

Supplementary Information

Surface Passivation of Perovskite by Atomic Layer Deposition: a Mechanism Investigation Enabling Efficient Inverted Planar Solar Cells

Ran Zhao,^{a,†} Kai Zhang,^{b,†} Jiahao Zhu,^{a,†} Shuang Xiao,^{b,*} Wei Xiong,^a Jian Wang,^b Tanghao Liu,^c
Guichuan Xing,^c Kaiyang Wang,^c Shihe Yang,^{b,*} and Xinwei Wang^{a,*}

^a Dr. R. Zhao, J. Zhu, W. Xiong, Prof. X. Wang

School of Advanced Materials, Shenzhen Graduate School, Peking University, Shenzhen
518055, China

Email: wangxw@pkusz.edu.cn

^b K. Zhang, Prof. S. Xiao, Dr. J. Wang, Prof. S. Yang

Guangdong Key Lab of Nano-Micro Material Research, School of Chemical Biology and
Biotechnology, Shenzhen Graduate School, Peking University, Shenzhen 518055, China

Email: xiaoshuang@pku.edu.cn (S.X.), chsyang@pku.edu.cn (S.Y.)

^c Dr. T. Liu, Prof. G. Xing, K. Wang

Institute of Applied Physics and Materials Engineering, University of Macau, Avenida da
Universidade, Taipa, Macau, China

([†]These authors contributed equally to this work.)

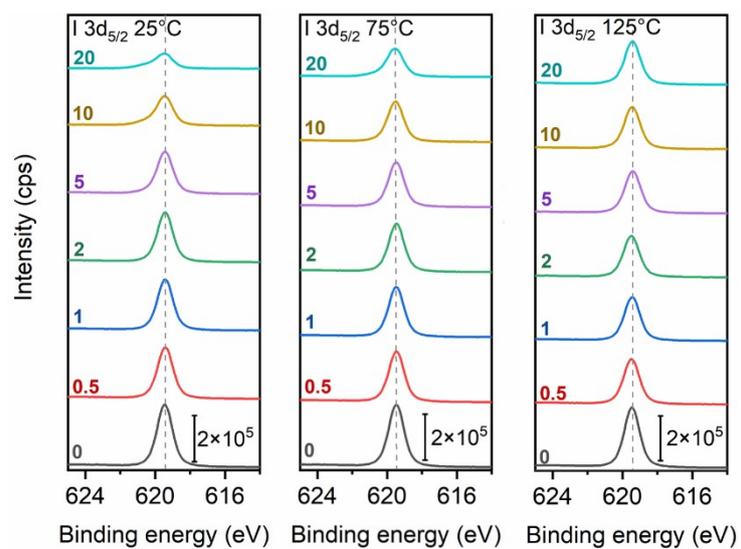


Figure S1 High-resolution XPS core-level spectra of I $3d_{5/2}$ taken from 0 cycles (i.e., initial surface) through 20 cycles of ALD Al_2O_3 on $\text{CH}_3\text{NH}_3\text{PbI}_3$. The deposition temperatures were at 25 °C, 75 °C and 125 °C.

