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Interfacial passivation with 4−chlorobenzene sulfonyl chloride for stable and efficient planar perovskite solar cells

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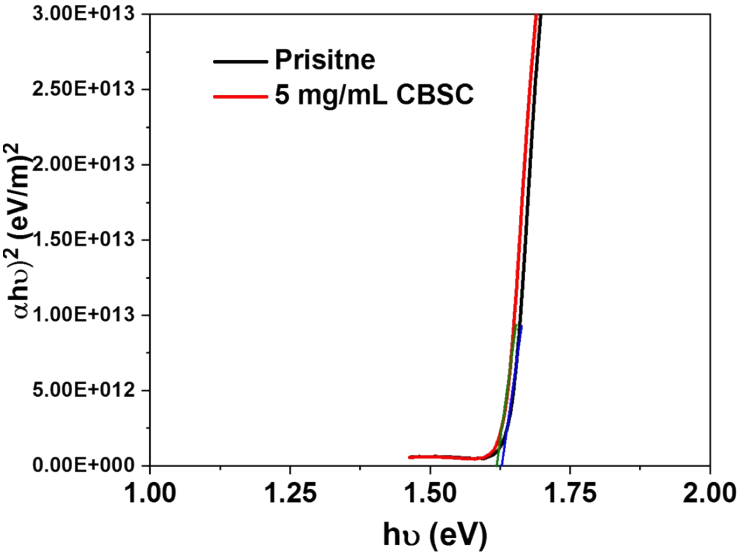

Figure S1. Tauc plots of the pristine and CBSC passivated peroskite films.

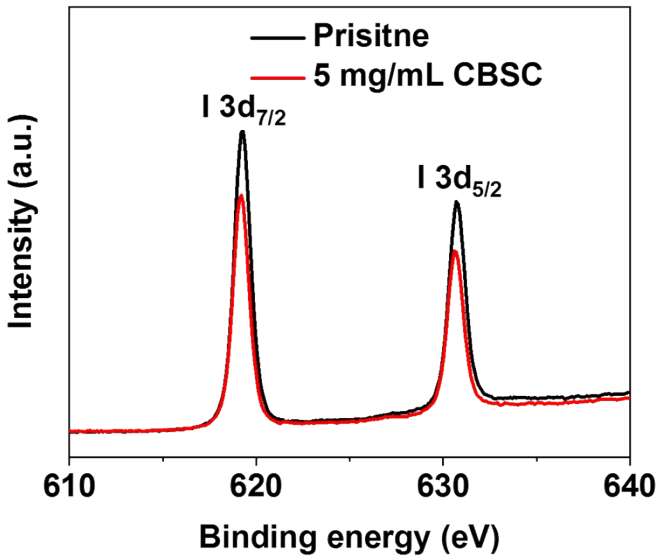

Figure S2. XPS spectra of the pristine and 5 mg/mL CBSC passivated films.

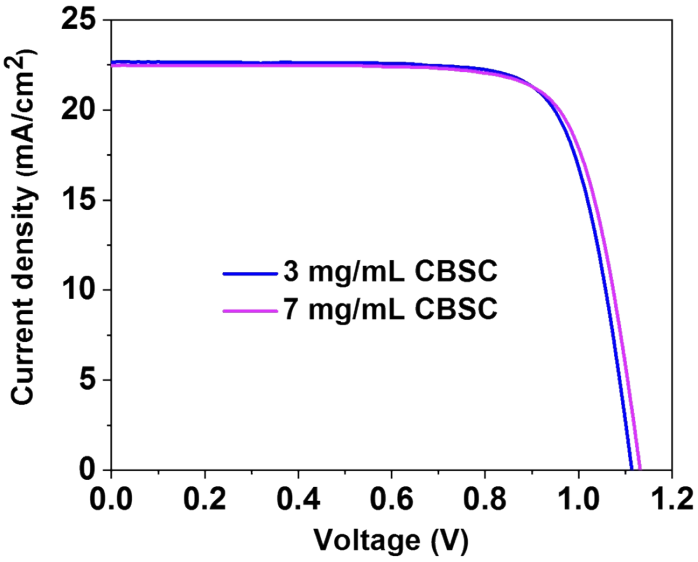

Figure S3. J-V curves of 3 mg/mL and 5 mg/mL CBSC passivated perovskite devices.

