Supporting information

Boosting Charge Transfer with MoS_2-Grafted MXene Interlayer for High-Efficiency All-Inorganic $CsPbBr_3$ Perovskite Solar Cells with an Ultrahigh Voltage of 1.701V

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Characterizations

The morphologies were obtained by a field emission SEM (Hitachi S4800) and TEM (Tecnai G2 F20). The X-ray photo electron spectroscopy (XPS) spectra were characterized using a multifunctional imaging electron spectrometer (Thermo ESCALAB 250XI) with an Al Kα x-ray source. The element analysis was carried out using SEM (FEI QUANTA250 and Zeiss Gemini300). The AFM image was obtained by AFM (Seiko SPA400). The surface potential was characterized by KPFM (Multimode 8, Bruker, German). PL spectra were recorded via a fluorescence spectrometer excited by a 350 nm laser and the TRPL spectra were characterized using a Horiba spectrometer with an excitation wavelength of 500 nm. The characteristic *J-V* curves of PSCs were recorded on an electrochemical workstation (CHI660E) under irradiation of simulated solar light (Newport, Oriel Class 3A, 91195A). The light intensity was controlled at 100 mW cm^{-2} calibrated by a standard silicon solar cell. The IPCE spectra of various devices were obtained using an IPCE kit from Enli Technology Co., Ltd. The V_{oc} decay curves were measured at open-circuit mode by illuminating the device for several seconds, and then instantaneously switching off the light. Tafel curves and Mott–Schottky curves of various devices were measured on CHI660E electrochemical workstation.

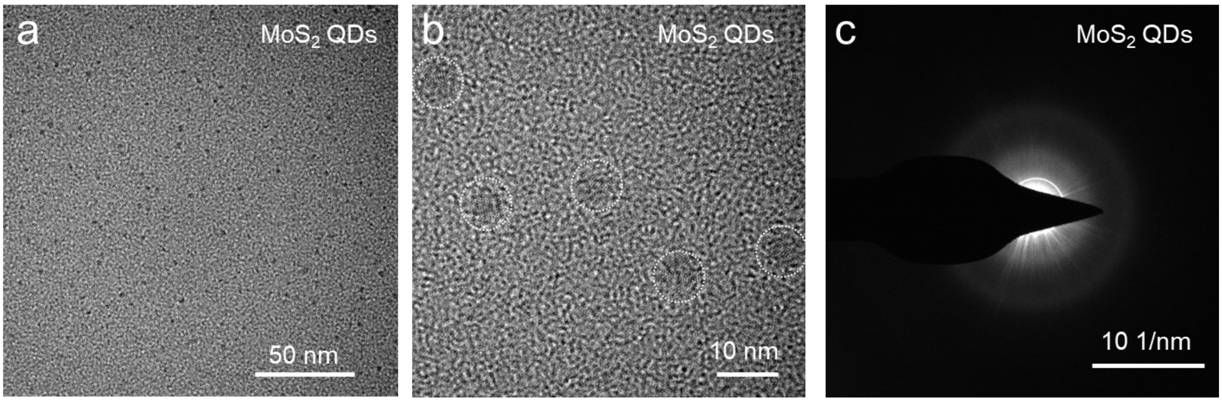

Fig. S1. (a,b)TEM images and (c) SAED patterns of MoS_2 QDs.

