

Supporting Information

Advanced Co-Self-Assembled Monolayers for Stress Relief and Performance Optimization in Methylammonium-Free Perovskite Solar Cells

Che-Chia Hsu¹ and Sheng-Hsiung Yang^{*,2}

¹Institute of Photonic System and ²Institute of Lighting and Energy Photonics, College of Photonics, National Yang Ming Chiao Tung University, No. 301, Section 2, Gaofa 3rd Road, Guiren District, Tainan 711010, Taiwan, ROC

*Correspondence: yangsh@nycu.edu.tw

Table S1. Atomic percentage of P, Sn, and O atoms measured by EDS of the pristine MeO-2PACz, Co-SAM (4-PA), and Co-SAM (4-PAA) on FTO substrates.

	P atom (%)	Sn atom (%)	O atom (%)
MeO-2PACz	1.38	31.82	66.80
Co-SAM (4-PA)	1.52	31.47	67.01
Co-SAM (4-PAA)	1.58	32.08	66.34

Table S2. TR-PL fitting parameters of perovskite films deposited on MeO-2PACz, Co-SAM (4-PA), and Co-SAM (4-PAA).

Sample	A ₁ (%)	τ_1 (ns)	A ₂ (%)	τ_2 (ns)	τ_{avg} (ns)
MeO-2PACz	49	10.1	39.7	702.5	690.4
Co-SAM (4-PA)	52.7	7.97	31.3	342.2	329.6
Co-SAM (4-PAA)	66.8	5.68	25.6	287.3	273.5

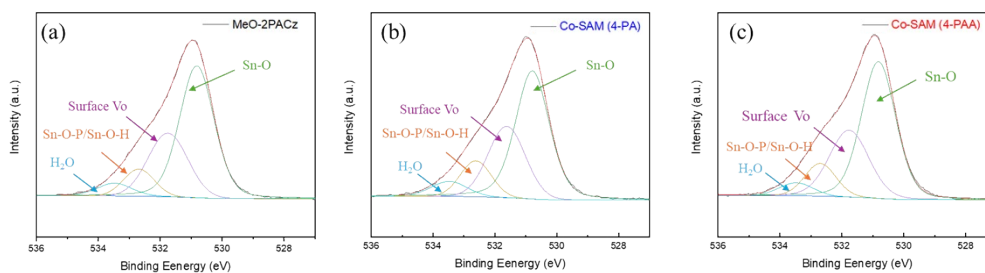


Fig. S1. O 1s XPS spectra of (a) MeO-2PACz, (b) Co-SAM (4-PA), and (c) Co-SAM (4-PAA) on FTO substrates.

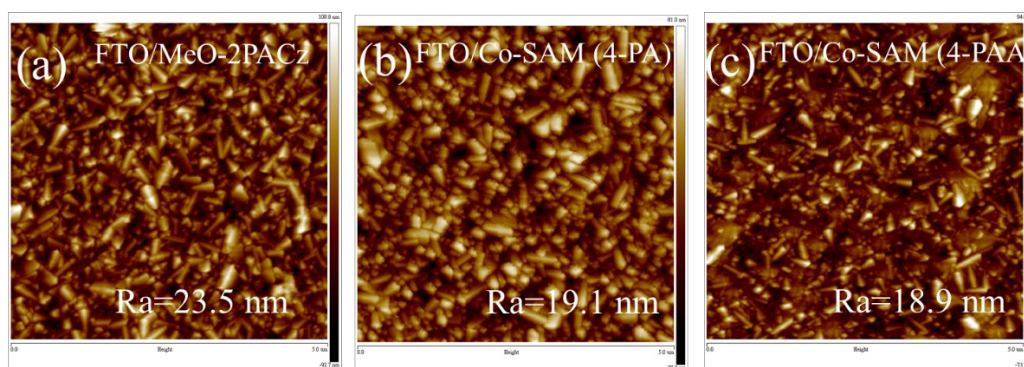


Fig. S2. Topographic AFM images with R_a values of MeO-2PACz, Co-SAM (4-PA), and Co-SAM (4-PAA) on FTO substrates.