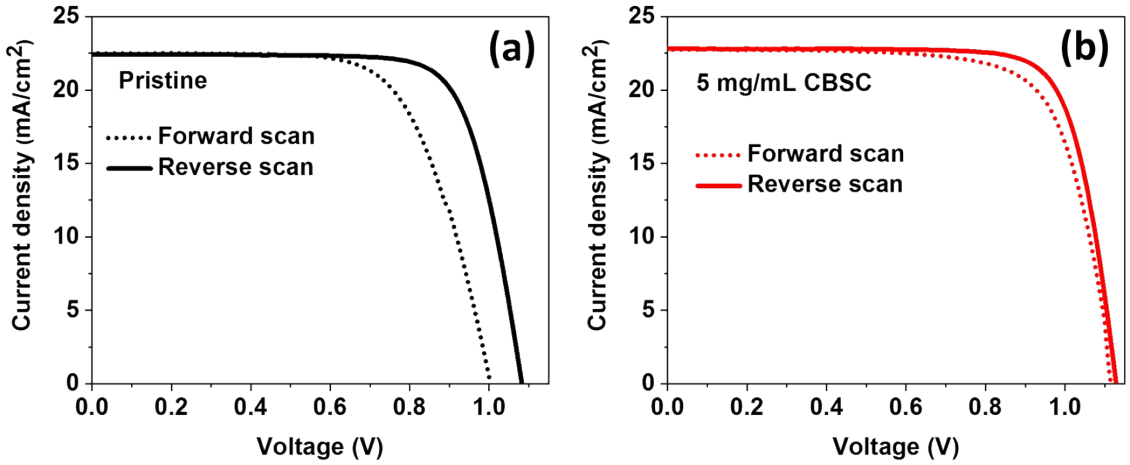

Figure S4. J-V curve of (a) the pristine and (b) the CBSC passivated device under reverse and forward direction.

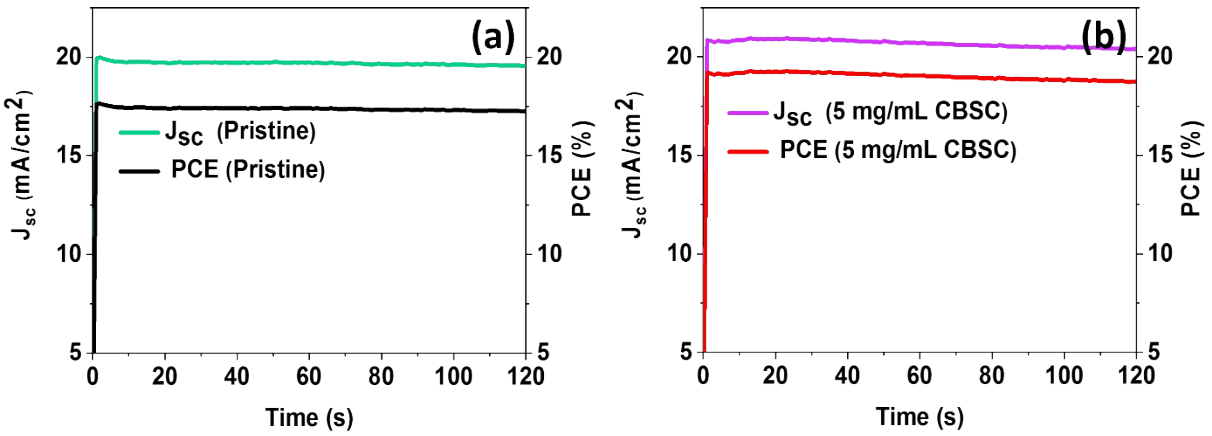

Figure S5. The stabilized PCE at the maximum power point (MPP) of a) the pristine device and (b) the CBSC passivated device.