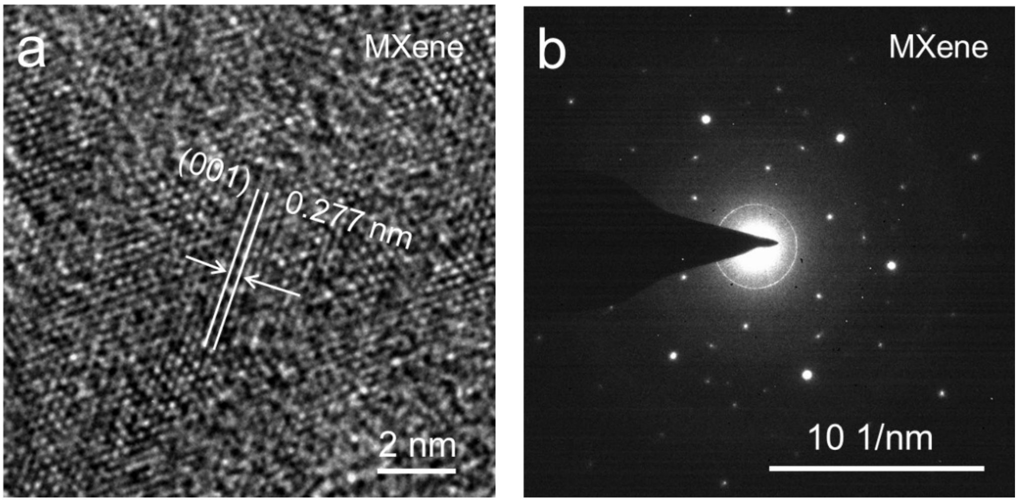

Fig. S2. (a) HRTEM image and (b) SAED patterns of MXene nanoflakes

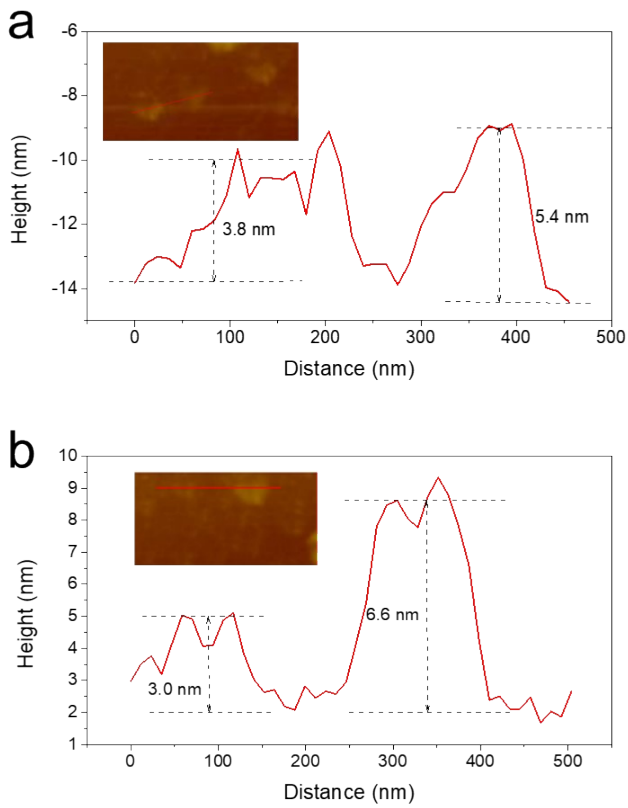

Fig. S3. Height profile of (a) MXene nanoflakes and (b) MoS_2@MXene nanoflakes, insert is the corresponding AFM image.

