

Supporting Information

Stabilizing all-inorganic CsPbI₃ perovskite with polyacrylonitrile for
photovoltaic solar cells

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Experimental Details

Materials. Dimethylammonium iodine (DMAI) and bis(trifluoromethane) sulfonamide lithium salt (Li-TFSI) were purchased from TCI. Cesium iodide (CsI), Lead (II) iodide (PbI₂), FK209 Co(III) bis(trifluoromethane) sulfonimide salt and Spiro-OMeTAD (2,2',7,7'-tetrakis[N,N-di(4-methoxyphenyl) amino]-9,9'-spirobifluorene) were purchased from Xi'an Polymer Light Technology Corp. Polyacrylonitrile (PAN) was purchased from Shanghai Macklin Biochemical Co., Ltd (Mw 50,000). Anhydrous N, N-dimethylformamide (DMF) was purchased from Innochem. 4-tert-butylpyridine (tBP) and acetonitrile were purchased from Sigma-Aldrich. Other materials were purchased from Sinopharm Chemical Reagent Co. Ltd. And all materials used without any further purification.

Solar cell fabrication. The FTO glasses were cleaned by deionized water, ethyl alcohol, acetone, and isopropanol with ultra-sonication for 20 min respectively, then dried by the flow N₂. Afterwards, a compact TiO₂ film was prepared by immersing the FTO glasses in 200 mM TiCl₄ aqueous solution at 70 °C for 1 hour, then washed with deionized water and ethanol before annealing at 100 °C for 1 hour.

The CsI, PbI₂ and DMAI were mixed in anhydrous DMF at the molar ratio of 1:1:1 to form a 0.6 M precursor solution. 43.3 mg of PAN was dissolved in 1ml DMF, and a varied volume of the PAN solution was added into the precursor solution. The resultant precursor solution was spin-coated at 3000 r.p.m for 30 s on the TiO₂/FTO substrates treated by O₃/ultraviolet for 20 min, followed by annealing at 210°C for 5min. The hole transport layer was formed by spin-coating Spiro-OMeTAD solution at 3000 r.p.m for 30 s. Spiro-OMeTAD solution was prepared by dissolving 72.3 mg of Spiro-OMeTAD, 28.8 μL of 4-tert-butyl pyridine, 17.5 μL Li-TFSI solution (520 mg of Li-TFSI in 1 mL acetonitrile), 28 μL of FK209 Co (III) (300 mg of FK209 Co (III) in 1 mL acetonitrile). Finally, a ~80 nm thick Au electrode layer was deposited using thermal evaporation under vacuum.

Measurement and characterization. The morphologies of the perovskite films were evaluated by the field-emission scanning electron microscopy (SEM, JEOL, JSM-

7500F, Japan). Absorption spectra were conducted by a UV/Vis spectrometer (SHIMADZU, UV-1800 UV/Vis Spectrophotometer) in the wavelength range of 300-900 nm. The XRD patterns were collected by using a X'Pert powder X-ray diffractometer (Bruker D8) with monochromatic Cu K α radiation ($\lambda = 1.5418 \text{ \AA}$) operated at 40 kV and 40 mA. Current density-voltage characteristics of the PSCs were measured under 1 sun illumination in a glovebox filled with N₂, using a programmable Keithley 2400 source meter under AM 1.5G solar irradiation at 100 mW cm⁻² (Enli Tech, Class AAA solar simulator). The EQE was measured by illumination with monochromatic (Enli Tech, Class AAA solar simulator, QE-mini).

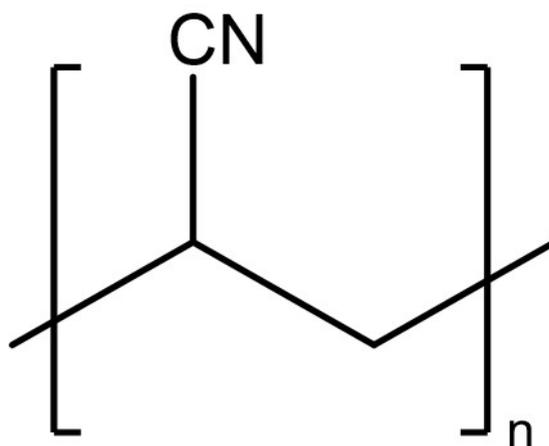


Fig. S1. The chemical structure of PAN.

