

Stress Regulation via Surface Micro-etching and Reconstruction for Enhancing Triple-Cation Perovskite Solar Cells with the Efficiency of 25.54%

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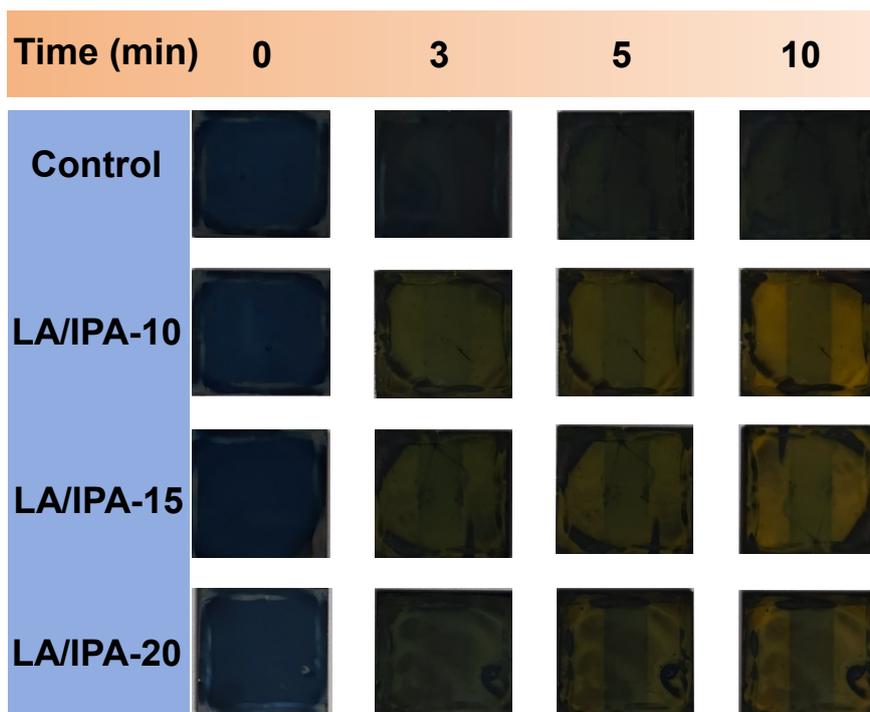


Figure S1. The state change of perovskite films soaked in mixed solution with the different LA/IPA ratio for 10 minutes.

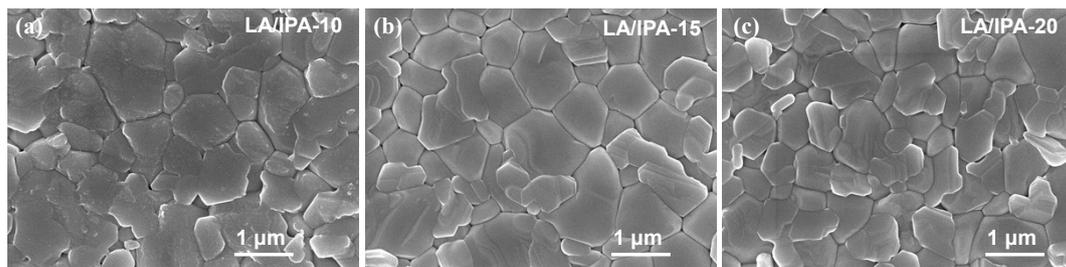


Figure S2. Surface SEM images of perovskite films etched by mixed solutions with the different LA/IPA ratios of a) 1:10, b) 1:15 and c) 1:20.

