Supporting Information

Surface Engineering Based on Ionic Liquids for Efficient and Stable $CsPbI_3$ Perovskite Solar Cells

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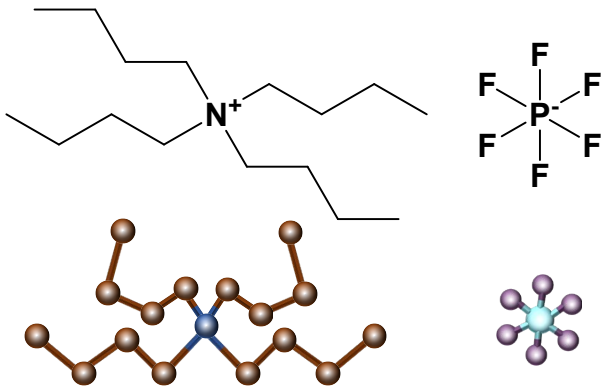

Fig. S1. Chemical structures and corresponding structural diagrams of $TBAPF_6$.

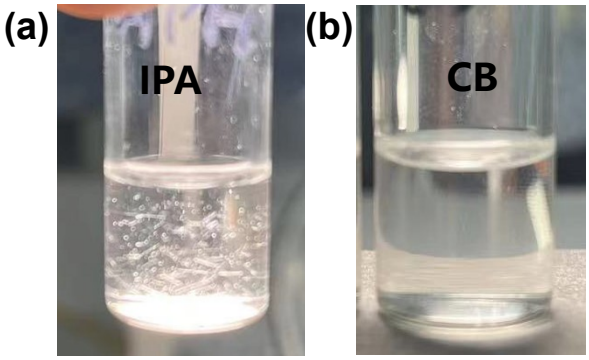

Fig. S2. The solubility of $TBAPF_6$ in (a) isopropanol and (b) chlorobenzene.

According to previous reports, isopropyl alcohol (IPA) and chlorobenzene (CB) were common solvents for Surface treatment of as-deposited $CsPbI_3$ films and were used in this work.[1-3] The same amount of $TBAPF_6$ was added in equal volume of IPA or CB. After stirring, $TBAPF_6$ couldn't dissolve in IPA and there was a large amount of precipitation at room temperature. With heating, $TBAPF_6$ gradually dissolved in IPA and a colorless and transparent solution would be observed. However, crystal particles would precipitate rapidly after cooling down (Fig. S2a). In contrast, $TBAPF_6$ could well dissolve in CB to form a colorless and transparent solution at room temperature (Fig. S2b).

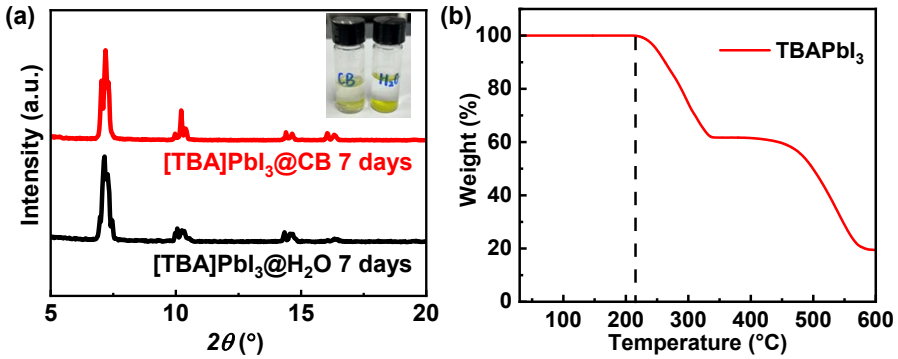

Fig. S3. (a) X-ray diffraction patterns of the $[TBA]PbI_3$ single crystal immersed in deionized water or CB for 7 days. (b) TGA curve of the low-dimensional material

[TBA]PbI_3.

On one hand, under the consideration of moisture stability of synthetic [TBA]PbI_3 single crystals, [TBA]PbI_3 was immersed in deionized water at room temperature for 7 days. On the other hand, the using of hole transport material (HTM) in this work is Spiro-OMeTAD and CB is the common solvent for Spiro-OMeTAD.[4-6] Therefore, the spinning coating of hole transport layer (HTL) could cause damage to perovskite layer, and the similar experiment was conducted by soaking [TBA]PbI_3 into CB. Herein, we used XRD to estimate the degradation of [TBA]PbI_3 single crystals (Fig. S3a).