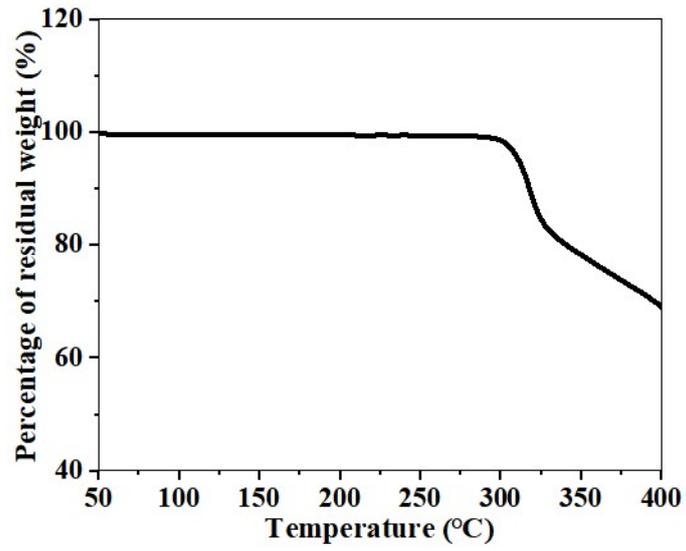


Fig. S2. Thermogravimetric analysis (TGA) of PAN.

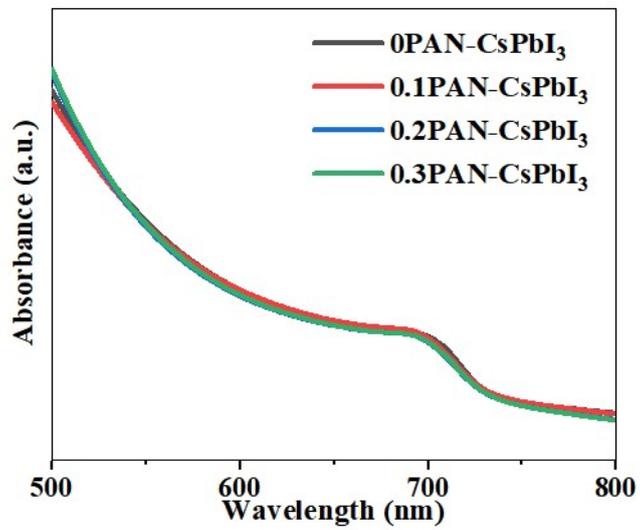


Fig. S3. UV-vis spectra of xPAN-CsPbI₃.

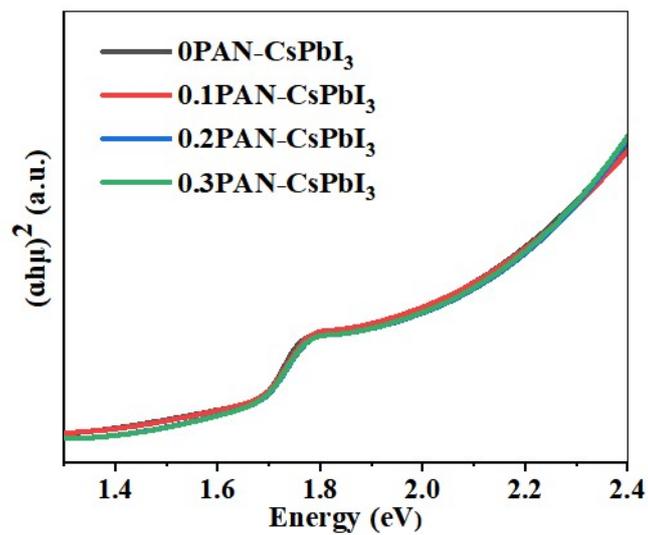


Fig. S4. Tauc Plots of xPAN-CsPbI₃ films.

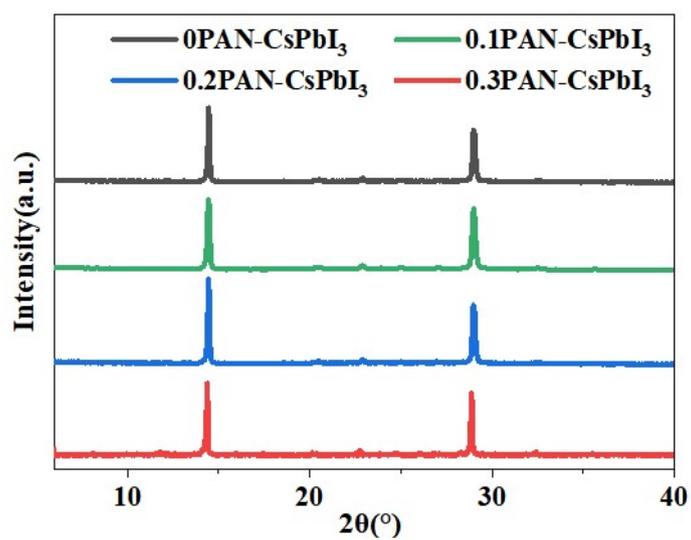


Fig. S5. XRD patterns of xPAN-CsPbI₃.

