Tailoring buried interface of tin oxide-based n-i-p perovskite solar cells via bidirectional and multifunctional metal ion chelating agent modification

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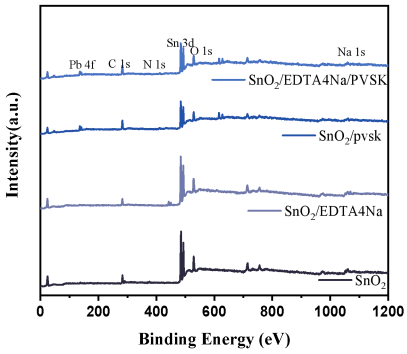
(a)



(b)

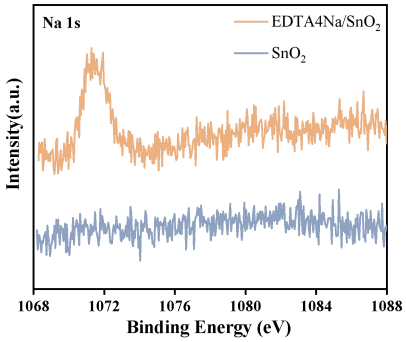


Figure S1 (a)XPS survey spectra of SnO_2, SnO_2/EDTA4Na, and SnO_2 coated with particularly low concentration perovskite solution before and after EDTA4Na modification. (b) Na 1s XPS spectra of SnO_2, SnO_2/EDTA4Na films.

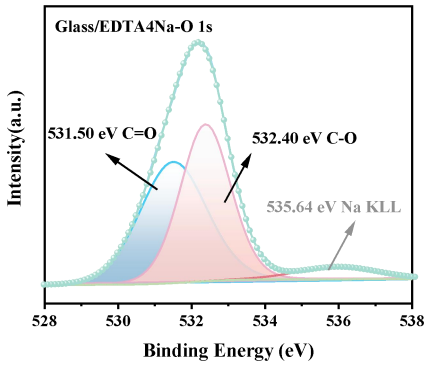


Figure S2 O 1s XPS spectra of EDTA4Na film deposited on glass substrate.

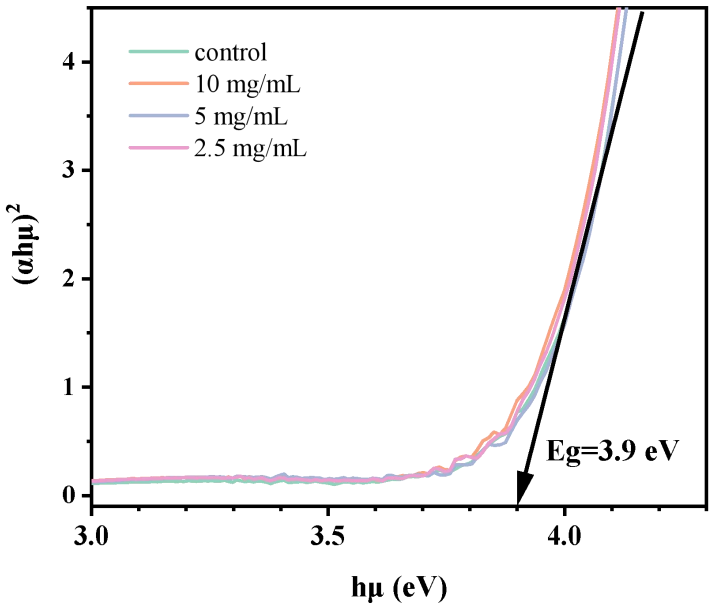


Figure. S3. Optical band gap of SnO_2 before and after EDTA4Na modification, detected by $(\alpha h\mu)^2$ as a function of photon energy.

