

SnO₂ 表面卤化提高钙钛矿太阳能电池光伏性能

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SnO₂ Surface Halogenation to Improve Photovoltaic Performance of Perovskite Solar Cells

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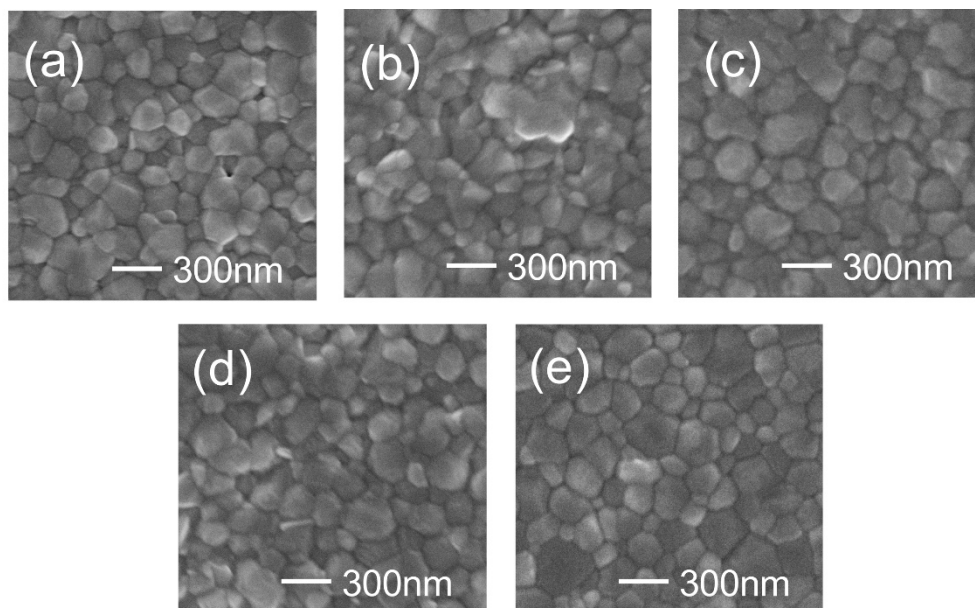


图 S1 (a)无钝化层和加入(b) $1 \text{ mg}\cdot\text{mL}^{-1}$ 、(c) $2.5 \text{ mg}\cdot\text{mL}^{-1}$ 、(d) $5 \text{ mg}\cdot\text{mL}^{-1}$ 、(e) $10 \text{ mg}\cdot\text{mL}^{-1}$ 不同浓度 TBAC 钝化层后钙钛矿的 SEM 顶视图

Fig. S1 SEM images of perovskite films (a) without and with (b) $1 \text{ mg}\cdot\text{mL}^{-1}$, (c) $2.5 \text{ mg}\cdot\text{mL}^{-1}$, (d) $5 \text{ mg}\cdot\text{mL}^{-1}$, (e) $10 \text{ mg}\cdot\text{mL}^{-1}$ TBAI passivation layer.

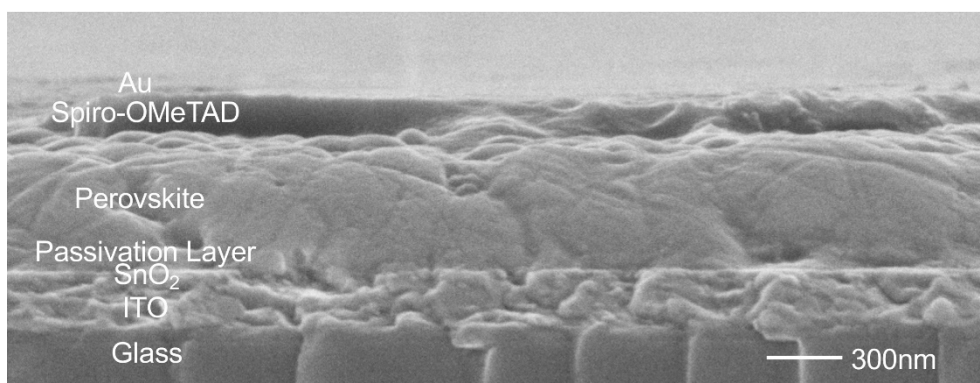


图 S2 钙钛矿太阳能电池器件的 SEM 截面图

Fig. S2 Cross-sectional SEM image of PSCs.

