

Supplementary Materials: Dual Strategy Based on Quantum Dot Doping and Phenylethylamine Iodide Surface Modification for High-Performance and Stable Perovskite Solar Cells

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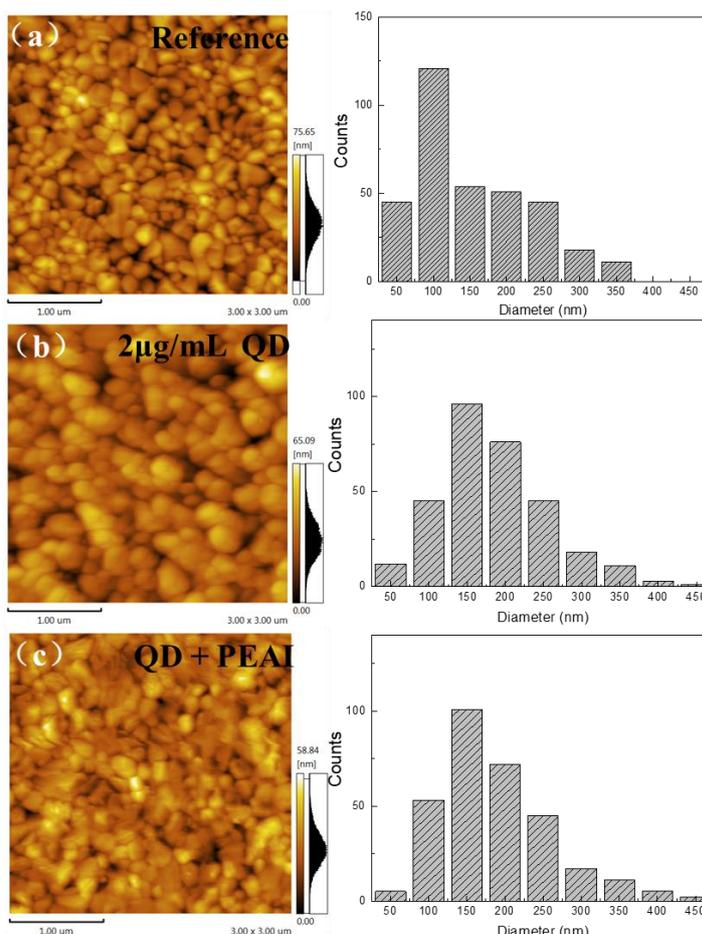
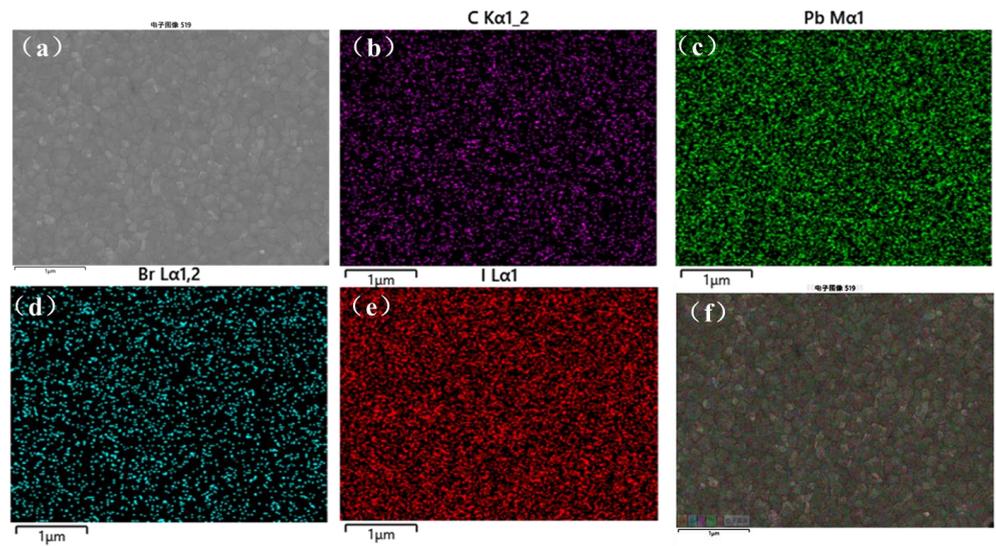


Figure S1. AFM images and grain size statistics of perovskite films modified with different conditions: (a) reference, (b) doped with 2 $\mu\text{g/mL}$ CsPbBr₃ QDs, (c) jointly modified with 2 $\mu\text{g/mL}$ CsPbBr₃ QDs and 2 mg/mL PEAI.