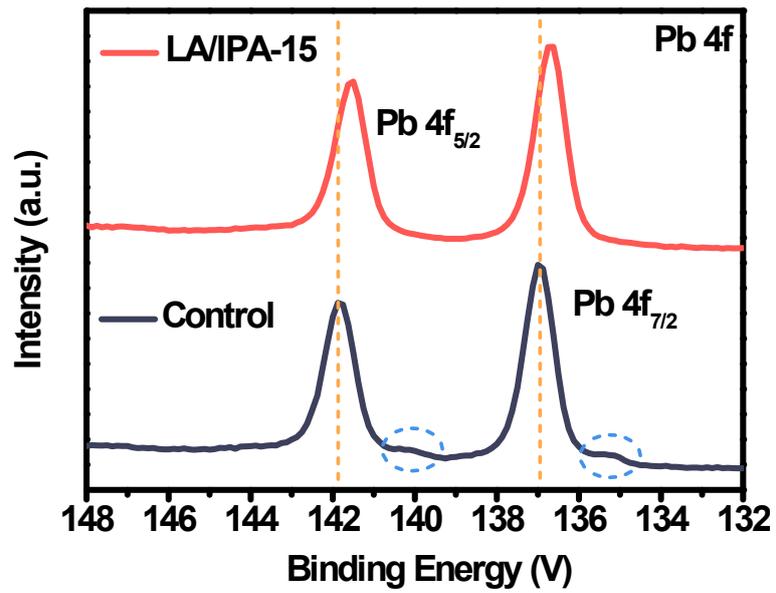


Figure S3. The XPS spectra of Pb 4f for control and LA/IPA-15 treated perovskite films.

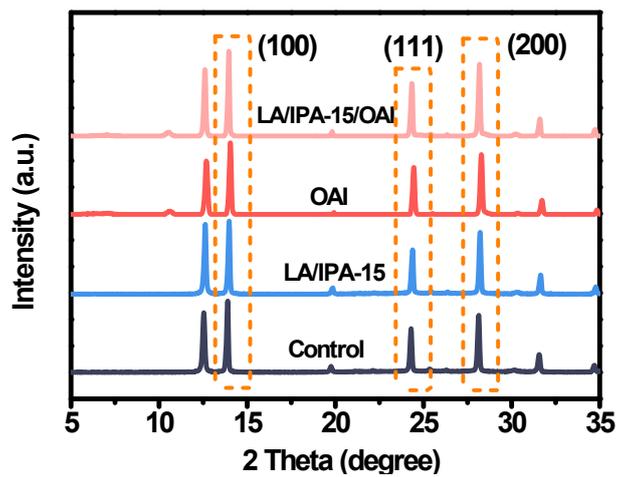


Figure S4. XRD pattern of control, LA/IPA-15, OAI and LA/IPA-15/OAI treated perovskite films.

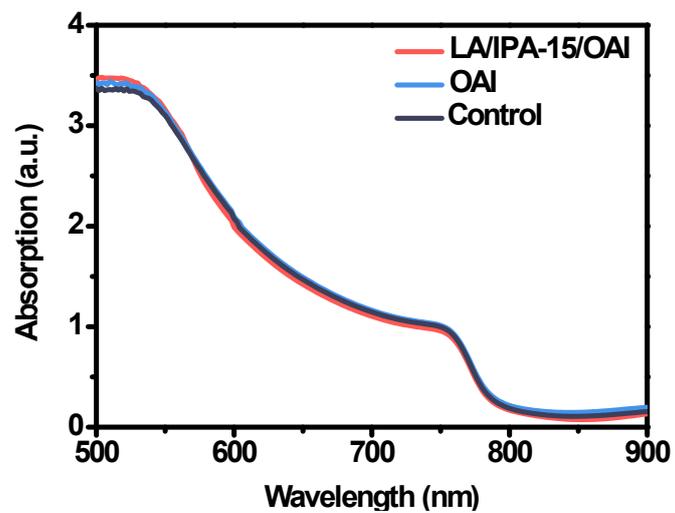


Figure S5. UV-vis light absorption spectrum of different perovskite films.