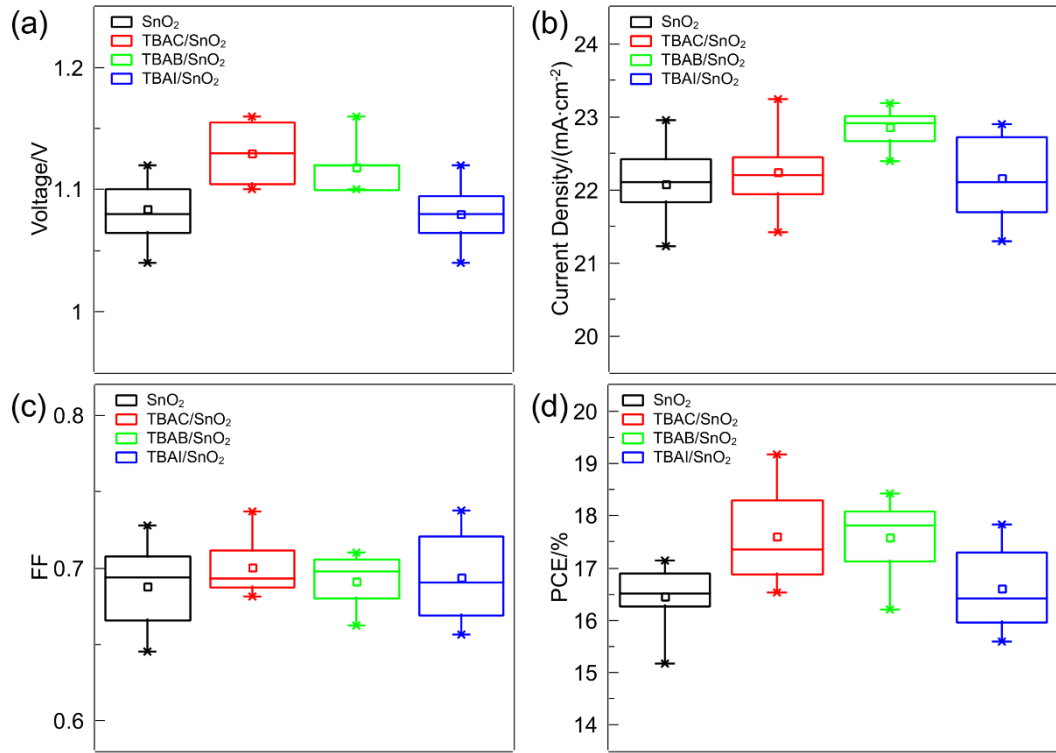


图 S3 无钝化层和加入不同钝化层后 10 组钙钛矿太阳能电池器件的(a)开路电压(V_{oc})统计图、(b)短路电流(J_{sc})统计图、(c)填充因子(FF)统计图和(d)为能量转换效率(PCE)统计图

Fig. S3 Statistical distribution of (a) V_{oc} , (b) J_{sc} , (c) FF, and (d) PCE of PSCs without and with different passivation layers (each condition has 10 cells).

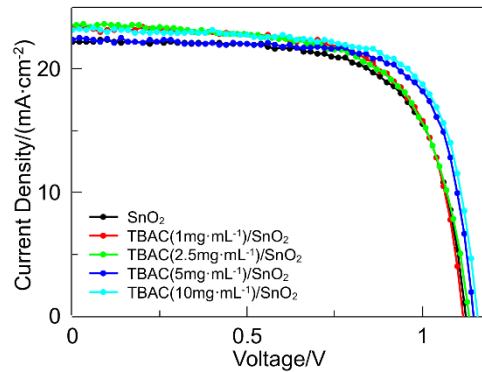


图 S4 无钝化层和加入不同浓度 TBAC 钝化层后太阳能电池器件的电流密度-光电压($J-V$)图

Fig. S4 $J-V$ curves of PSCs without and with TBAC passivation layer treated by different concentrations.

表 S1 无钝化层和加入不同浓度 TBAC 钝化层后钙钛矿太阳能电池器件光伏性能参数

Table S1 Photovoltaic parameters of PSCs without and with TBAC passivation layer treated by different concentrations.

