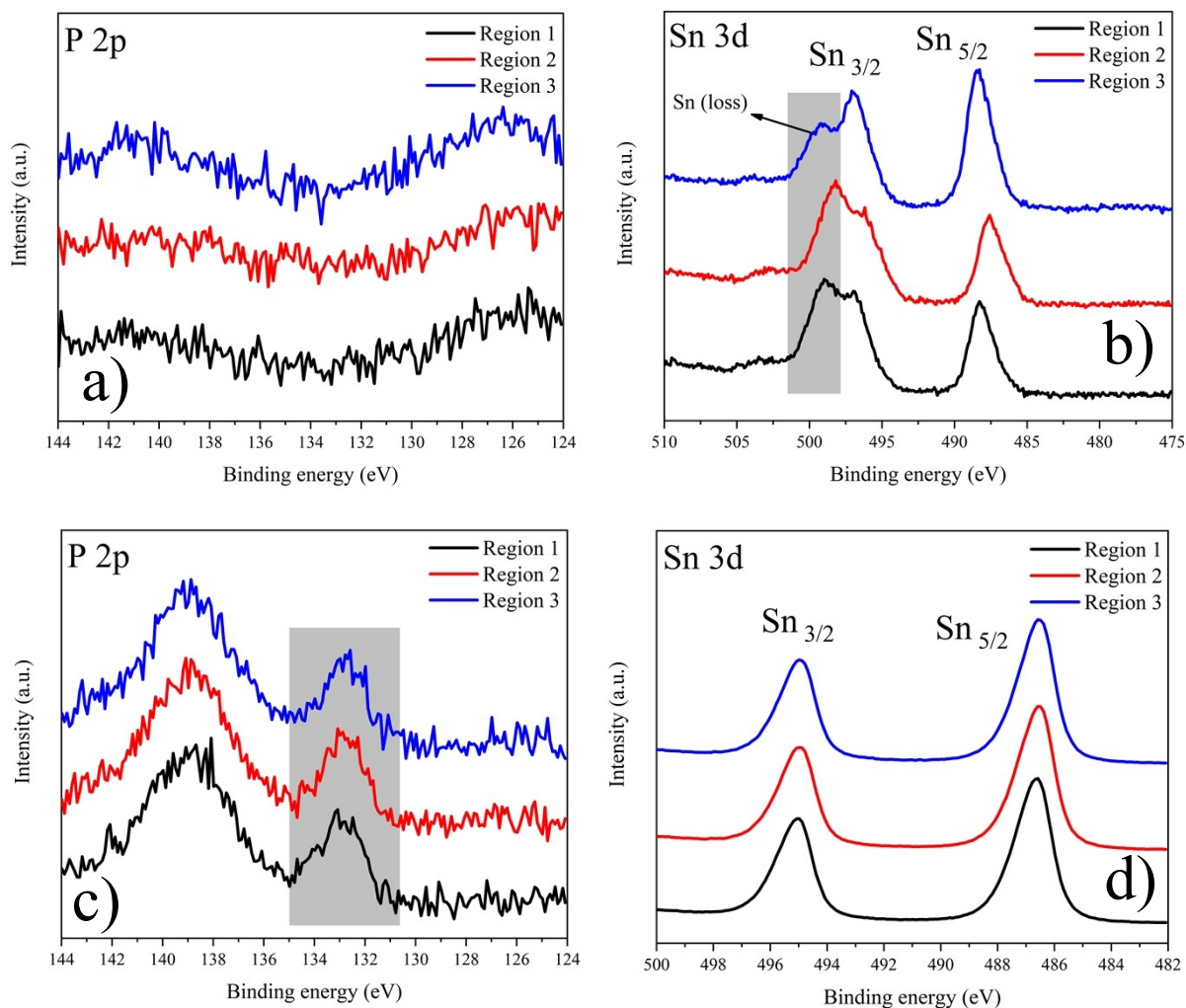


Figure S6. High-resolution a) P 2p and b) Sn 3d XPS spectra collected from three different spots (Region 1–3) on high-haze FTO/mixed-SAM (IPA rinsed) substrate. High-resolution c) P 2p and d) Sn 3d XPS spectra collected from three different spots (Region 1–3) on low-haze FTO/mixed-SAM (IPA rinsed) substrate.