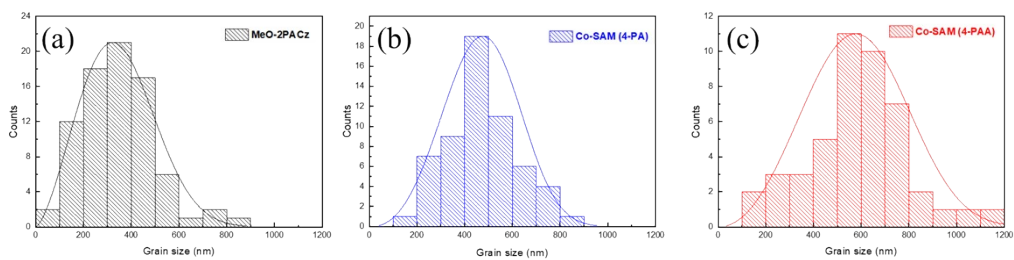


Fig. S3. Grain-size distributions of perovskite layers on (a) MeO-2PACz, (b) Co-SAM (4-PA), and (c) Co-SAM (4-PAA).

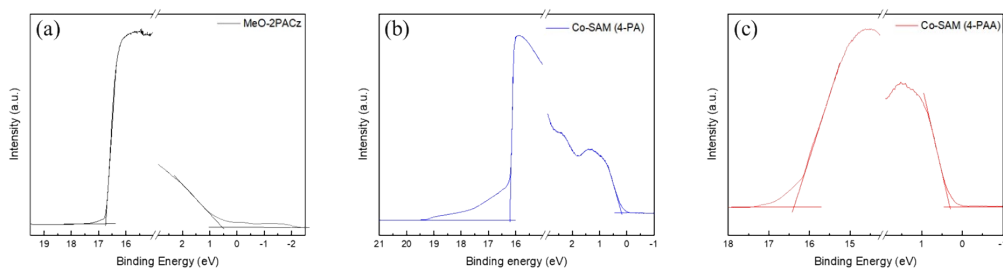


Fig. S4. UPS spectra of (a) MeO-2PACz, (b) Co-SAM (4-PA), and (c) Co-SAM (4-PAA)

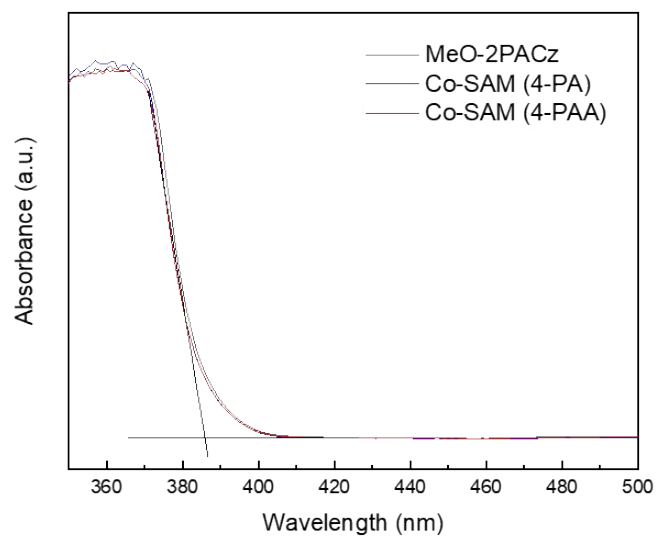


Fig. S5. UV-vis absorption spectra of MeO-2PACz, Co-SAM (4-PA), and Co-SAM (4-PAA)

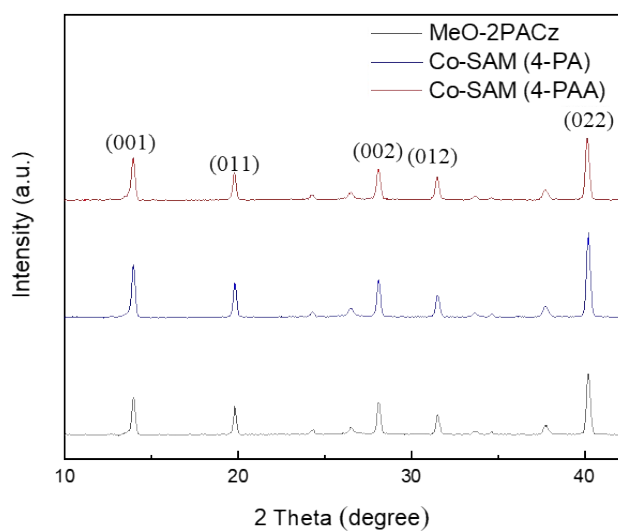


Fig. S6. XRD analysis of perovskite films deposited on various SAM-modified substrates.