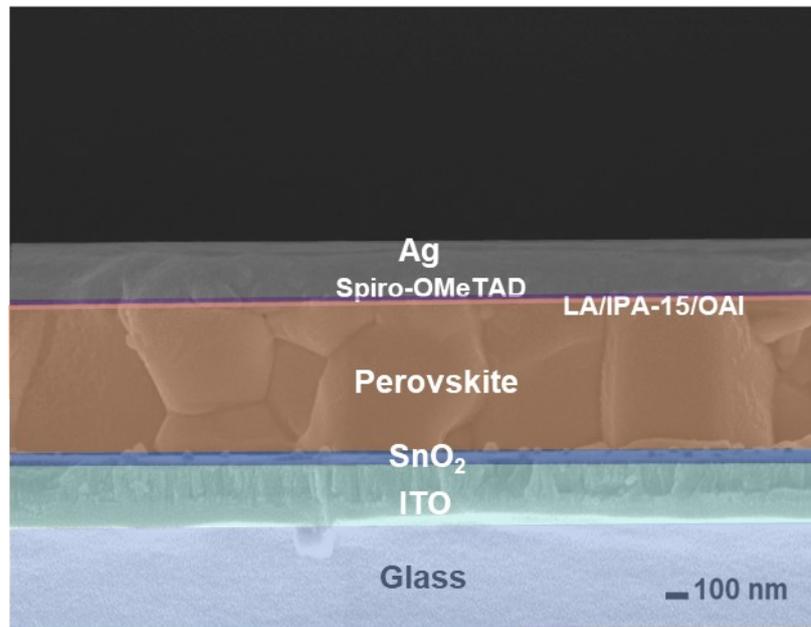


Figure S6. Cross-section SEM images of the LA/IPA-15/OAI treated device.

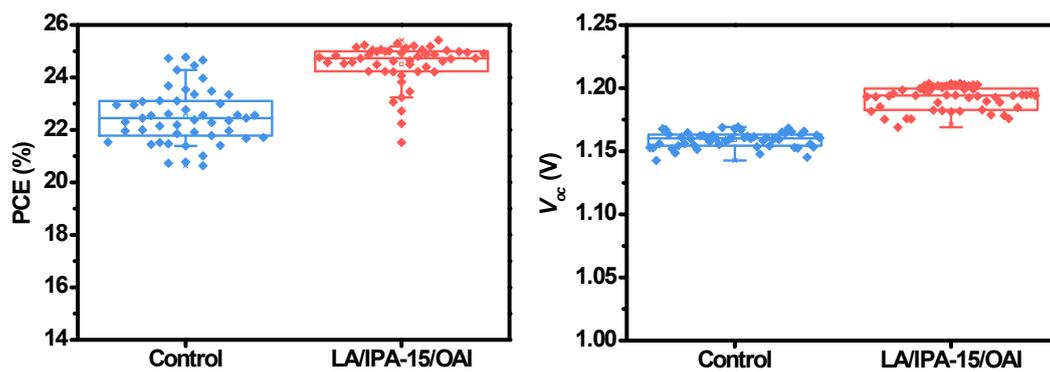


Figure S7. Statistical diagram of PCE and V_{oc} for the control and LA/IPA-15/OAI treated PSCs.

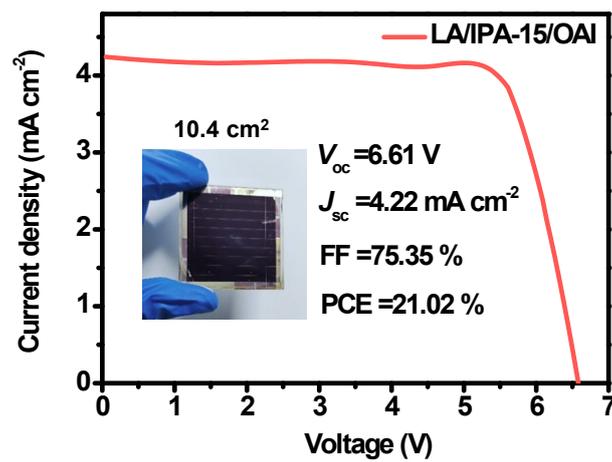


Figure S8. J - V curve of LA/IPA-15/OAI treated PSC mini-module with an area of 10.4 cm^2 .



Figure S9. Water contact angle (CA) of perovskite films with different treatments.

Table S1. The fitting parameters of TRPL spectra for the control and target samples.

Samples	A_1	τ_1 (ns)	A_2	τ_2 (ns)	τ_{ave} (ns)
Control	1.04	21.90	0.16	127.04	77.47
LA/IPA-15/OAI	0.34	58.84	0.27	359.90	308.52

Table S2. The fitting data of EIS for the control and target devices.

