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Building UV filter and interfacial bridge with multifunctional molecule for enhancing the performance and stability of $MAPbI_3$ solar cells

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Supplementary note 1

Materials: Indium Tin Oxides (ITO) glass substrates, lead iodide (PbI_2), Methylammonium iodide (CH_3NH_3I, MAI), 4-tert-butypyridine and lithium bis (trifluoromethanesulfonyl) imide (Li-TFSI), SnO_2 aqueous colloidal dispersion (15wt%, ALFA), 2,2′,7,7′-tetrakis (N,N-dip-methoxyphenylamine) 9,9′-Spirobifluorene (Spiro-OMeTAD) and all anhydrous solvents were purchased from YOUXUAN Technology Co. Ltd. (China). 2-hydroxy-4-methoxybenzophenone-5-sulfonic acid (BP-4) was purchased by Beijing InnoChem Science & Technology Co., Ltd. All chemicals and reagents were used as received from chemical companies without any further purification.

Supplementary note 2

Fabrication of perovskite solar cells: SnO_2 was used as ETL, which was coated on the ITO glass sheet by spin-coating. The deposited ITO glass is transferred to a nitrogen-filled glove box (H_2O and O_2 <1 ppm). 0-0.3 mg ml^{-1} of BP-4 dissolving in Dimethyl formamide (DMF) were spin-coated on ETL at 4000 rpm for 30 s. 462 mg of PbI_2 and 163 mg of MAI were dissolved in a mixed solvent of Dimethyl sulfoxide (DMSO) and DMF (v: v = 3:7). The 90 μL of the the $MAPbI_3$ precursor solution was deposited on the ITO/SnO_2 layer by a spin coating process, i.e., 500 rpm for 10 s and 4500 rpm for 30 s. During the second step, 400 μL of CB was poured on the spinning substrate 15 s prior to the end of the program. Subsequently, the obtained films were dried at 60 ^oC for 5 min and at 100 ^oC for 10 min. The 75 μL of the mixture hole transport layer solution prepared by mixing 72.3 mg of Spiro-OMeTAD, 18.5 μL with a

solution of 500 mg/mL Li-TFSI in acetonitrile and 28.5 μL of 4-tertbutylpyridine in 1 mL of CB was spin-coated on the prepared $MAPbI_3$ films at 3000 rmp for 30 s. Finally, 100 nm Ag was thermally deposited under vacuum condition.

Supplementary note 3

Characterization: The scanning electron microscope (SEM) images was taken using a Hitachi S-4800. AFM was measured by Park NX20, Korea. The optical properties of the films were analyzed using a UV-Vis-near-infrared (NIR) spectrophotometer (Shimadzu, UV-3600Plus, Japan). Fourier transform infrared spectroscopy (FTIR) was measured by Nicolet iS10, America. Electron-only devices (ITO/SnO_2/perovskites/PCBM/Ag) was fabricated to calculate trap state density of the devices. The defect density was determined by the equation for the trap-filled limit voltage. The crystal structure of the control and UV-F/perovskite films was carried out by X-ray diffraction (XRD) (PANalytical X-ray Spectrometer Empyrean DY01660 ID206161). PL spectra were obtained using a PL microscopic spectrometer (FLS1000, China) with a 385 nm CW laser excitation source. The TRPL (FLS1000, China) was measured by using an excitation wavelength of 385nm. The main corresponding setup consisted of perovskite, and mica-flakes. The transient photovoltage spectrum (TPV) was measured by CEL-TPV2000 (CEAULIGHT, China). X-ray photoelectron spectroscopy (XPS) was used to obtain the chemical states information (measured by Escalab250Xi, Germany). *J-V* characterizations was carried out under AM 1.5 G simulated sunlight illuminations (100 mW cm^{-2}, Model 94043A, Oriel, American). Electrical impedance spectroscopy (EIS) was performed by using the electrochemical workstation (CHI660C, Chen Hua, China) with a frequency range from 1 Hz to 0.1MHz in the dark. The spectral responses were obtained from

an EQE measurement system (Newport PV measurement, American).

