

Electronic supplementary information

Electron Transport Layer Assisted by Nickel Chloride Hexahydrate for Open-Circuit Voltage Improvement in MAPbI₃ Perovskite Solar Cells

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Table S1. The main parameters of O 1s peak in different SnO₂ films.

SnO ₂ films	Peak type	Peak position (eV)	Percentage (%)
SnO ₂	O (vacancies)	531.70	35.35
	O (lattice)	530.46	64.65
SnO ₂ - NiCl ₂	O (vacancies)	531.76	31.08
	O (lattice)	530.53	68.92

Table S2. Fitting parameters of the exponential decay function in TRPL spectra.

Samples	A_1	τ_1	A_2	τ_2	τ_{ave}
FTO/PVK	0.423	11.74	0.577	198.3	119.4
SnO ₂ /PVK	0.088	22.96	0.881	75.35	70.62
SnO ₂ - NiCl ₂ /PVK	0.084	47.48	0.867	112.9	107.1

Table S3. Fitted parameters for the EIS measurements acquired under dark for different samples.

Sample	R_s ($\Omega \text{ cm}^2$)	R_{rec} ($\Omega \text{ cm}^2$)
SnO_2	1.06	8.17×10^3
$\text{SnO}_2 - \text{NiCl}_2$	2.63	1.47×10^4

Table S4. Band gaps (E_g), secondary–electron cutoff (E_{cutoff}), fermi edge ($E_{F, \text{edge}}$), fermi level (E_F), valence band (E_{VB}) and conduction band (E_{CB}) for SnO₂ and SnO₂-NiCl₂ films.

Samples	E_g (eV)	E_{cutoff} (eV)	E_F (eV)	$E_{F, \text{edge}}$ (eV)	E_{VB} (eV)	E_{CB} (eV)
SnO ₂	4.12	16.76	4.46	3.51	7.97	3.85
SnO ₂ -NiCl ₂	4.15	16.68	4.54	3.41	7.95	3.80

The E_{cutoff} of SnO₂ and SnO₂-NiCl₂ films are 16.76 and 16.68 eV, respectively. we calculate as $E_F = E_{\text{cutoff}} - 21.22$ eV, where E_{cutoff} is the high binding energy cutoff to get the Fermi level (E_F), and 21.22 eV is emission energy from He irradiation. The E_F of SnO₂ and SnO₂-NiCl₂ films are calculated as -4.46 and -4.54 eV, respectively. The $E_{F, \text{edge}}$ of SnO₂ and SnO₂-NiCl₂ films are 3.51 and 3.41 eV, respectively. The E_{VB} of SnO₂ and SnO₂-NiCl₂ films are -7.97 and -7.95 eV, calculating as $E_{\text{VB}} = E_F - E_{F, \text{edge}}$ (Fermi edge). According to the absorption spectrum and Tauc plot, we get the band gap (E_g) of SnO₂ (4.12 eV) and SnO₂-NiCl₂ (4.15 eV). E_{CB} obtained from E_g and E_{VB} is -3.85 and -3.80 eV, respectively.

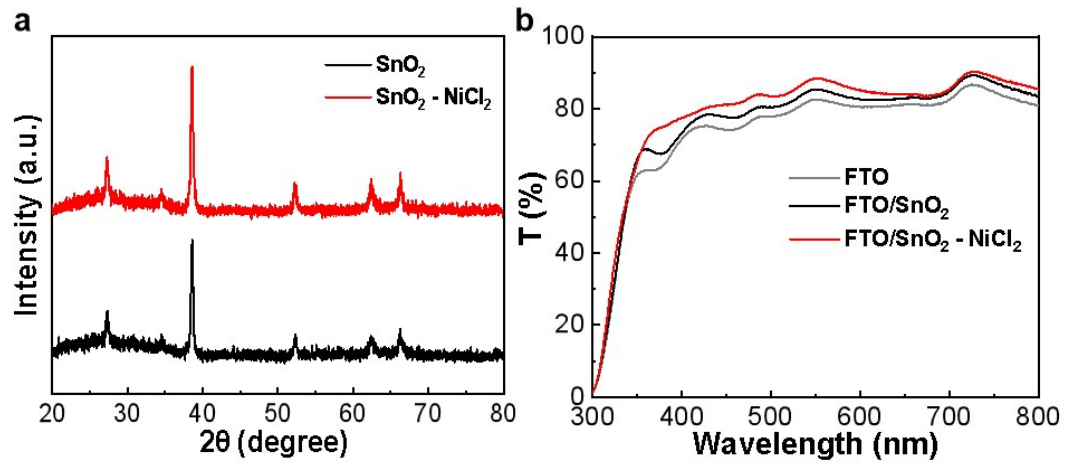


Figure S1. (a) The XRD pattern of SnO_2 without and with NiCl_2 . (b) The Transmission spectrum of FTO, FTO/ SnO_2 and FTO/ $\text{SnO}_2\text{-NiCl}_2$ substrate, respectively.