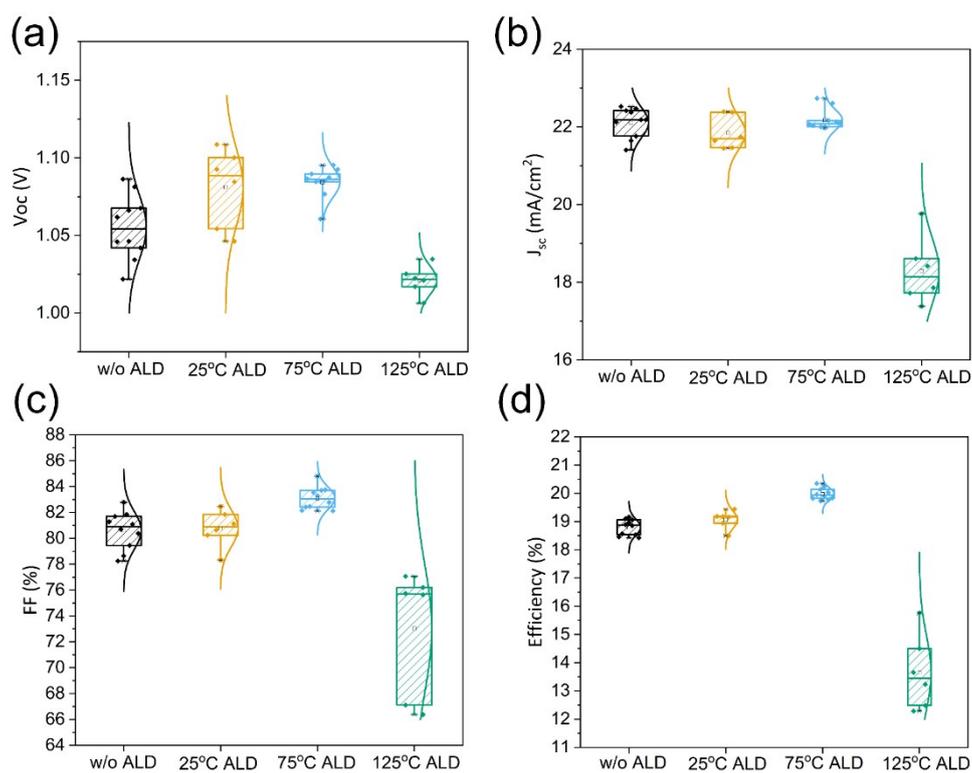


Figure S2 Statistical distributions of open circuit voltage (V_{oc}), short circuit current density (J_{sc}), fill factor (FF), and power conversion efficiency for the perovskite solar cells (PSCs) without ALD and with the ALD Al₂O₃ deposited at 25 °C, 75 °C and 125 °C.

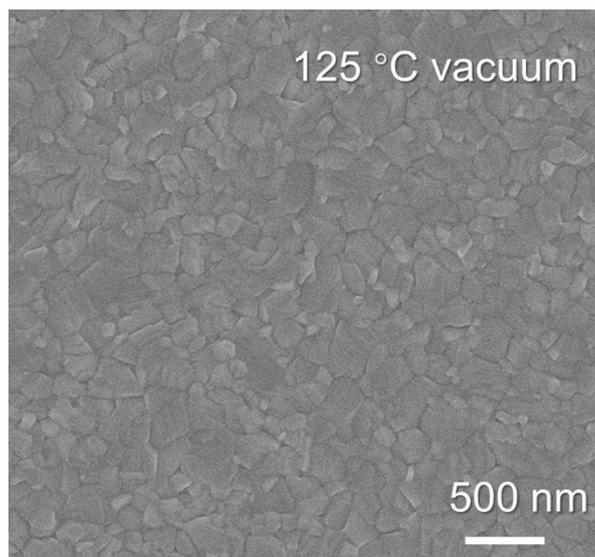


Figure S3 SEM image taken on the $\text{CH}_3\text{NH}_3\text{PbI}_3$ film annealed under vacuum at 125 °C.