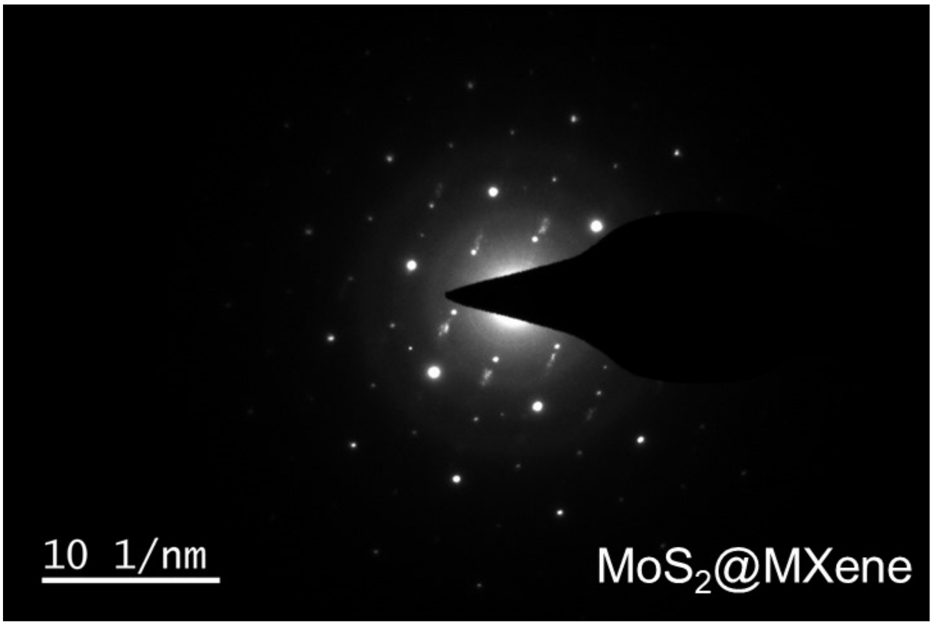

Fig. S4. SAED patterns of MoS_2@MXene nanoflakes.

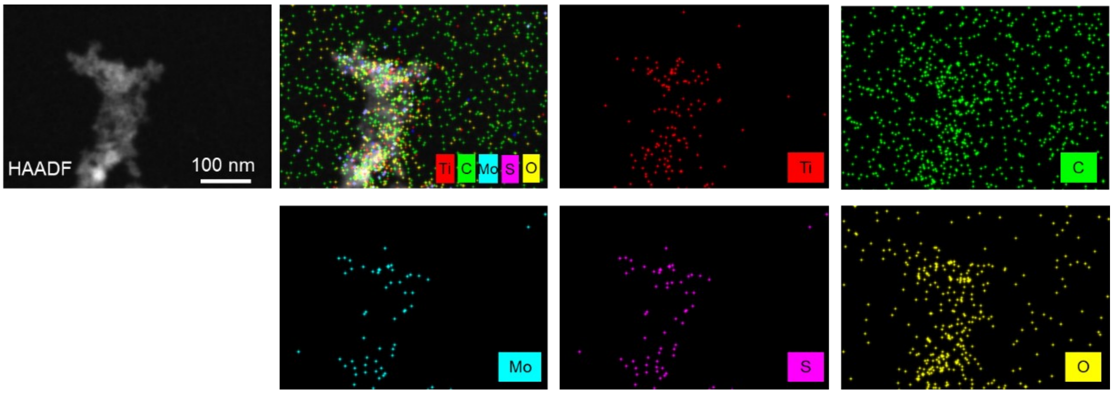

Fig. S5. HAADF image and the corresponding EDS mapping of MoS_2@MXene nanoflakes.