[TBA]PbI_3 single crystals exhibited excellent thermal stability by thermogravimetric analysis (TGA) measurement. The weight loss of synthetic [TBA]PbI_3 single crystals was only 1 wt% when temperature increased up to 220 °C, and the apparent weight losses happened at temperature ranges from 220 °C to 400 °C and from 400 °C to 600 °C, corresponding to volatilization of TBAI and sublimation of PbI_2, respectively.[7]

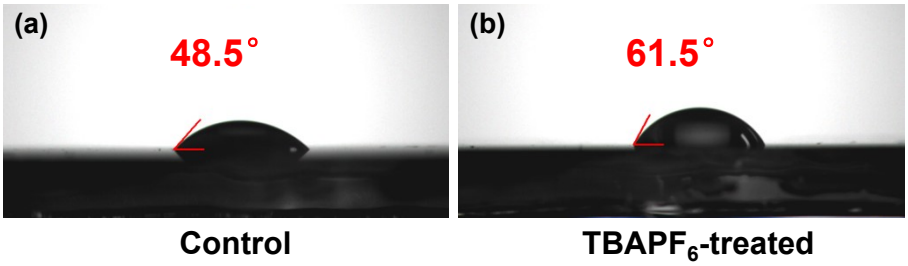

Fig. S4. Water contact angle measurements on the surface of (a) control and (b) $TBAPF_6$-treated films.

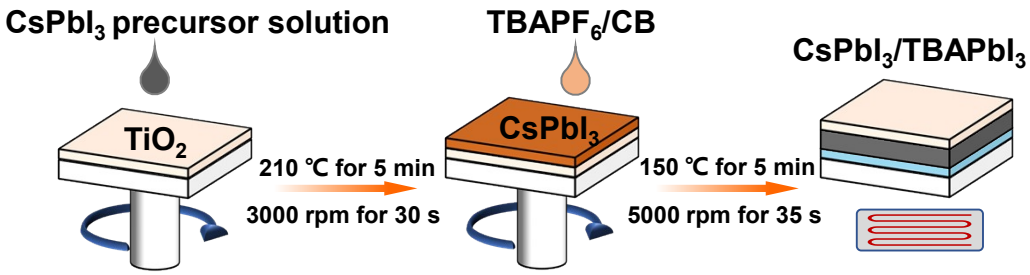

Fig. S5. Schematic diagram of the preparation of $CsPbI_3$ films with surface treatment of $TBAPF_6$.

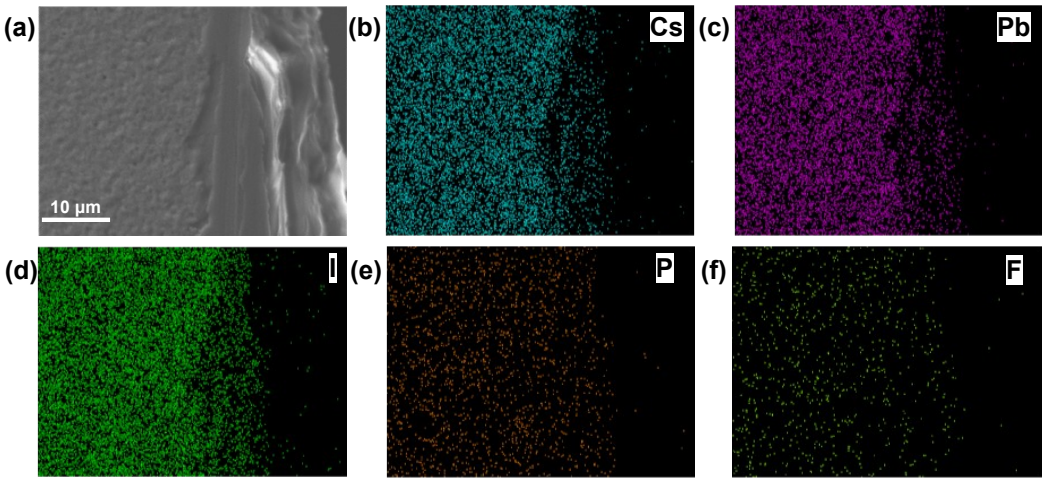

Fig. S6. (a) SEM image of $TBAPF_6$-treated film, (b-f) Elemental analysis spectra of Cs, Pb, I, P, and F.