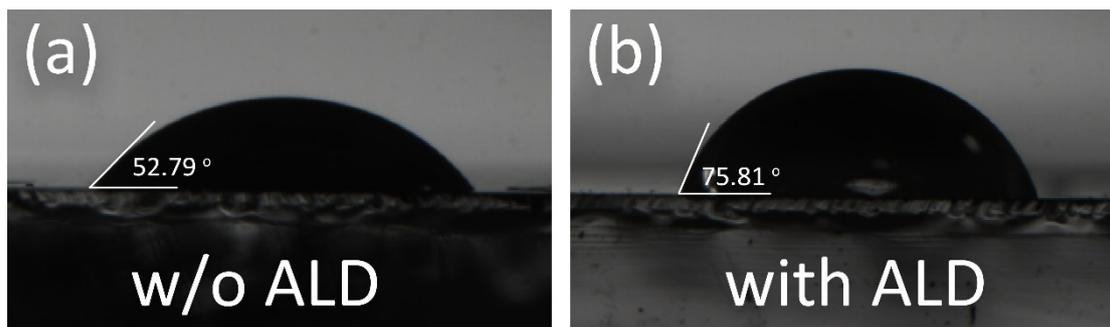


Figure S4 Contact angle measurement for the MAPbI₃ film (a) without ALD-Al₂O₃ and (b) with 10 cycle ALD-Al₂O₃ at 75 °C.

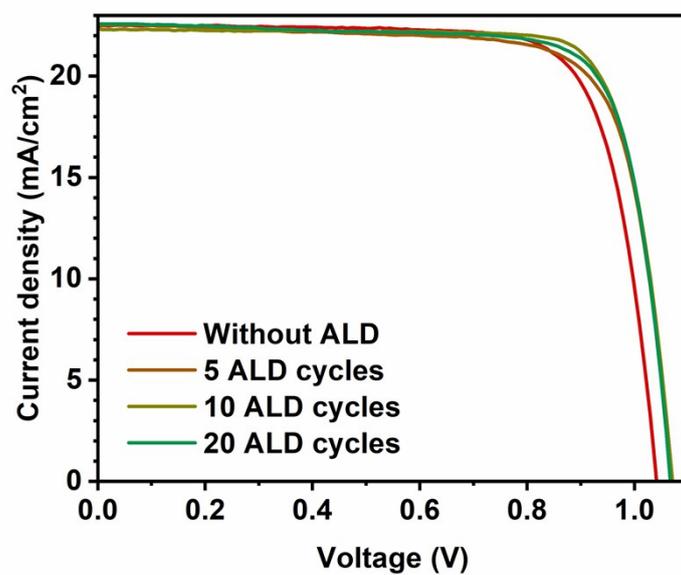


Figure S5 Curves of current density versus voltage for the PSCs without ALD (red) and with 5- (brown), 10- (dark yellow), and 20-cycle (green) ALD Al₂O₃ deposited at 75 °C.

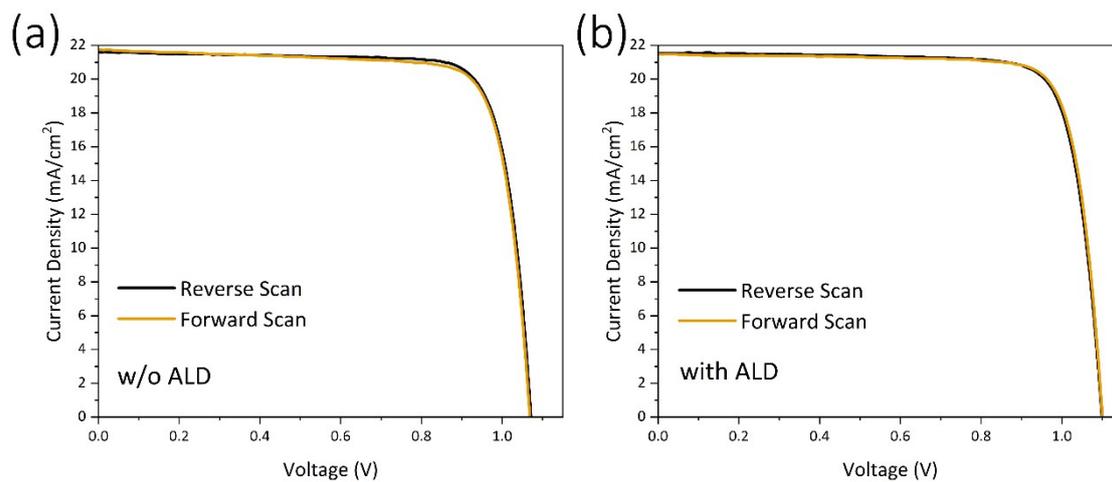


Figure S6 The reverse and forward scan J-V curves for the PSCs (a) without ALD-Al₂O₃ and (b) with 10 cycle ALD-Al₂O₃ at 75 °C.