Supplementary note 4

Theoretical calculation: In this paper, the theoretical calculations were performed by density function (DFT) methods. The calculations of electrostatic potential (ESP) and the dipole moment were conducted on the Gaussian 09 program by using B3PW91 and the all-electron double-ξ valence basis sets of 6-31G*.

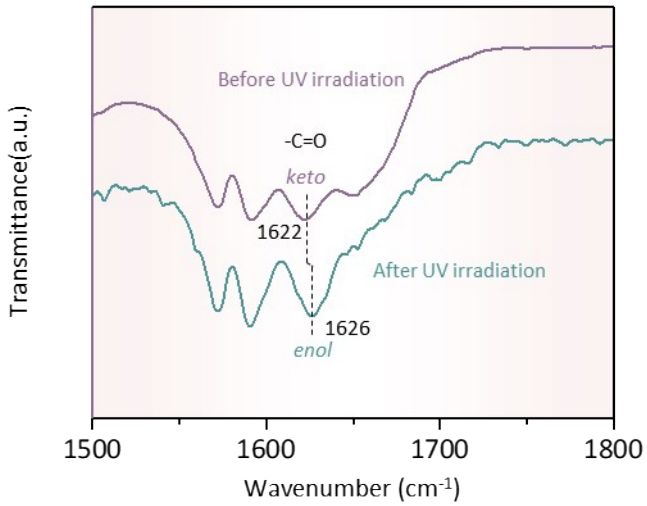

Figure S1 FTIR spectra of the –C=O group of the pure BP-4 sample (before and after UV irradiation).

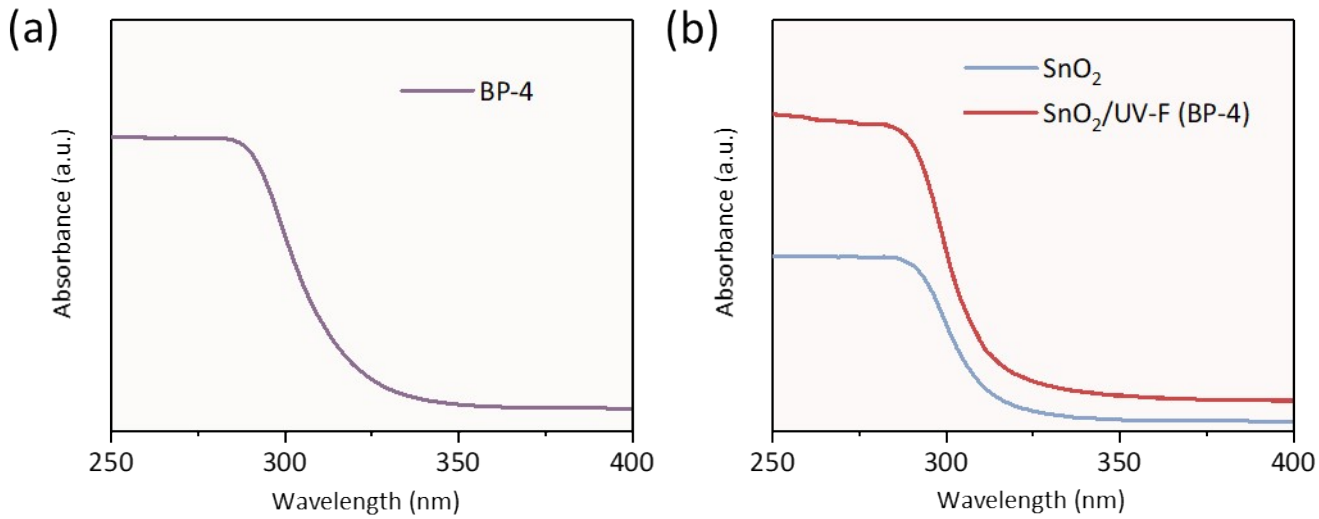

Figure S2 (a) UV–vis absorption spectra of the BP-4 film. (b) UV–vis absorption spectra of the SnO_2 and the SnO_2/UV-F film, respectively.