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Figure S2. EDS mappings of PFs jointly modified with CsPbBr₃ QDs and PEA1: (a) SEM pattern, (b) C element, (c) Pb element, (d) Br element, (e) I element, (f) the combination of SEM and mappings.

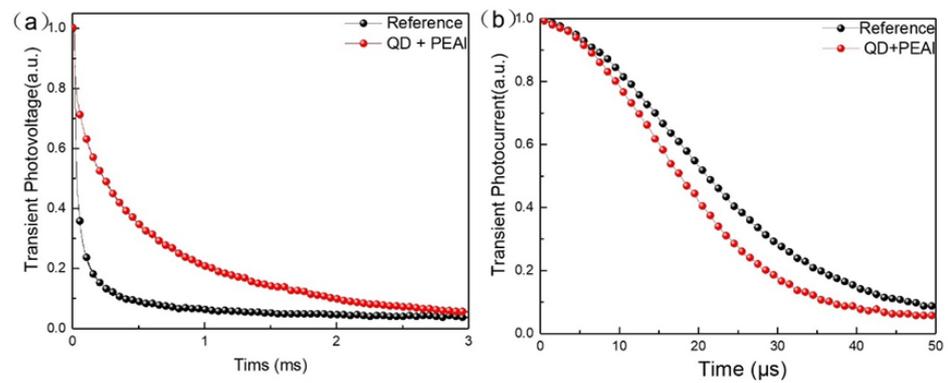
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Table S1 The parameters of (110) diffraction peak of PFs modified at different conditions.

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Samples	Peak location (°)	Intensity (a.u.)	FWHM (°)
reference	13.97	1506	0.193
0.2 μg/mL QDs	13.99	1713	0.185
2 μg/mL QDs	14.01	2398	0.178
10 μg/mL QDs	14.04	1968	0.183
QDs+PEAI	14.01	2396	0.178



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Figure S3. TPV (a) and TPC (b) decay curves of original and jointly-modified PSCs.

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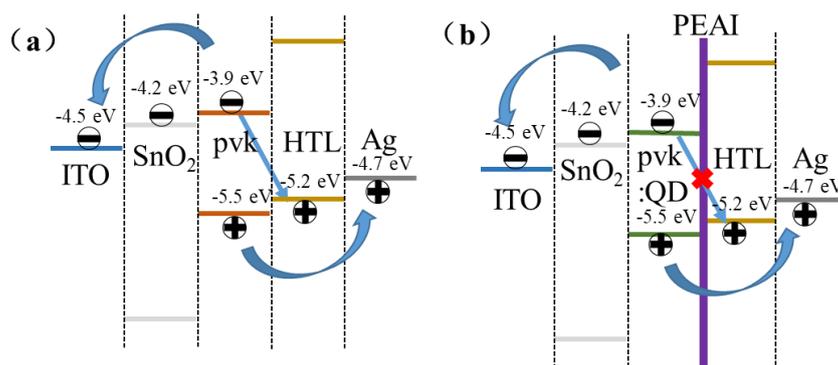


Figure S4. The energy alignment of reference and CsPbBr₃ QDs + PEAI modified PSCs.

The quantum tunneling effect is described as follows:

$$T = (C / A)^2 = \text{Exp} \left[-2 d \sqrt{\frac{2m_n(qV_0 - E)}{\hbar^2}} \right] \quad (\text{S-1})$$

where T represents the transmission coefficient, C represents the transmission wave function, A represents the incident wave function, m_n represents the effective mass of the electron, \hbar represents the reduced Planck constant, qV_0 represents the barrier height, and d represents the thickness of the tunneling layer.