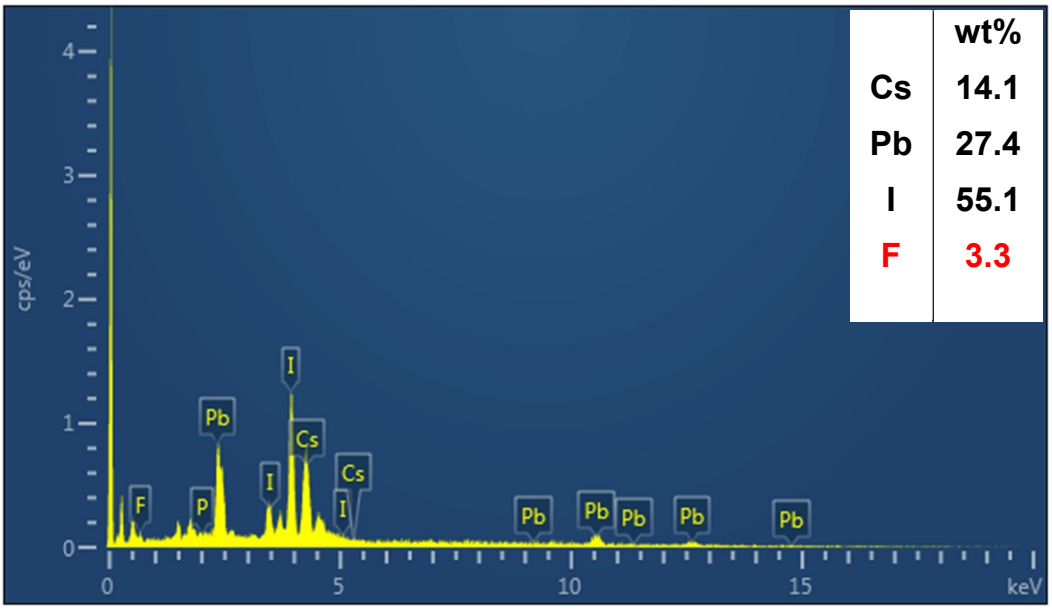

Fig. S7. Relative content analysis results of different elements on the surface of the $TBAPF_6$-treated film.

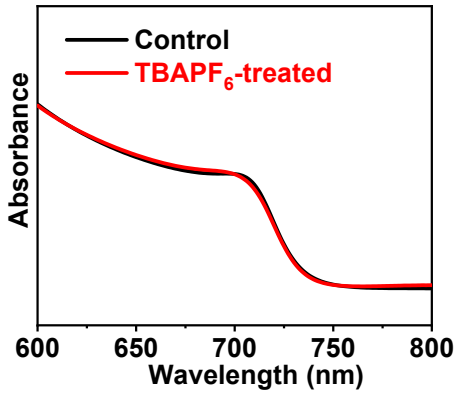

Fig. S8. UV–vis absorption spectra of the control and $TBAPF_6$-treated films.

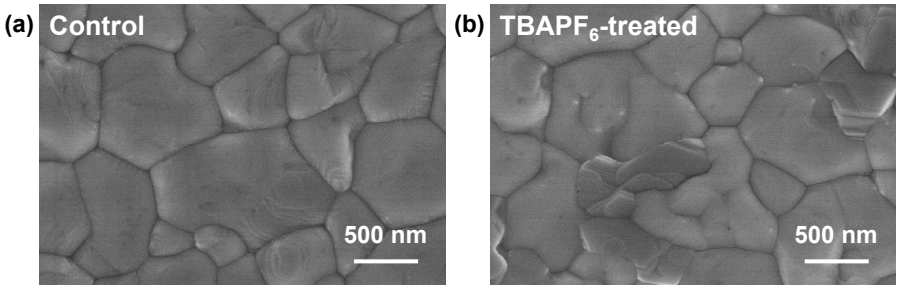

Fig. S9. SEM images of (a) control and (b) $TBAPF_6$-treated films.