Samples	R_s (Ω)	R_{tran} (Ω)	R_{rec} (Ω)
Control	68	4390	11425
LA/IPA-15/OAI	34	2141	21587

Table S3. Photovoltaic performance statistics of representative triple-cation PSCs during the past three years.

Perovskite component	V_{oc} (V)	J_{sc} (mA cm ⁻²)	FF (%)	PCE (%)	Year	Ref.
$\text{Cs}_{0.05}(\text{FA}_{0.98}\text{MA}_{0.02})_{0.95}\text{Pb}(\text{I}_{0.98}\text{Br}_{0.02})_3$	1.17	24.85	81.33	23.68	2022	[S1]
$(\text{CsPbI}_3)_{0.05}[(\text{FAPbI}_3)_{0.97}(\text{MAPbBr}_3)_{0.03}]_{0.9}$	1.21	25.21	80.12	24.43	2022	[S2]
$(\text{Cs}_{0.05}\text{FA}_{0.95}\text{PbI}_3)_{0.975}(\text{MAPbBr}_3)_{0.025}$	1.18	25.58	82.11	24.78	2023	[S3]
$\text{Cs}_{0.07}\text{FA}_{0.9}\text{MA}_{0.03}\text{Pb}(\text{I}_{0.92}\text{Br}_{0.08})_3$	1.20	24.50	81.80	24.20	2023	[S4]
$(\text{Cs}_{0.05}\text{FA}_{0.75}\text{MA}_{0.20})\text{Pb}(\text{I}_{0.96}\text{Br}_{0.04})_3$	1.20	25.58	82.68	25.43	2023	[S5]
$\text{Cs}_{0.03}\text{FA}_{0.945}\text{MA}_{0.025}\text{Pb}(\text{I}_{0.975}\text{Br}_{0.025})_3$	1.16	25.07	84.88	24.74	2024	[S6]
$\text{Cs}_{0.07}\text{FA}_{0.9}\text{MA}_{0.03}\text{Pb}(\text{I}_{0.975}\text{Br}_{0.025})_3$	1.20	25.25	82.99	25.04	2024	[S7]
$\text{Cs}_{0.03}\text{FA}_{0.945}\text{MA}_{0.025}\text{Pb}(\text{I}_{0.975}\text{Br}_{0.025})_3$	1.20	25.40	83.79	25.54	2024	This work

- [S1] S. You, H. Zeng, Z. Ku, X. Wang, Z. Wang, Y. Rong, Y. Zhao, X. Zheng, L. Luo, L. Li, S. Zhang, M. Li, X. Gao, X. Li, *Adv. Mater.* **2020**, 32, 2003990.
- [S2] J.-H. Kim, Y. R. Kim, J. Kim, C.-M. Oh, I.-W. Hwang, J. Kim, S. Zeiske, T. Ki, S. Kwon, H. Kim, A. Armin, H. Suh, K. Lee, *Adv. Mater.* **2022**, 34, 2205268.
- [S3] X. Wang, D. Liu, R. Liu, X. Du, B. Zhang, X. Sun, C. Chen, Z. Li, Q. Zhao, Z. Shao, X. Wang, G. Cui, S. Pang, *Adv. Energy Mater.* **2023**, 2203635.
- [S4] J. Deng, K. Wei, L. Yang, L. Lin, Y. Xiao, X. Cai, C. Zhang, D. Wu, X. Zhang, J. Zhang, *Adv. Mater.* **2023**, 35, 2300233.
- [S5] L. Shen, P. Song, L. Zheng, L. Wang, X. Zhang, K. Liu, Y. Liang, W. Tian, Y. Luo, J. Qiu, C. Tian, L. Xie, Z. Wei, *Adv. Mater.* **2023**, 35, 2301624.
- [S6] Y. Ding, X. Feng, E. Feng, J. Chang, H. Li, C. Long, Y. Gao, S. Lu, J. Yang, *Small* **2024**, 2308836.
- [S7] D. Liu, C. Chen, X. Wang, X. Sun, B. Zhang, Q. Zhao, Z. Li, Z. Shao, X. Wang, G. Cui, S. Pang, *Adv. Mater.* **2024**, 36, 2310962.