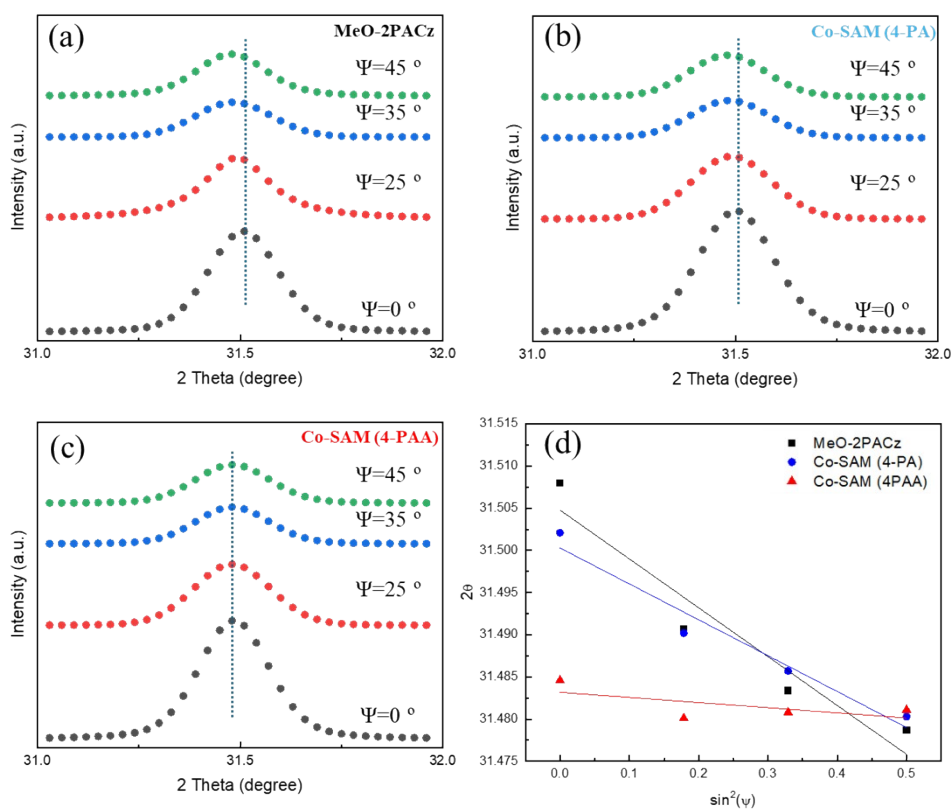


Fig. S7. GIXRD patterns of the perovskite films deposited on (a) MeO-2PACz, (b) Co-SAM (4-PA), and (c) Co-SAM (4-PAA), measured at different ψ angles from 5° to 45° ; (d) 2θ versus $\sin^2(\psi)$ plots for the corresponding perovskite films on FTO/MeO-2PACz, FTO/Co-SAM (4-PA), and FTO/Co-SAM (4-PAA).

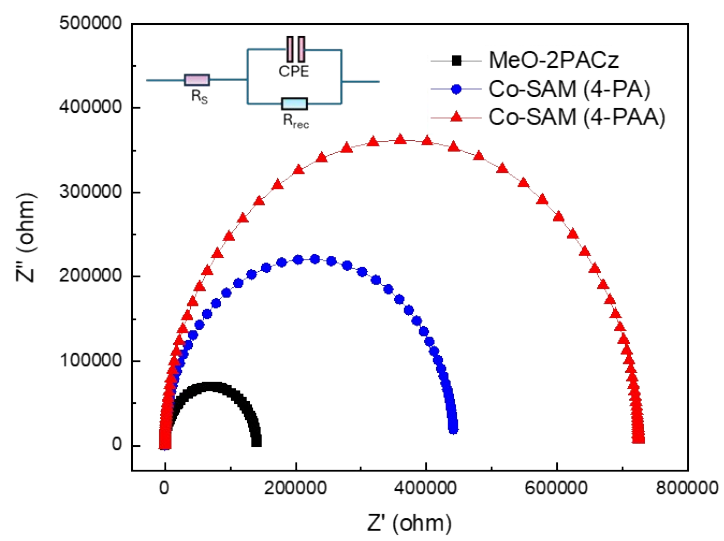


Fig. S8. Nyquist plots of PSCs without or with Co-SAM modification.