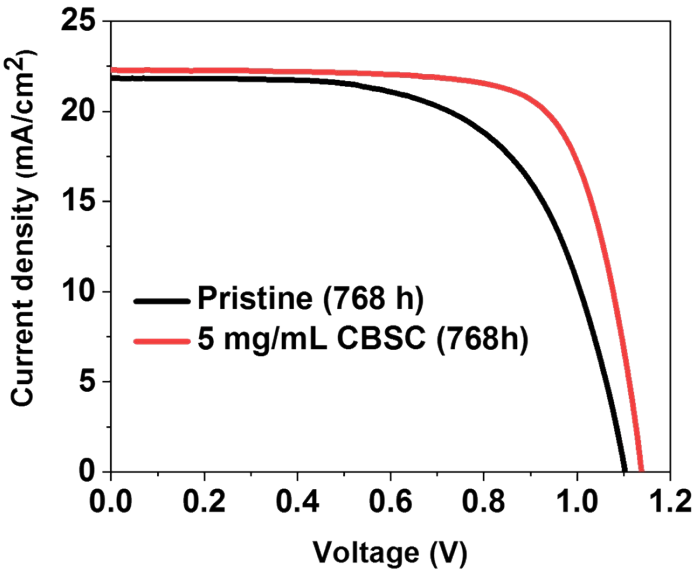

Figure S6. J-V curve of pristine and CBSC passivated devices after storing in a dried box (30% humidity and room temperature) for 768 hours.

Table S1: The fitting results of TRPL decay curves for 0 mg/mL (pristine), 5 mg/mL, and 7 mg/mL CBSC passivated perovskite film.

Samples	**A_1**	**τ_1 (ns)**	**A_2**	**τ_2 (ns)**	**$\tau_{average}$ (ns)**
Perovskite	1.05	20.15	0.53	104.29	48.40
Perovskite /5 mg/mL CBSC	0.80	26.81	0.54	140.02	72.42
Perovskite /7 mg/mL CBSC	0.94	24.49	0.50	131.50	61.73

Table S2. Photovoltaic parameters of champion devices with the pristine and CBSC passivated under reverse and forward scan.

Devices	Scan direction	Voc [V]	Jsc [mA cm^{-2}]	FF [%]	PCE [%]	Hysteresis index (HI)
Pristine	Reverse	1.08	22.43	75.4	18.29	0.17
	Forward	1.00	22.48	67.34	15.18	
5 mg/mL CBSC	Reverse	1.13	22.80	77.79	20.02	0.07
	Forward	1.11	22.74	72.66	18.47	

Table S3. Photovoltaic parameters of perovskite solar cells of pristine and CBSC passivated devices stored under a controlled environment (in dark, 30% RH, and room temperature).

Devices	Aging time	Voc [V]	Jsc [mA cm^{-2}]	FF [%]	PCE [%]
Pristine	0 h	1.08	22.43	75.4	18.29
	768 h	1.10	21.83	62.87	15.09
5 mg/mL CBSC	0 h	1.13	22.80	77.79	20.02
	768 h	1.13	22.28	73.65	18.66

Experimental Section;

Materials: Fluorine−doped tin oxide (FTO) substrates were purchased from Nippon sheet glass Co., Ltd. (Japan). lead (II) iodide (PbI_2, 99.99%) and Lead (II) bromide ($PbBr_2$, 99.99%) and were purchased from Tokyo Chemical Industry (TCI). Methylammonium bromide (MABr, > 99.5%) and Formamidinium iodide (FAI, > 99.5%) were purchased from Dyesol. Tin (II) chloride ($SnCl_2$, 99.99%), absolute ethanol, acetylacetone (≥ 99.8%), titanium (IV) butoxide (97%), 2-methoxyethanol (99.8%), 4−chlorobenzene sulfonyl chloride (97%), chlorobenzene (99.8%), acetonitrile (99.8%), 4−tert−Butylpyridine (TBP, 98%), tris(2-(1H-pyrazol-1-yl)-4-tert-butylpyridine)cobalt(III) tri[bis(trifluoromethane)sulfonimide] (FK209 Co (III) TFSI salt, 98%), **s**piro−OMeTAD, Bis(trifluoromethylsulfonyl)amine lithium salt (99%), dimethyl sulfoxide (DMSO, 99.99%), Cesium iodide (CsI, 99.99%) and Dimethylformamide (DMF, > 99.9%) were purchased from Sigma Aldrich company.

Preparation of TiO_2 compact layer. A compact titanium dioxide (c-TiO_2) layer was deposited on the surface of the cleaned FTO glass substrate using the spin coating technique of the precursor solution (0.767 µL of titanium (IV) butoxide and 0.230 µL of acetylacetone into 7.5 mL of 2-methoxyethanol) at 3000 rpm for 40 s and heated to 500 ºC for an hour.

Preparation of SnO_2 layer: a thin tin−oxide (SnO_2) layer was deposited by spin coating the precursor solution (22.5 mg of tin (II) chloride dissolved in 1 mL of absolute ethanol) at 5000 rpm for 20 s and annealed at 200 ºC for an hour.