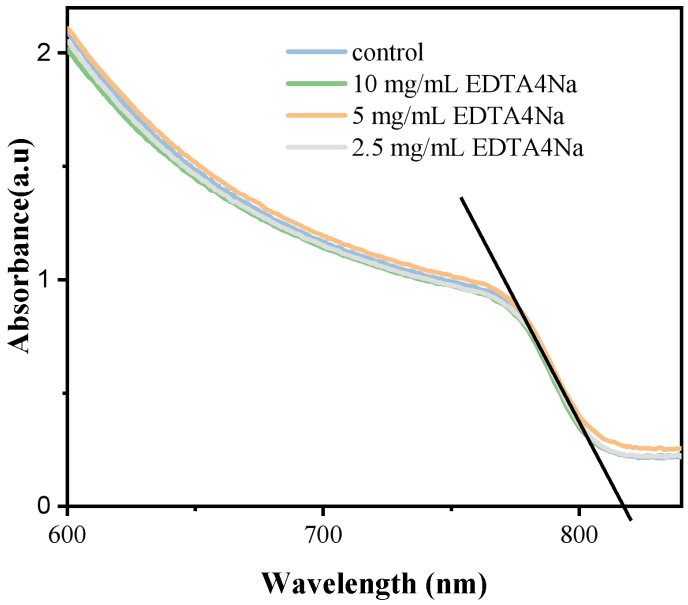


Figure.S4. UV-Vis absorption spectrum of perovskite thin films deposited on SnO_2 and SnO_2/EDTA4Na.