Sample	V_{oc}/V	$J_{sc}/(mA \cdot cm^{-2})$	FF	PCE/%
SnO ₂	1.120	22.206	0.690	17.150
TBAC (1 mg·mL ⁻¹)/SnO ₂	1.120	23.387	0.674	17.667
TBAC (2.5 mg·mL ⁻¹)/SnO ₂	1.130	23.502	0.659	17.492
TBAC (5 mg·mL ⁻¹)/SnO ₂	1.140	22.256	0.737	18.693
TBAC (10 mg·mL ⁻¹)/SnO ₂	1.160	23.111	0.715	19.170

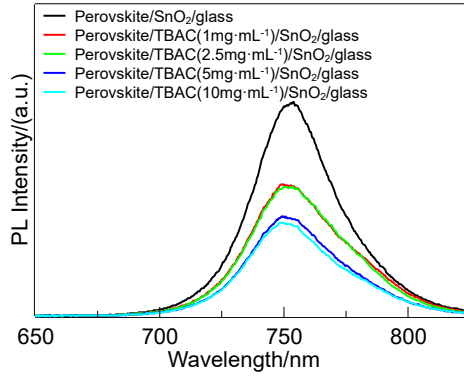


图 S5 无钝化层和加入不同浓度 TBAC 钝化层后钙钛矿层的稳态荧光光谱

Fig. S5 SSPL spectra of perovskite films without and with TBAC passivation layer treated by different concentrations.

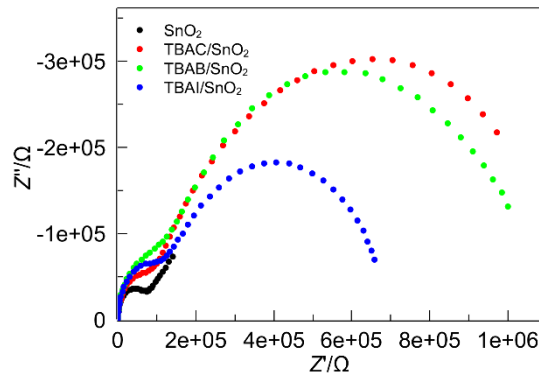


图 S6 无钝化层和加入不同钝化层后钙钛矿太阳能电池器件在无偏压下的电化学交流阻抗谱

Fig. S6 EIS spectra of PSCs with no bias without and with different passivation layers.

表 S2 无钝化层和加入不同钝化层后钙钛矿太阳能电池器件等效电路拟合参数

Table S2 Parameters of the equivalent circuit of PSCs without and with different passivation layers.

Sample	$R_s/(\Omega \cdot \text{cm}^2)$	$R_{co}/(\Omega \cdot \text{cm}^2)$	$\text{CPE}_1\text{-T}/(\text{F} \cdot \text{cm}^{-2})$	$\text{CPE}_1\text{-P}/(\text{F} \cdot \text{cm}^{-2})$	$R_{rc}/(\Omega \cdot \text{cm}^2)$	$\text{CPE}_2\text{-T}/(\text{F} \cdot \text{cm}^{-2})$	$\text{CPE}_2\text{-P}/(\text{F} \cdot \text{cm}^{-2})$
SnO ₂	7.87	123580	1.02E-8	0.96	131550	9.53E-8	0.87
TBAC/SnO ₂	7.34	210550	1.73E-8	0.99	499010	2.78E-8	0.86
TBAB/SnO ₂	7.88	246680	1.04E-8	0.98	279920	4.84E-8	0.86
TBAI/SnO ₂	7.46	140240	7.83E-9	1.03	145430	4.72E-8	0.85

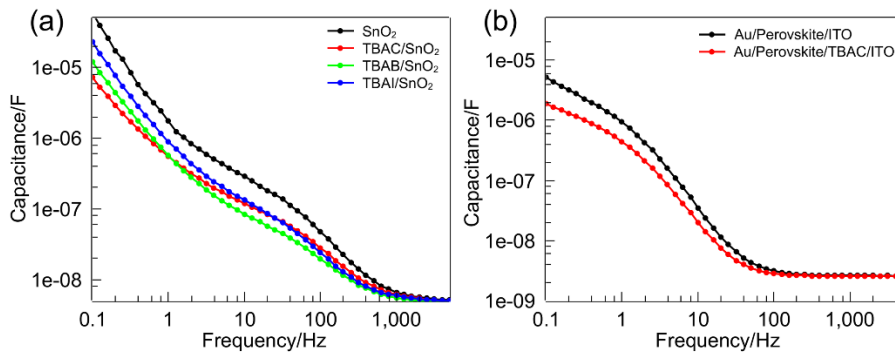


图 S7 (a)无钝化层和加入不同钝化层后钙钛矿太阳能电池器件在无偏压下的 $C-f$ 图; (b)无钝化层和加入 TBAC 钝化层后无电荷传输层器件在无偏压下的 $C-f$ 图

Fig. S7 (a) $C-f$ curves of PSCs with no bias without and with different passivation layers; (b) $C-f$ curves of Au/Perovskite/ITO devices with no bias without and with TBAC passivation layers.