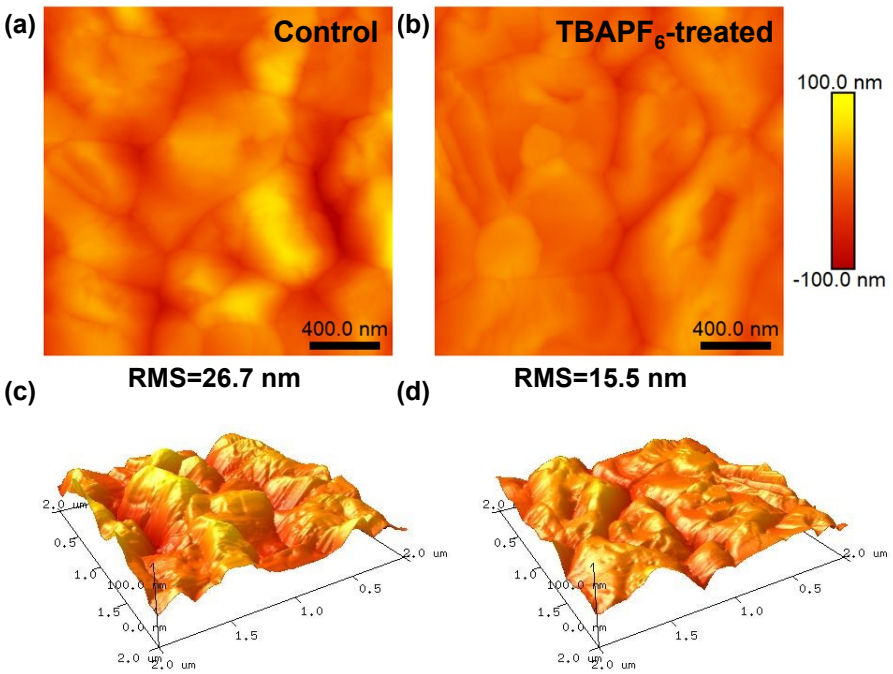

Fig. S10. AFM images of (a), (c) control and (b), (d) $TBAPF_6$-treated films.

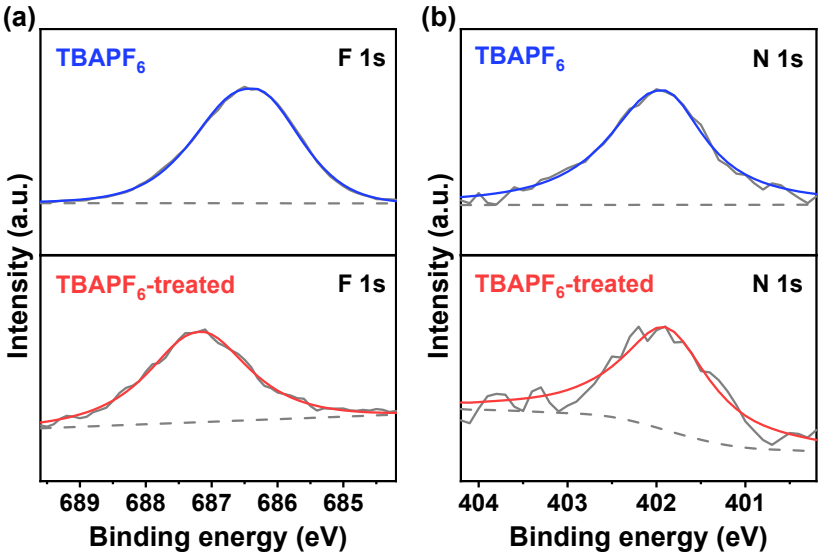

Fig. S11. XPS spectra of $TBAPF_6$ sample and $TBAPF_6$-treated films. (a) F 1s, (b) N 1s.

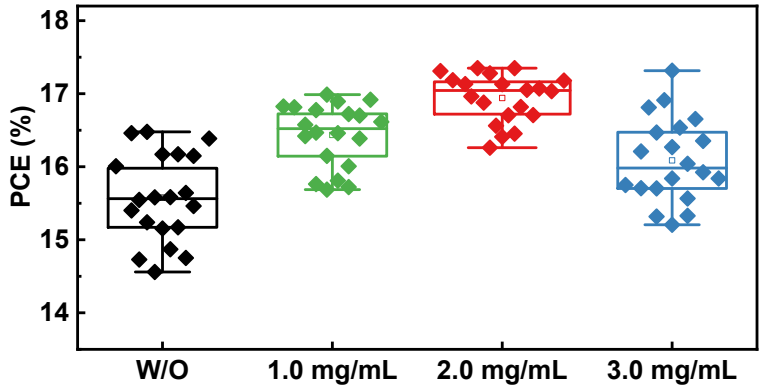

Fig. S12. PCEs statistics of C-PSCs treated with different concentrations of $TBAPF_6$.