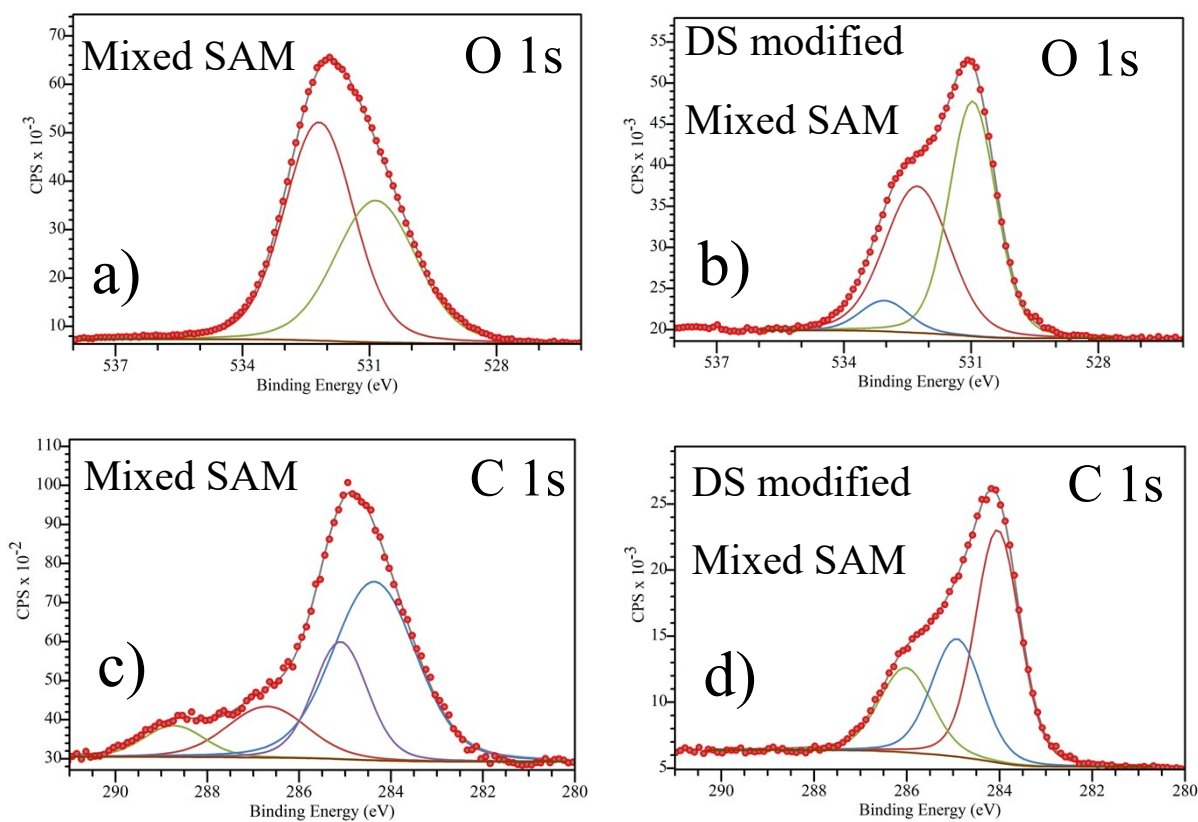


Figure S7. (a, b) O 1s and (c, d) C 1s XPS core-level spectra of (a) FTO/mixed-SAM and FTO/DS-modified mixed-SAM films.

Table S2. Peak fitting results of the O 1s XPS spectra for mixed SAM and DS modified SAM samples.

O 1s	Mixed SAM	Relative area (%)	FWHM (eV)
lattice O ²⁻ (Sn–O)	530.87 eV	43.08	2.24
Surface –OH / adsorbed H ₂ O/O _x species	532.09 eV	56.92	1.92
O 1s	DS modified	Relative area (%)	FWHM (eV)
lattice O ²⁻ (Sn–O)	530.98 eV	49.93	1.30
interfacial O (P–O–Sn)/surface –OH/adsorbates	532.27 eV	43.29	1.80
hydroxyl-rich oxygen (polyol-related and/or strongly H-bonded)	533.04 eV	6.78	1.35

adsorbates			
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Table S3. Peak fitting results of the C 1s XPS spectra for mixed SAM and DS modified SAM samples.

C 1s	Mixed SAM	Relative area (%)	FWHM (eV)
C–C / C=C (hydrocarbon/aromatic)	284.36	54.61	2.12
C–N and/or C–O (heteroatom-adjacent carbon)	285.10	23.27	1.38
C–O (ether/alcohol; methoxy-rich and/or H-bonded C–O)	286.70	15.13	2.05
Carbonate/carboxylate-like surface adsorbates; possible adventitious carbon	288.72	6.99	1.54
C 1s	DS modified	Relative area (%)	FWHM (eV)
C–C / C=C (hydrocarbon/aromatic)	284.14	44.86	1.14
C–C/C–H shoulder + heteroatom-adjacent C (C–N/C–O overlap)	284.91	35.64	1.54
Oxygenated carbon (C–O-dominant; alcohol/ether/polyol/methoxy environments; possible H-bonded C–O)	286.09	19.50	1.41