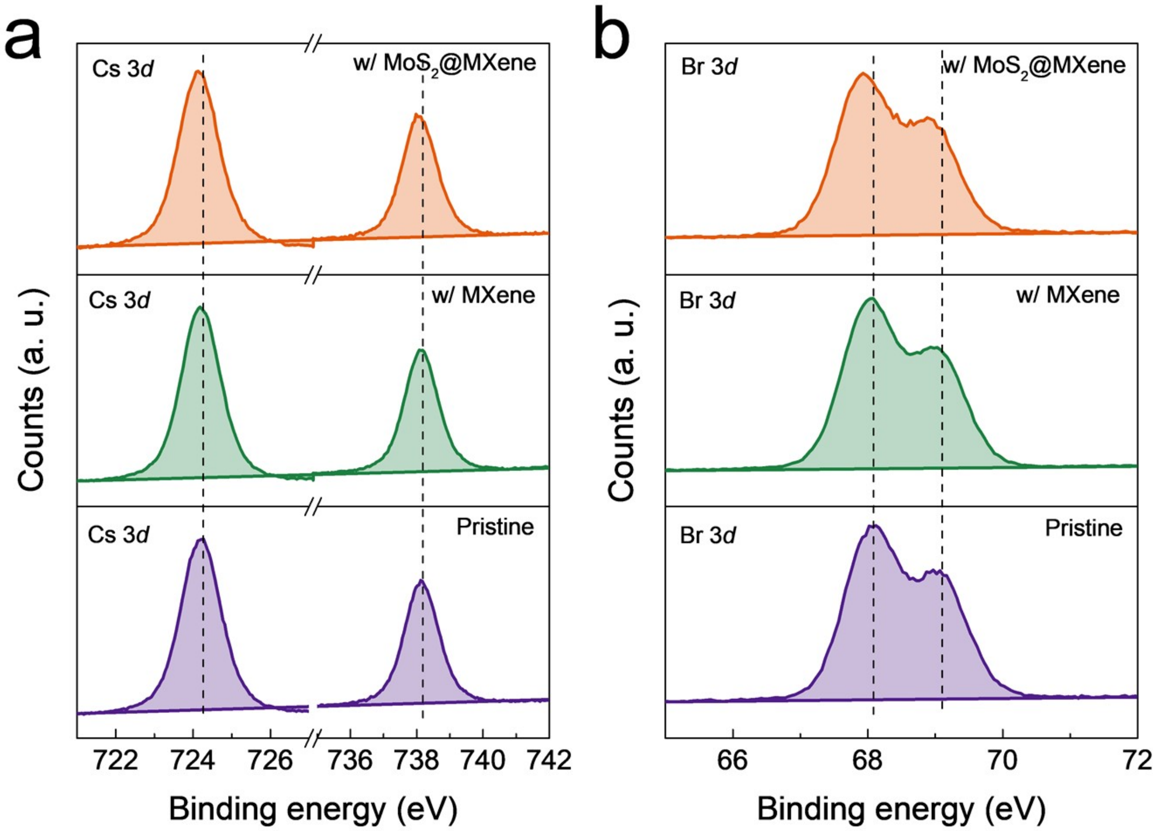

Fig. S6. XPS spectra of (a) Cs 3*d* and (b) Br 3*d* for $CsPbBr_3$ films with different modifications.

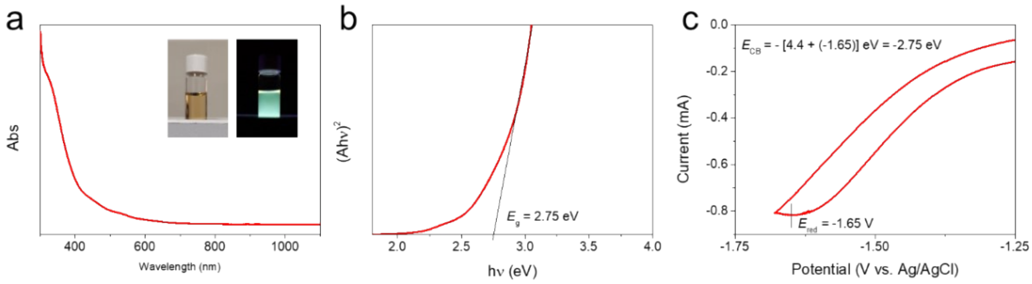

Fig. S7. (a, b) UV-Vis absorption spectra and (c) CV curves of (a) MoS_2 QDs. The inset image is the photographs of the MoS_2 QDs before and after illumination (365 nm).

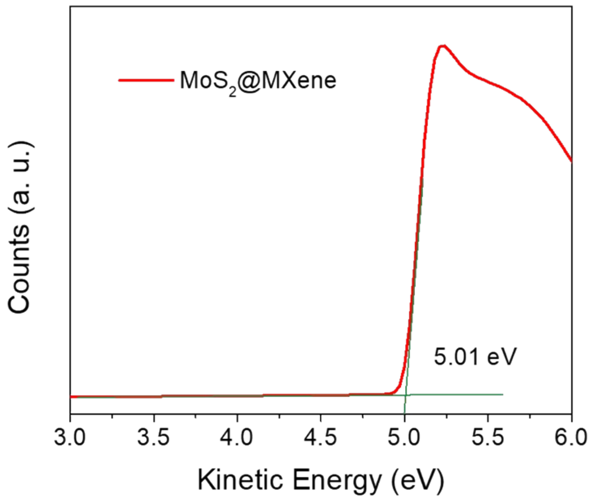

Fig. S8. Ultraviolet photoelectron spectrum of MoS_2@MXene with a work function of -5.01 eV.