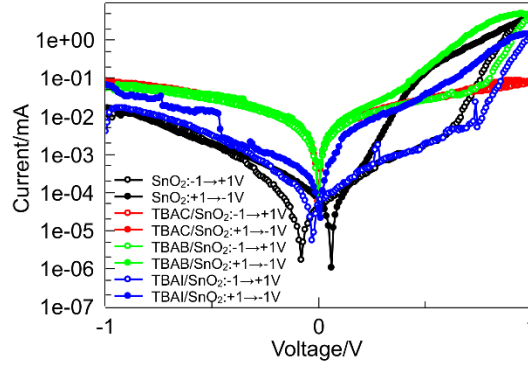


图 S8 无钝化层和加入不同钝化层后无电荷传输层器件在暗场下的对数电流-电压图

Fig. S8 The logarithmic I - V curves of Au/Perovskite/ITO devices without and with different passivation layers.

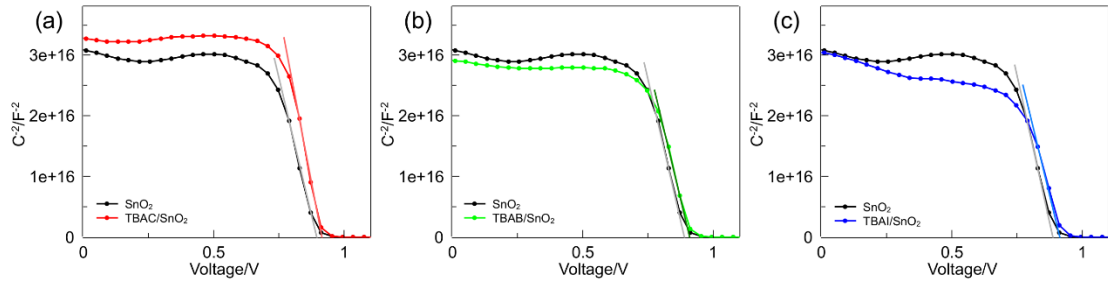


图 S9 无钝化层和加入不同钝化层后钙钛矿太阳能电池器件的 C^2 - V 图

Fig. S9 C^2 - V curves of PSCs without and with different passivation layers.

表 S3 无钝化层和加入不同钝化层钙钛矿太阳能电池器件 C^2 - V 图的平带电位(V_{bi})、斜率和掺杂浓度

Table S3 V_{bi} , Slope of the C^2 - V curves and doping densities (N) of ETLs of PSCs without and with different passivation layers.

Sample	V_{bi}/V	Slope/($F^{-2} V^{-1}$)	$N/(\text{cm}^{-3})$
SnO ₂	0.895	18.81×10^{16}	10.00×10^{15}
TBAC/SnO ₂	0.915	19.34×10^{16}	9.73×10^{15}
TBAB/SnO ₂	0.910	18.13×10^{16}	10.38×10^{15}
TBAI/SnO ₂	0.914	17.66×10^{16}	10.65×10^{15}

表 S4 无钝化层和加入不同钝化层后全电子传输层器件的陷阱填充限制电压(V_{TFL})和缺陷密度(n_t)

Table S4 V_{TFL} and n_t of electron-only devices without and with different passivation layers.

Sample	V_{TFL}/V	$n_t/(\text{cm}^{-3})$
SnO ₂	0.975	16.73×10^{15}
TBAC/SnO ₂	0.351	6.02×10^{15}
TBAB/SnO ₂	0.480	8.24×10^{15}
TBAI/SnO ₂	0.577	9.90×10^{15}

表 S5 [PbX₄]团簇与 SnO₂ (110)表面相互作用主要参数

Table S5 Interaction between the [PbX₄] clusters and the SnO₂ (110) surface.

	[PbCl ₄]	[PbBr ₄]	[PbI ₄]
$\Delta E/eV$	-4.68	-4.48	-4.26
$d_{X-Sn}/\text{\AA}$	2.58	2.74	2.97
$d_{Pb-Sn}/\text{\AA}$	3.41	3.49	3.50

表 S6 表面功函数

Table S6 Workfunction of interfaces.

	SnO ₂	SnO ₂ + [PbCl ₄]	SnO ₂ + [PbBr ₄]	SnO ₂ + [PbI ₄]
$E_{\text{fermi}}/\text{eV}$	-0.9585	-1.1746	-1.1744	-1.0856
E_{vac}/eV	3.3498	3.6089	3.6044	3.6583
E_{WF}/eV	4.308	4.783	4.779	4.744