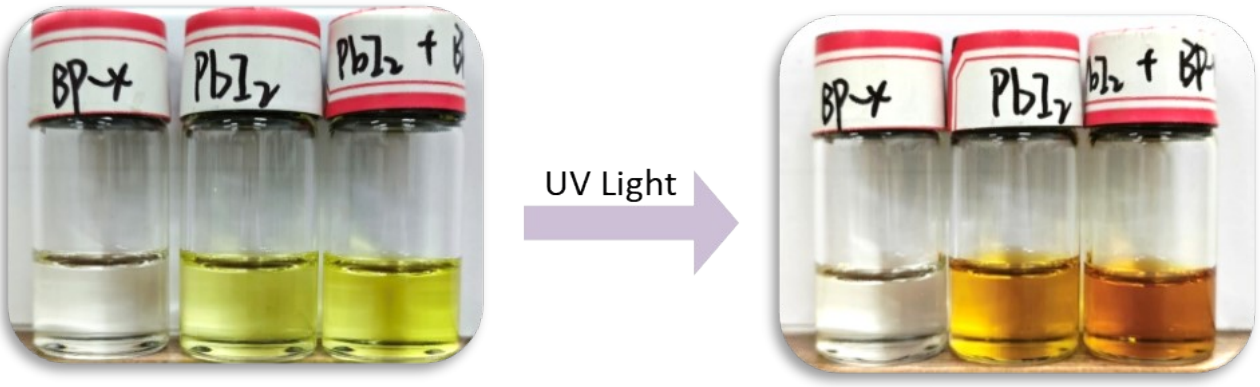

Figure S3 The color charge comparison of the PbI_2, BP-4, and PbI_2+BP-4 solutions during the UV irradiation.

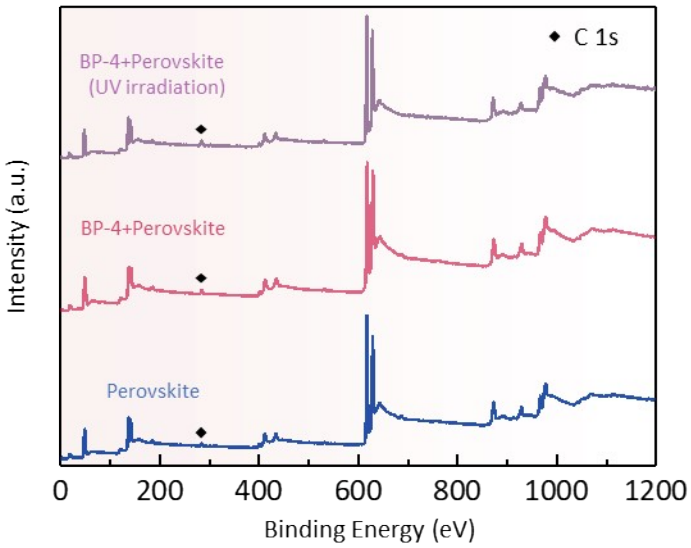

Figure S4 Full XPS data of the perovskite film, the BP-4+perovskite film, and the BP-4+perovskite film after UV irradiation, respectively.

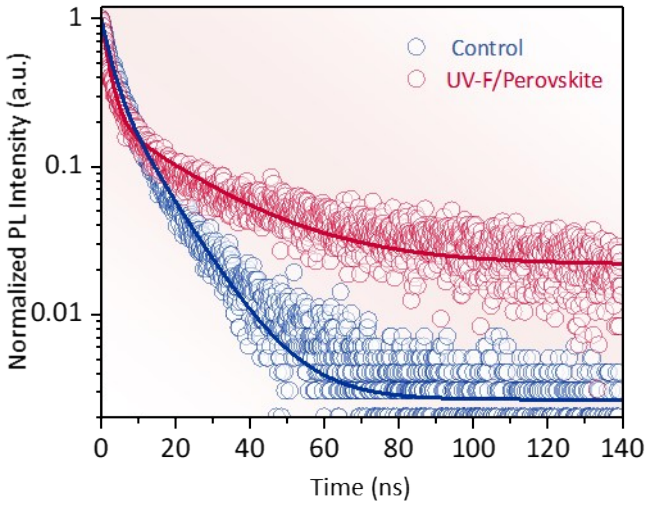

Figure S5 TRPL of the control and the UV-F/perovskite device with a structure of glass/perovskite structure.