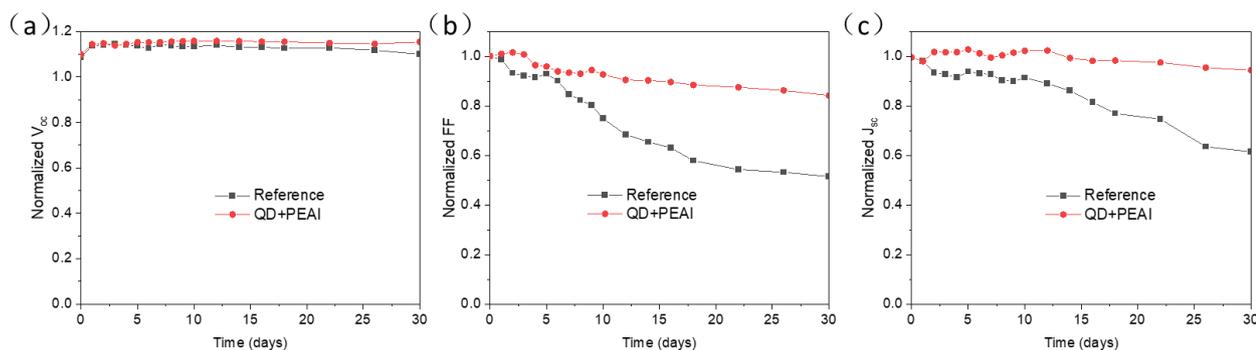


Figure S5. Aging curves of normalized Voc (a), FF(b) and Jsc (c) in air condition with a RH of 40% and RT (unpacked).

Table S2 Simple comparison of PCE MAPbI₃ perovskite solar cells.

Perovskite	PCE _{max} (%)	Reference
MAPbI ₃	19.11	[1]
MAPbI ₃	20.06	[2]
MAPbI ₃	20.22	[3]
MAPbI ₃	20.23	[4]
MAPbI ₃	20.46	[5]
MAPbI ₃	20.46	[6]
MAPbI ₃	20.46	[7]
MAPbI ₃	20.93	[8]
MAPbI ₃	21.04	This Work

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References

1. Liu, R.; Wang, J.; Mak, C.H.; Du, M.; Li, F.-F.; Shen, H.-H.; Santoso, S.P.; Yu, E.T.; Yu, X.; Chu, P.K.; et al. Optimizing Black Phosphorus/Halide Perovskite Compositions by Scanning Photoelectrochemical Microscopy. *J. Electrochem. Soc.* **2022**, *169*, 096510, doi:10.1149/1945-7111/ac8d34. 43
2. Feng, Z.; Weng, C.; Hua, Y.; Chen, X.; Huang, S. Efficient and Stable Perovskite Solar Cells: The Effect of Octadecyl Ammonium Compound Side-Chain. *Chem. Eng. J.* **2023**, *475*, 146498, doi:10.1016/j.cej.2023.146498. 44
3. Lu, R.; Liu, Y.; Zhang, J.; Zhao, D.; Guo, X.; Li, C. Highly Efficient (200) Oriented MAPbI₃ Perovskite Solar Cells. *Chem. Eng. J.* **2022**, *433*, 133845, doi:10.1016/j.cej.2021.133845. 45
4. Phase Control of Organometal Halide Perovskites for Development of Highly Efficient Solar Cells | ACS Applied Materials & Interfaces Available online: <https://pubs.acs.org/doi/10.1021/acsami.2c22769> (accessed on 24 March 2024). 46
5. Yao, Y.; Hang, P.; Wang, P.; Xu, L.; Cui, C.; Xie, J.; Xiao, K.; Li, G.; Lin, P.; Liu, S.; et al. CsPbBr₃ Quantum Dots Assisted Crystallization of Solution-Processed Perovskite Films with Preferential Orientation for High Performance Perovskite Solar Cells. *Nanotechnology* **2020**, *31*, 085401, doi:10.1088/1361-6528/ab55a1. 47
6. Azadipyrromethene Dye-Assisted Defect Passivation for Efficient and Stable Perovskite Solar Cells | ACS Applied Materials & Interfaces Available online: <https://pubs.acs.org/doi/full/10.1021/acsami.1c20923> (accessed on 24 March 2024). 48
7. Nguyen, M.H.; Kim, K.-S. Controlling the Grain Formation Process with Oleylamine and 4-Dimethylaminopyridine Additives for Efficient and Stable MAPbI₃ Solar Cells. *Mater. Today Chem.* **2023**, *34*, 101799, doi:10.1016/j.mtchem.2023.101799. 49
8. Reinforcing the Efficiency and Stability of Perovskite Solar Cells Using a Cesium Sulfate Additive | Journal of Materials Science: Materials in Electronics Available online: <https://link.springer.com/article/10.1007/s10854-023-10008-6> (accessed on 24 March 2024). 50

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