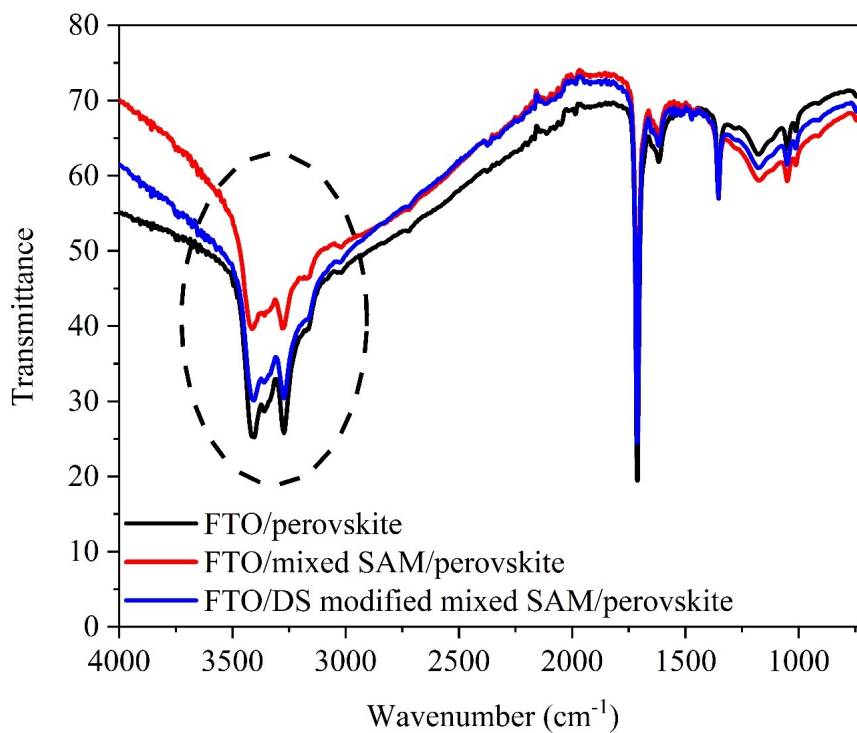
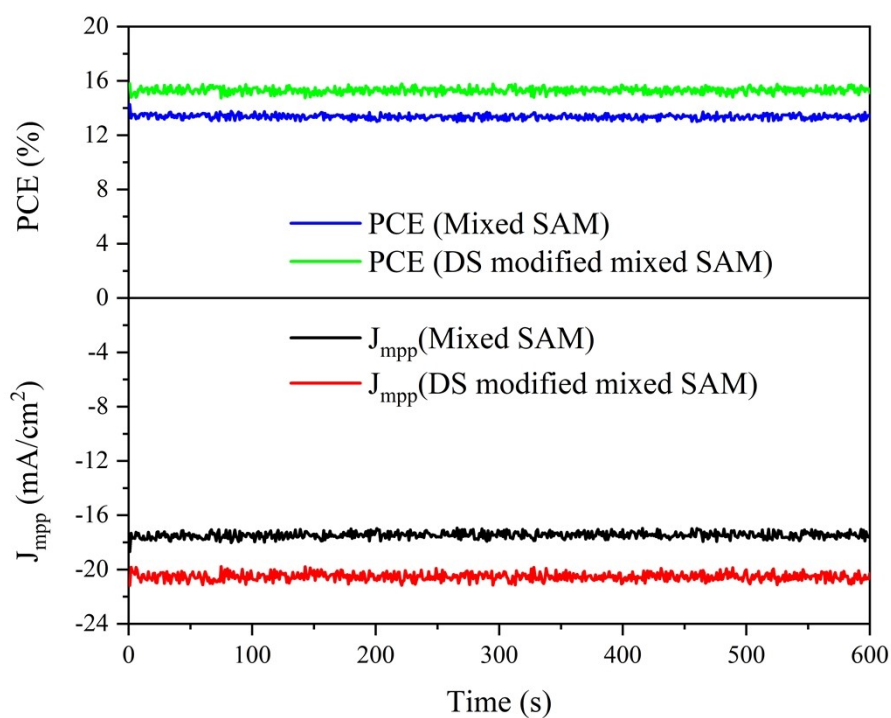


Figure S8. FTIR spectra of FTO/perovskite, FTO/mixed-SAM/perovskite, and FTO/DS-



modified mixed-SAM/perovskite films.

Figure S9. Time-dependent maximum power point tracking of mixed-SAM and DS-modified mixed-SAM based PSCs measured for 600 s under continuous illumination. (The MPPT measurements were performed on an independently fabricated set of devices prepared under the same optimized conditions as the representative devices in the main text.)