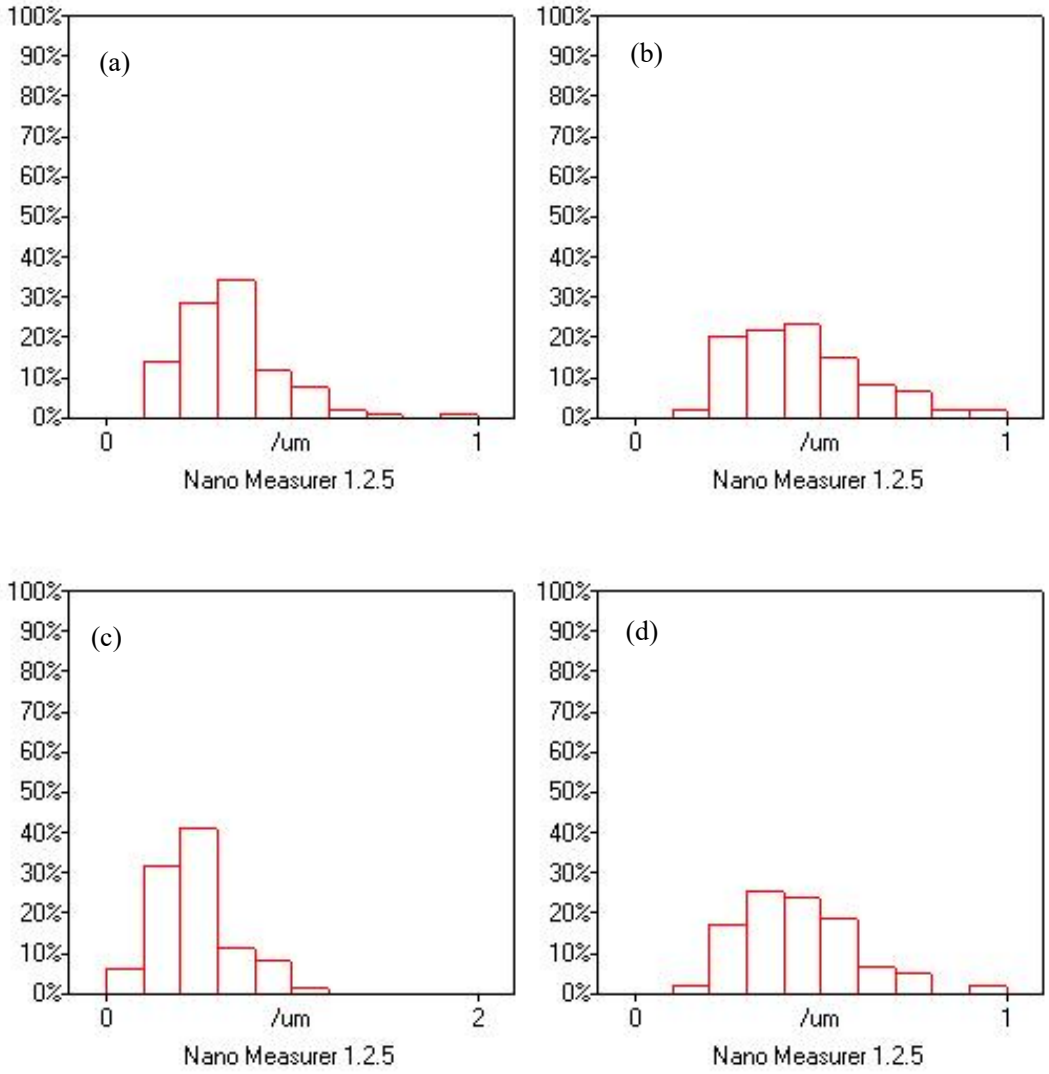


Figure S5 (a)-(d). The grain size distribution of perovskite films deposited on the SnO_2 and SnO2/EDTA4Na, corresponding to the FESEM images.

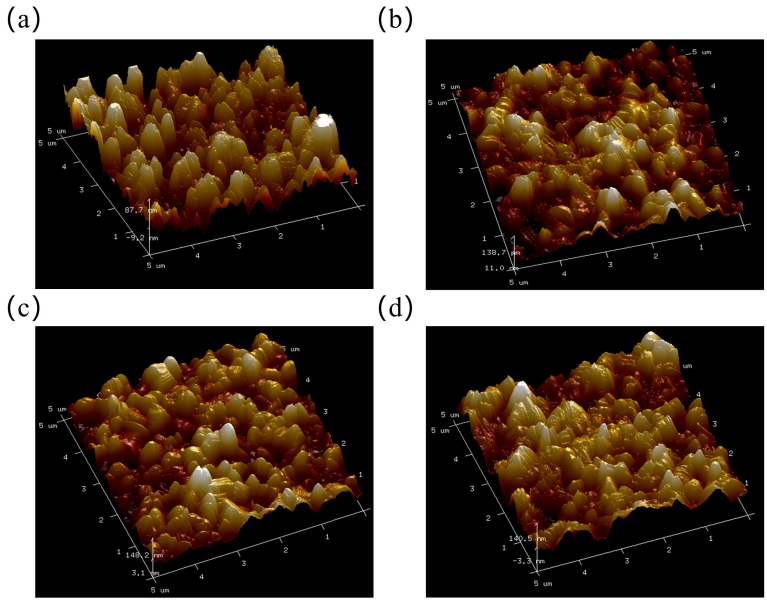


Figure S6 (a)-(d). AFM images of perovskite films deposited on SnO_2 and SnO_2/EDTA4Na.

Table S1. Photovoltaic parameters statistics of devices based on different concentrations of EDTA4Na modification

Devices	V_{OC} (V)	J_{SC} (mA cm^{-2})	FF (%)	PCE (%)
control	1.066	24.53	75.04	19.64
10 mg/mL	1.102	24.93	78.76	21.64
5 mg/mL	1.140	24.88	80.29	22.77
2.5 mg/mL	1.069	24.45	79.01	20.66

Table S2. Fitting parameters of TRPL decay curves of perovskite films based on ITO/SnO_2 and ITO/SnO_2/EDTA4Na substrate (refer to Figure. 6b).

Samples	τ_1 (ns)	$A_{1\ (\%)}$	τ_2 (ns)	A_2	τ_{avg} (ns)
ITO/SnO_2/perovskite	107.52	6.2%	543.45	93.8%	717.31
ITO/SnO_2/EDTA4Na	27.02	18.86%	185.36	81.14%	137.81

The trap-state density (N_t) can be calculated by the following equation：

$$N_{t=}\frac{2\varepsilon\varepsilon_0 V_{TFL}}{eL^2}$$

L = 5X10^{-5} cm	e =1.60 ×10^{-19} C	ε=53.69[1]	ε_0 ＝8.8542 × 10 $^{-14}$ F/cm

[1].Zhen Li, Bo Li, Xin Wu, Stephanie A. Sheppard, Shoufeng Zhang, Danpeng Gao, Nicholas J. Long, and Zonglong Zhu, *Organometallic-functionalized interfaces for highly efficient inverted perovskite solar cells.* 2022. **376**(6591): p. 416-420.