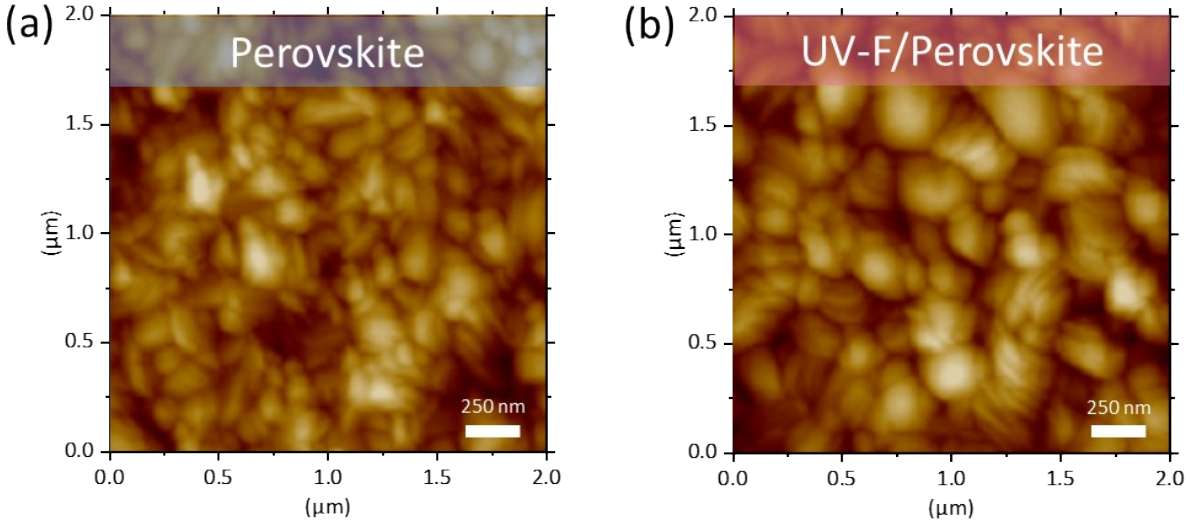

Figure S6 AFM images of (a) the control perovskite and (b) the UV-F/perovskite films.

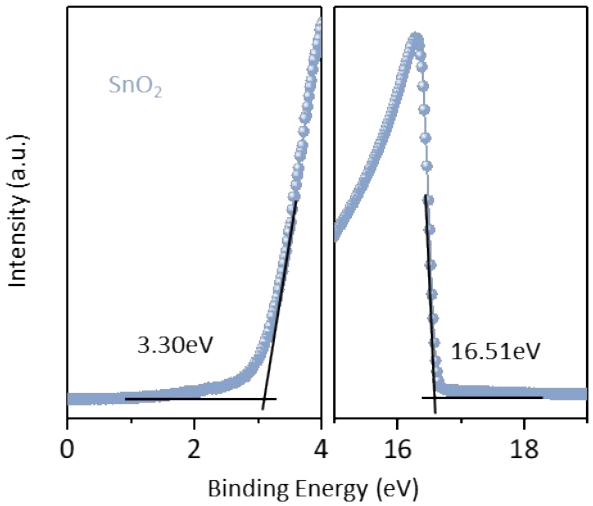

Figure S7 UPS spectra of cut-off energy region and valence band edge of SnO_2 film.