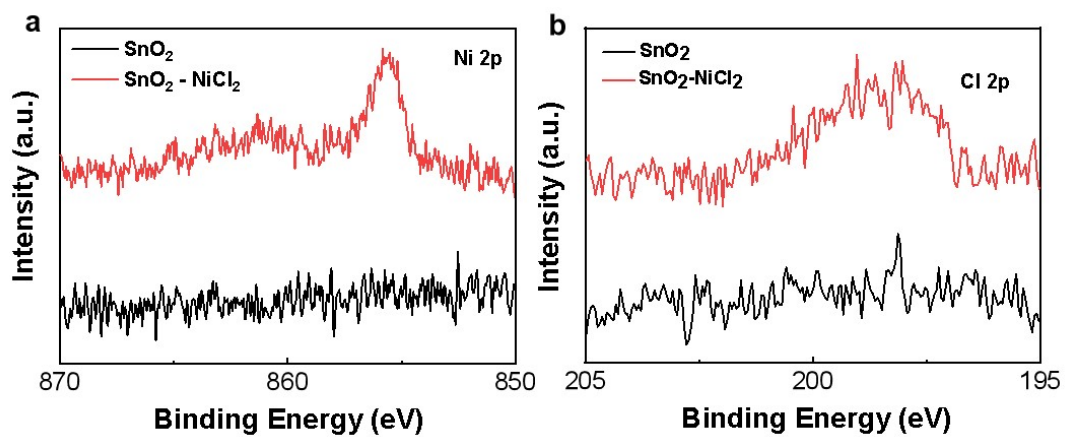


Figure S2. (a) X-ray photoelectron spectroscopy (XPS) of Ni 2p. (b) XPS of Cl 2p.

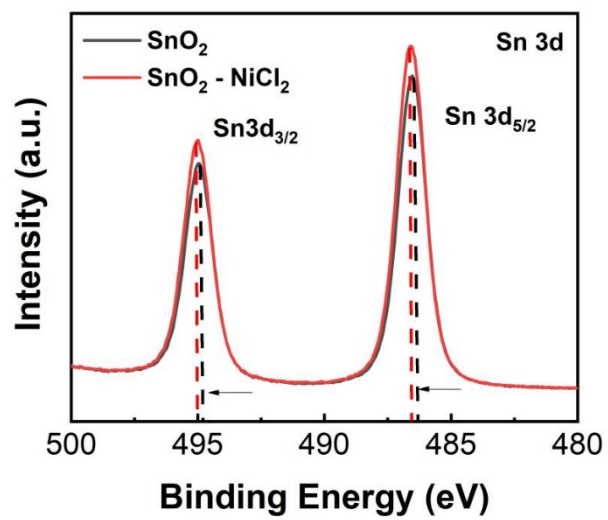


Figure S3. XPS of Sn 3d.