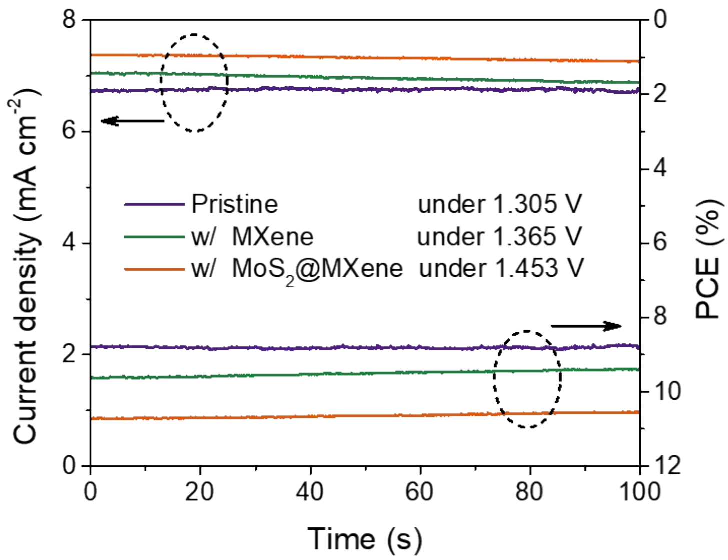

Fig. S9. Steady-state power output of the PSCs.

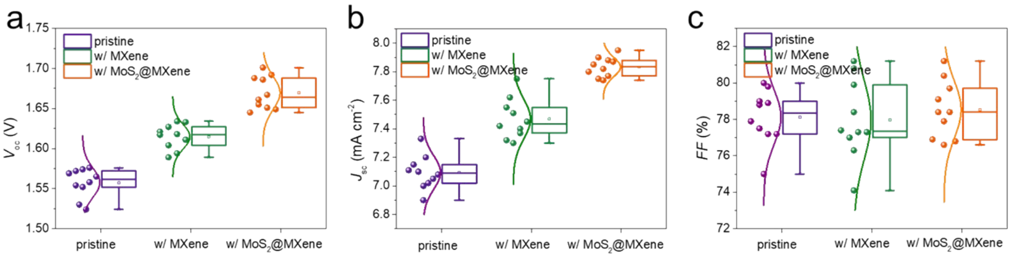

Fig. S10. Statistical distributions of V_{oc}, J_{sc} and FF for PSCs with different modifications.

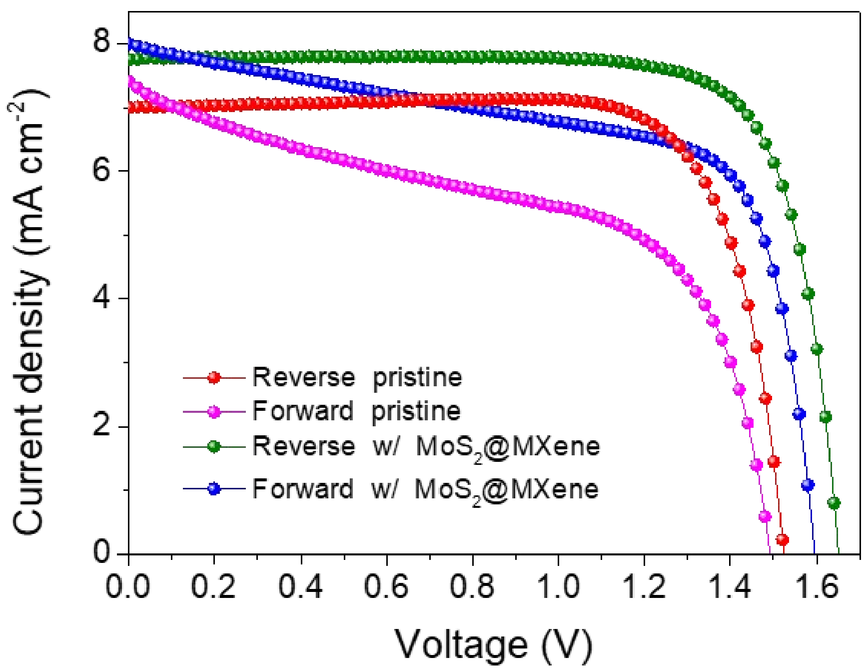

Fig. S11. *J-V* curves for the $CsPbBr_3$ PSCs with and without MoS_2@MXene under reverse and forward scans.