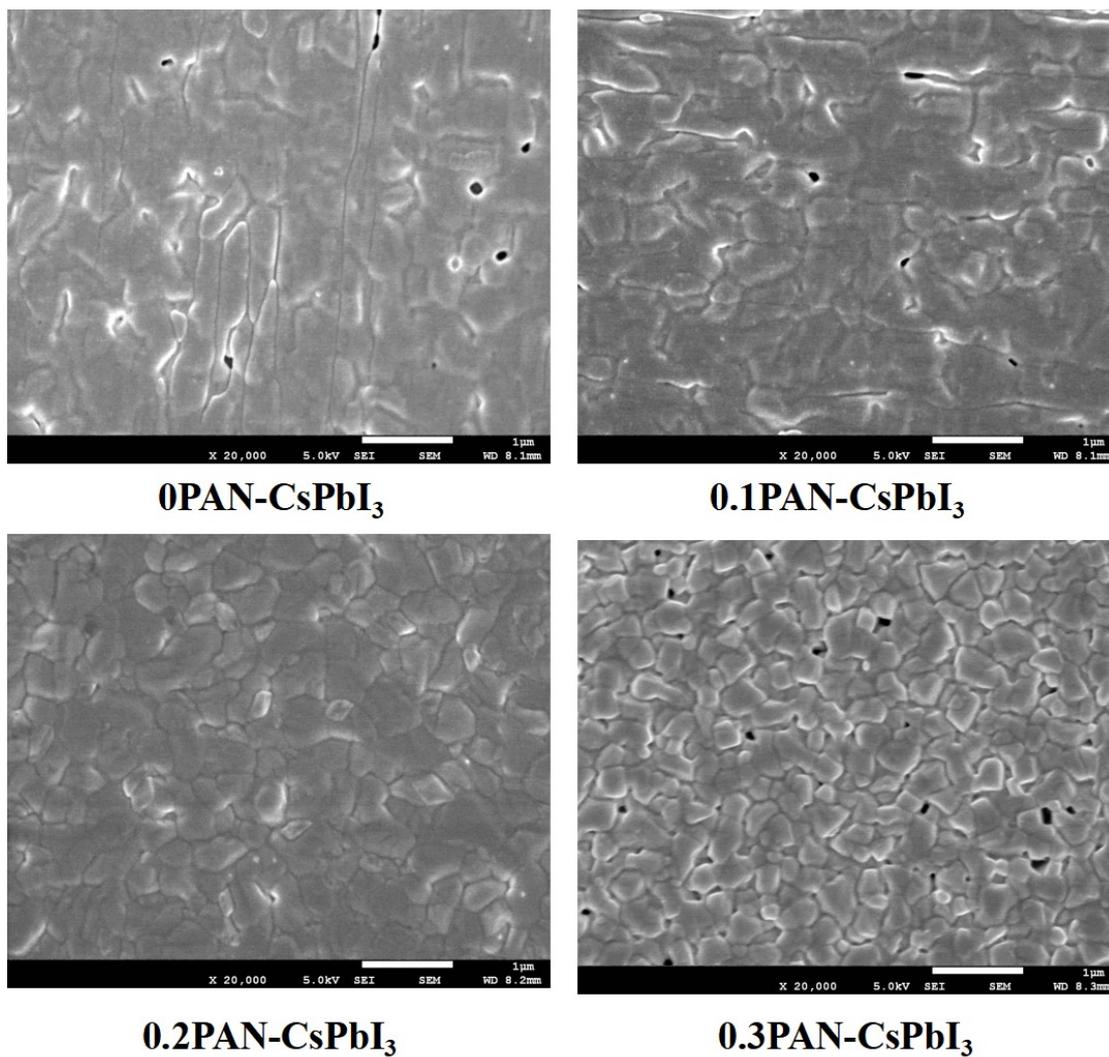


Fig. S6. Top-surface SEM images of xPAN-CsPbI₃ perovskite thin films. Scale bar, 1 μm.

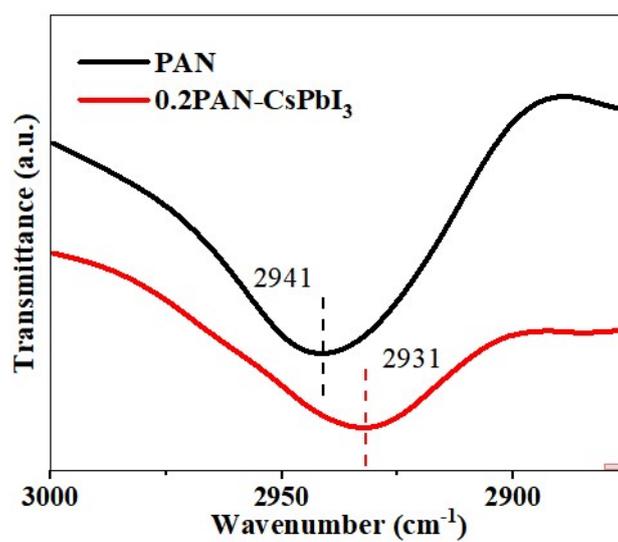


Fig. S7. The FTIR of the C-H of the PAN and the 0.2PAN-CsPbI₃.