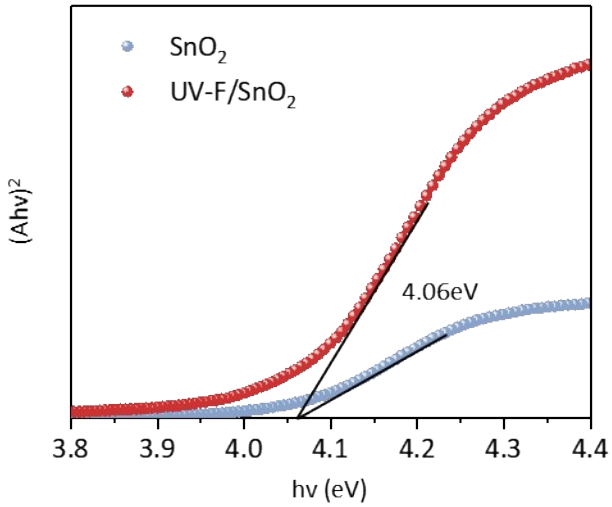

Figure S8 Optical band gaps of SnO_2 and UV-F/SnO_2 films.

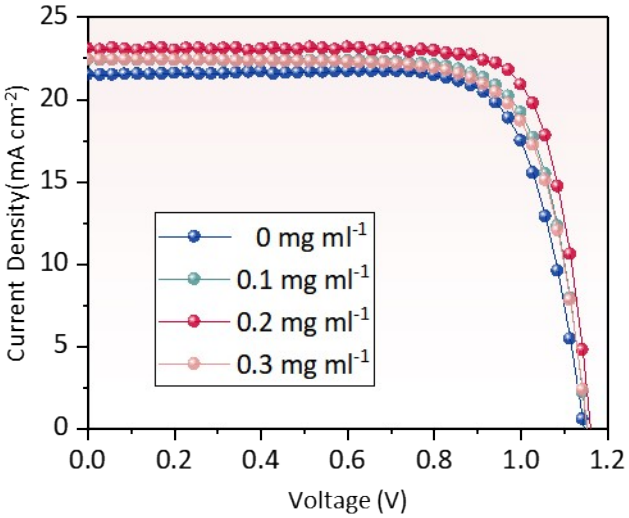

Figure S9 *J-V* curves for devices with different concentrations of BP-4.

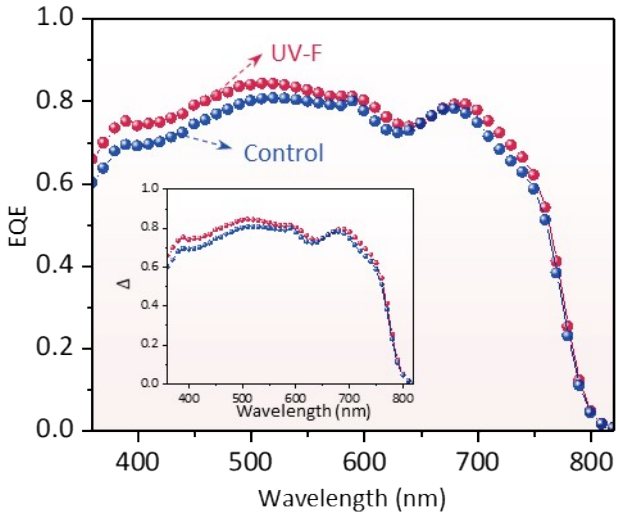

Figure S10 The EQE spectra of the control and the UV-F based device, respectively. The inset shows the EQE difference between the control device and UV-F based device.

Table S1. TRPL lifetimes of the control and the UV-F-based device. The test structure is Glass/perovskite

Sample	τ_1 (ns)	τ_2 (ns)
Control	2.70	10.50
UV-F	2.09	22.72

Table S2. TRPL lifetimes of the control and the UV-F sample. The test structure is Glass/SnO_2/perovskite

Sample	τ_1 (ns)	τ_2 (ns)
Control	21.65	51.13
UV-F	9.03	58.38

Table S3. Fitting results from the EIS of PSCs based on the control and UV-F-based device.

	R_S (Ω)	R_{tr} (Ω)	R_{rec} (Ω)
Control	329	83860	13830
UV-F-based device	227	10600	89220