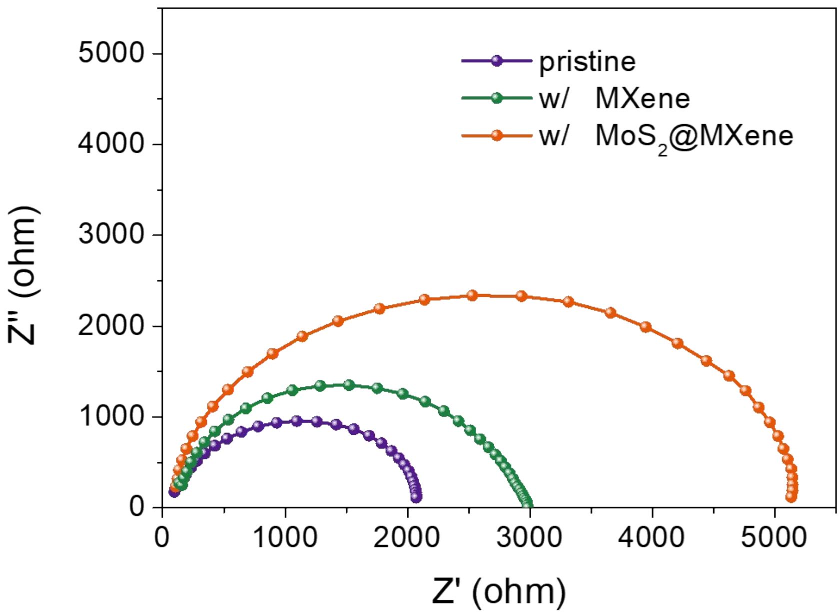

Fig. S12. EIS plots of various $CsPbBr_3$ PSCs.

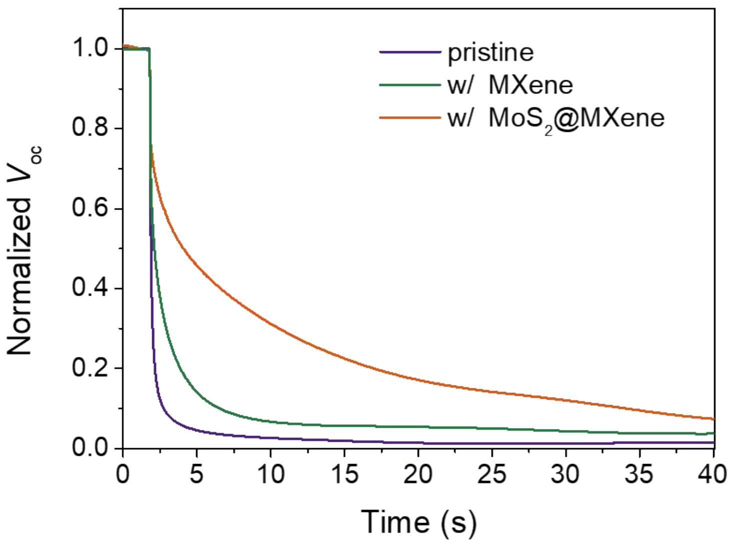

Fig. S13. V_{oc} decay curves of various $CsPbBr_3$ PSCs.