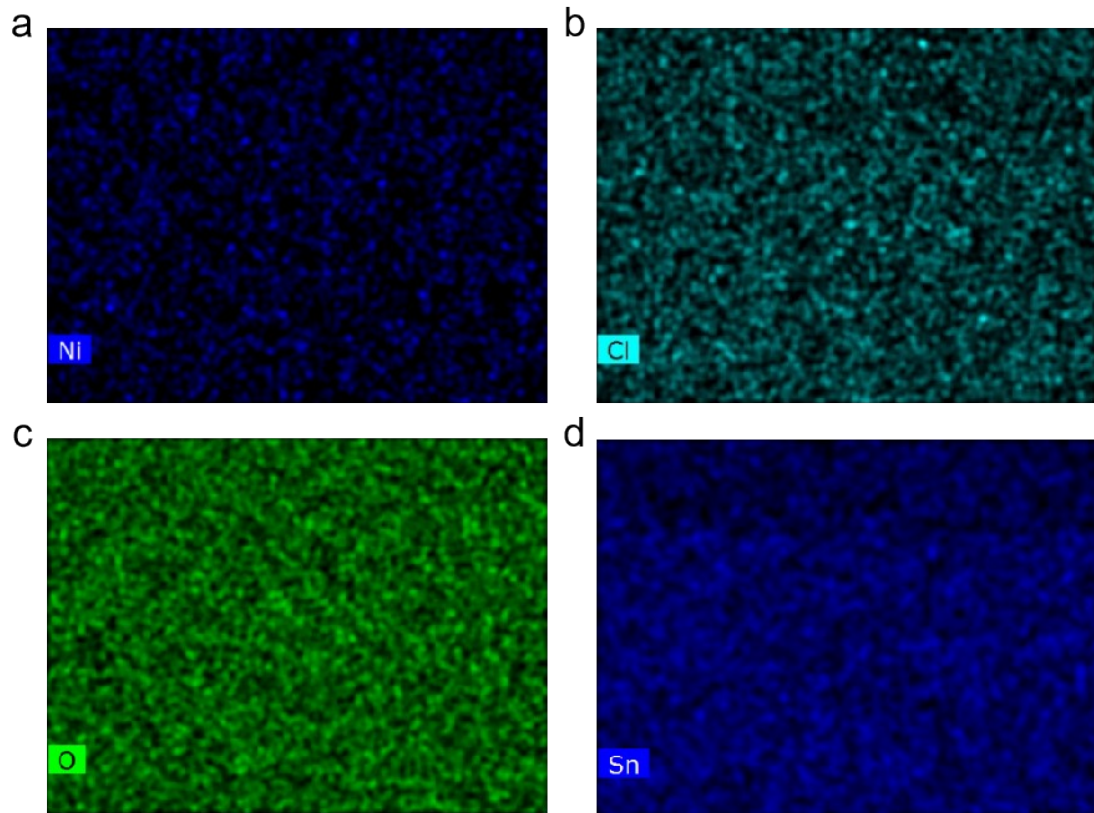


Fig. S4. Element distribution analysis of FTO/SnO₂-NiCl₂ film, EDS mapping of (a) Ni, (b)Cl, (c) O, d) Sn.

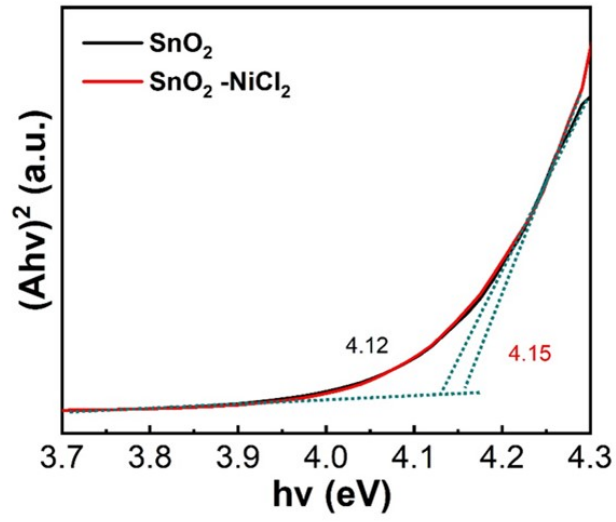


Figure S5. UV-Vis spectra of the SnO₂ and SnO₂-NiCl₂ films.

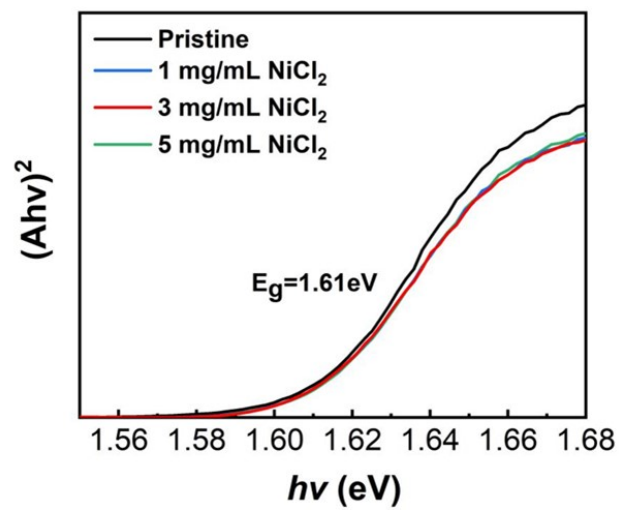


Figure S6. UV-Vis spectra of perovskite on the SnO₂ and SnO₂-NiCl₂ films.