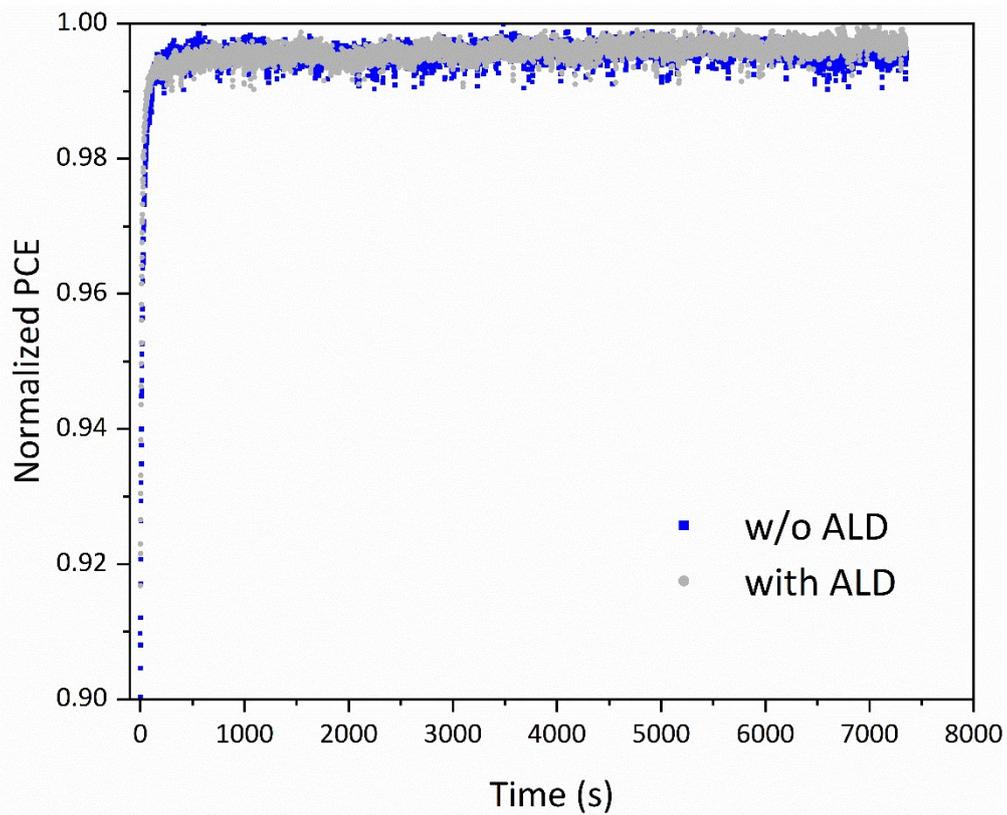


Figure S7 The maximum power point tracking measurement for the PSCs without and with 10 cycle ALD- Al_2O_3 at 75 °C.

Table S1 Fitted decay times of PSCs with and without ALD Al₂O₃ from time-resolved photoluminescence spectra. “Glass side” means that the incident light came from the glass side, and the “air side” means that the incident light came from the PVK side (PVK sample) or the Al₂O₃ side (PVK/Al₂O₃ sample).

Sample	τ_1 (ns)	A_1	τ_2 (ns)	A_2	τ_{ave} (ns)
PVK-air side	5.72	0.72	29.52	0.24	20.88
PVK/Al ₂ O ₃ -air side	9.10	0.45	84.30	0.29	73.39
PVK-Glass side	7.55	0.67	61.62	0.28	49.42
PVK/Al ₂ O ₃ -Glass side	8.86	0.53	89.52	0.29	77.52