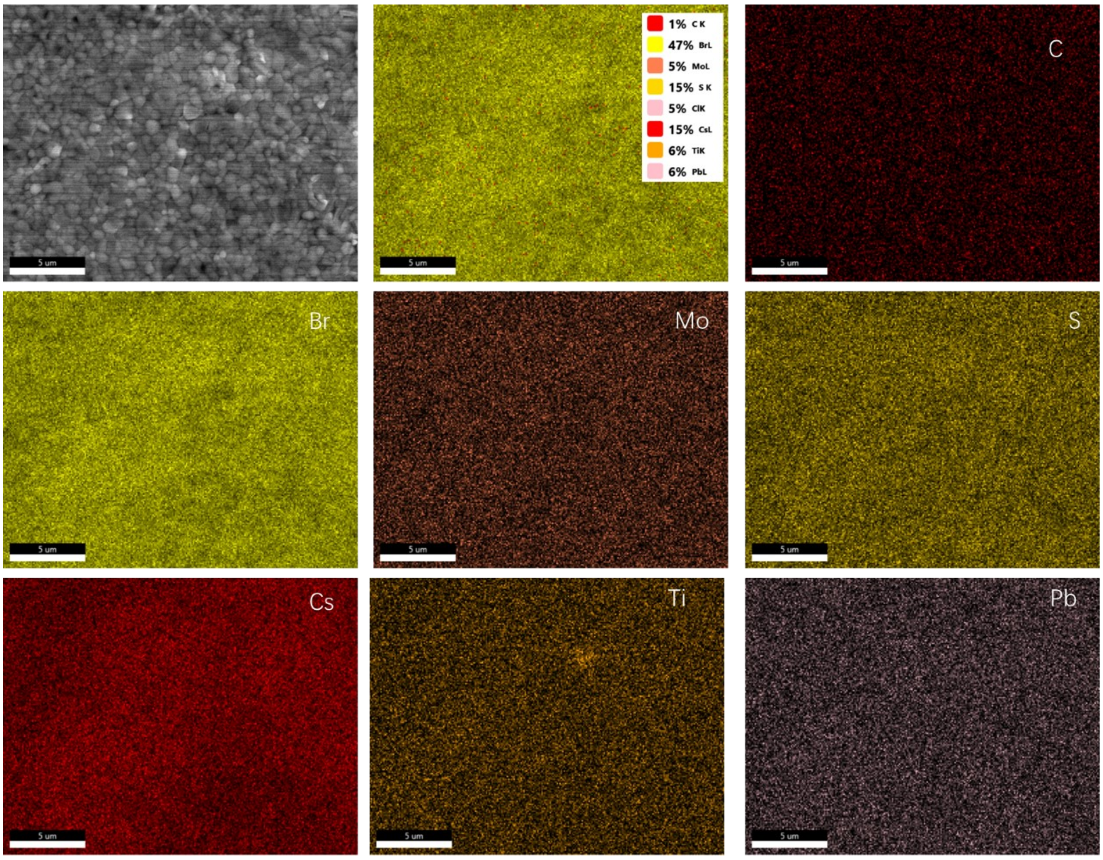

Fig. S14. SEM image and the corresponding EDS mapping images of $CsPbBr_3$ perovskite film with MoS_2@MXene modification.

Table S1. Photovoltaic parameters for PSCs under reverse and forward scans.

Devices	V_{oc} (V)	J_{sc} (mA/cm^2)	PCE (%)	FF (%)
Reverse pristine	1.524	7.00	8.24	77.2
Forward pristine	1.492	7.41	5.91	53.5
Reverse w/ MoS_2@MXene	1.651	7.75	10.03	78.4
Forward w/ MoS_2@MXene	1.595	8.00	8.39	65.8

Table S2. TRPL decay parameters of PSCs with and without modifications.

Device	τ_1 (ns)	a_1	τ_2 (ns)	a_2	τ_{ave} (ns)
Pristine	0.574	66.78%	10.446	33.22%	0.836
w/ MXene	0.527	69.76%	23.664	30.24%	0.749
w/ MoS_2@MXene	0.486	80.61%	8.369	19.39%	0.594

The TRPL decay curves in Figure 3h can be fitted by employing a biexponential function as follows:

$$I = Ae^{-(t-t_0)/\tau_1} + Be^{-(t-t_0)/\tau_2}$$

Here, τ_1 corresponds to the faster component associated with trap-mediated nonradiative recombination, while τ_2 is related to the slower component linked to radiative recombination. To assess the electron extraction ability, the average decay time (τ_{ave}) is calculated based on the formula $\tau_{ave} = (a_1\tau_1^2 + a_2\tau_2^2)/(a_1\tau_1 + a_2\tau_2)$, where a_1 and a_2 denote the amplitudes. The specific parameters of τ_1, τ_2, and τ_{ave} are listed in Table S2.