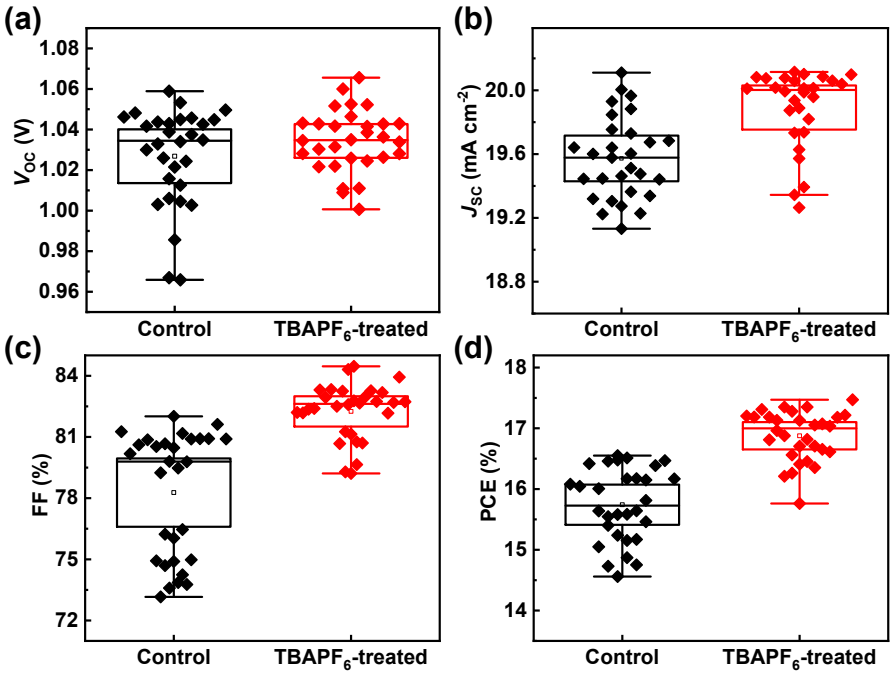

Fig. S13. Histograms of the (a) V_{OC}, (b) J_{SC}, (c) FF, and (d) PCE values based on the control and $TBAPF_6$-treated devices.

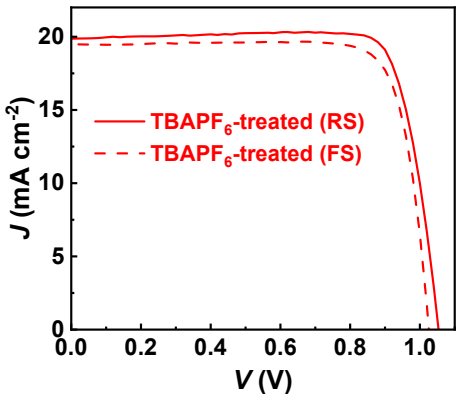

Fig. S14. Reverse scan (RS) and forward scan (FS) of $TBAPF_6$-treated devices.

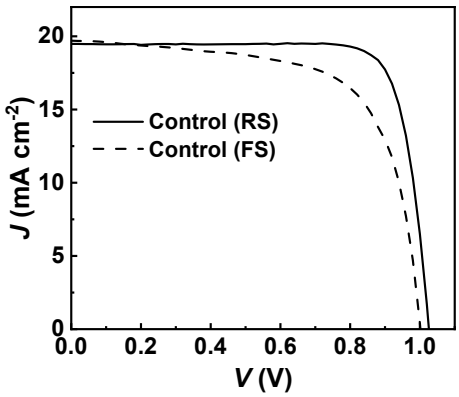

Fig. S15. Reverse scan and forward scan of control devices.

Table S1. Fitted parameters from TRPL spectra for the control and $TBAPF_6$-treated films.

	τ_1 (ns)	τ_2 (ns)	f_1 (%)	f_2 (%)	τ_{ave} (ns)
Control	2.4	28.2	12.1	87.9	27.9
$TBAPF_6$-treated	2.0	37.5	6.7	93.3	37.3

Table S2. Photovoltaic parameters of the control and $TBAPF_6$-treated devices.

	V_{OC} (V)	J_{SC} (mA cm)$^{-2}$	FF (%)	PCE_{best} (PCE_{avg}) (%)
Control	1.03	19.93	80.9	16.55 (15.69 ± 0.86)
$TBAPF_6$-treated	1.06	20.01	82.2	17.47 (16.72 ± 0.75)

Table S3. Photovoltaic parameters of the control and $TBAPF_6$-treated devices in the reverse scan and forward scan directions.

		V_{OC} (V)	J_{SC} (mA cm)$^{-2}$	FF (%)	PCE (%)	h[a]
Control	RS	1.03	19.48	80.9	16.17	18.6%
	FS	1.00	19.70	66.8	13.17	
$TBAPF_6$-treated	RS	1.05	19.87	83.2	17.41	8.5%
	FS	1.03	19.59	79.2	15.94	

[a] $h = (PCE_{RS} - PCE_{FS}) / PCE_{RS}$, where RS and FS represent the reverse and forward scan directions, respectively.

References

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