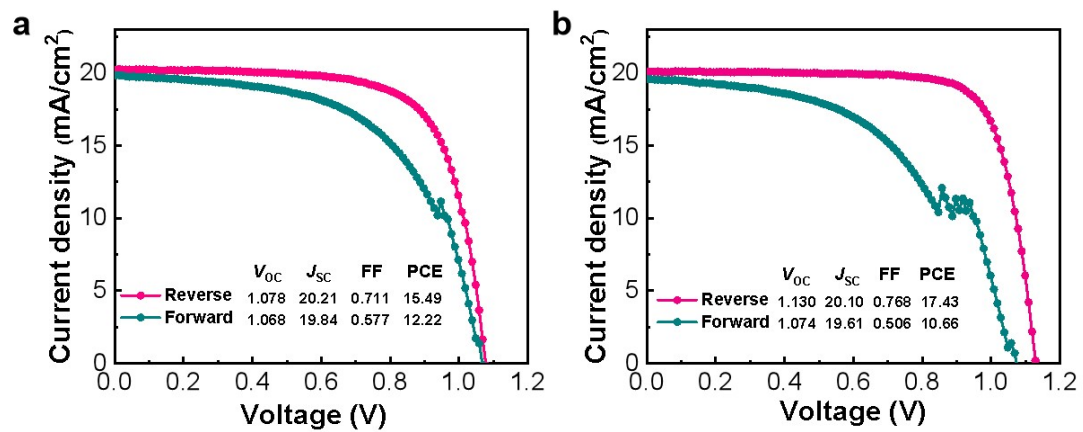


Figure S7. J - V curves of the device of without and with $NiCl_2$.

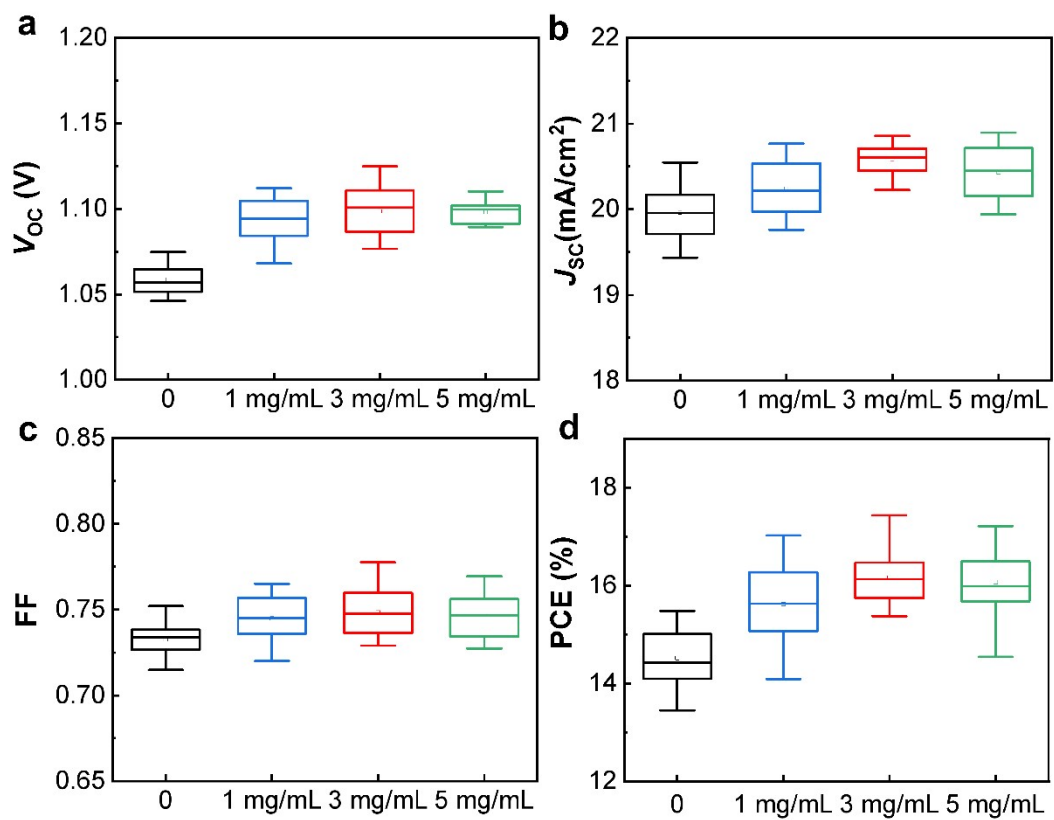


Figure S8. (a) Measured V_{OC} , (b) J_{SC} , (c) FF, and (d) PCE statistical parameters based on PSCs of different additive concentrations and unmodified PSCs (20 cells for each type).