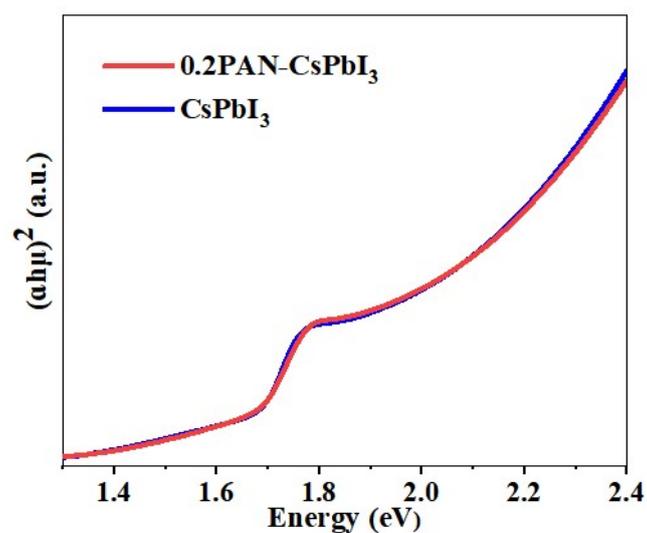


Fig. S8. The Tauc plots of the Control and the Target films.

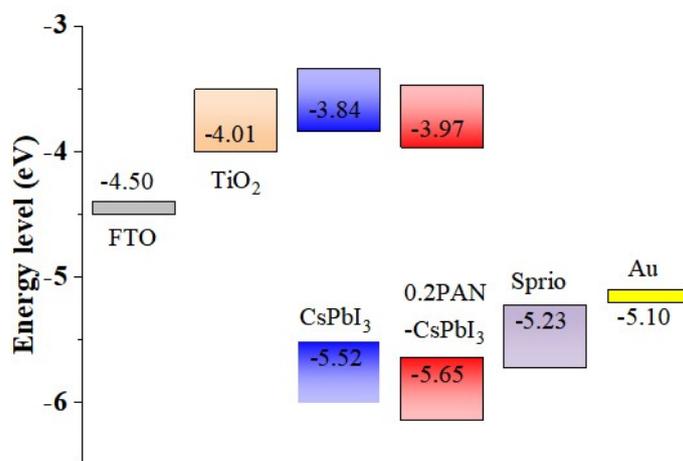


Fig. S9. The corresponding Energy diagram of each layer that constitute the solar cells.

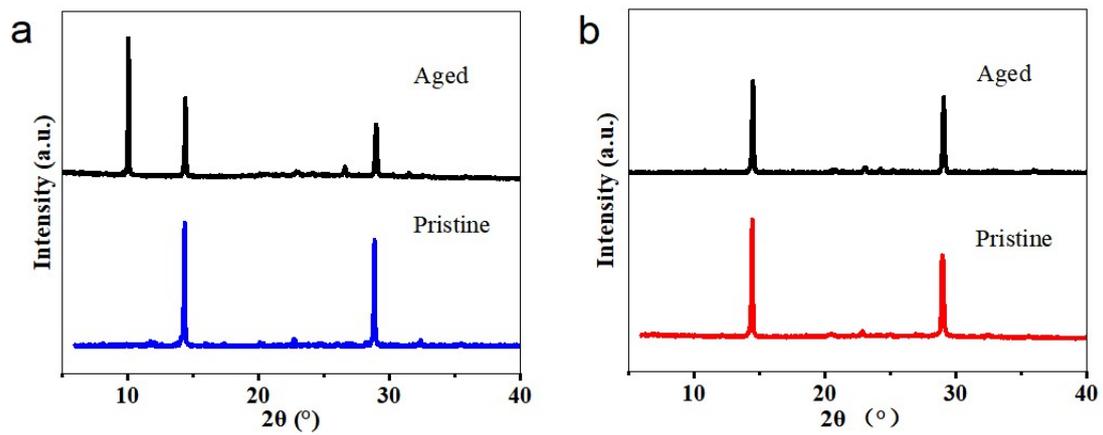


Fig. S10. The XRD spectra of the films after and before aging for 24 hours. (a) the CsPbI₃ and (b) the 0.2PAN-CsPbI₃ (at the ambient conditions with $30\pm 5\%$ RH and at 25°C).

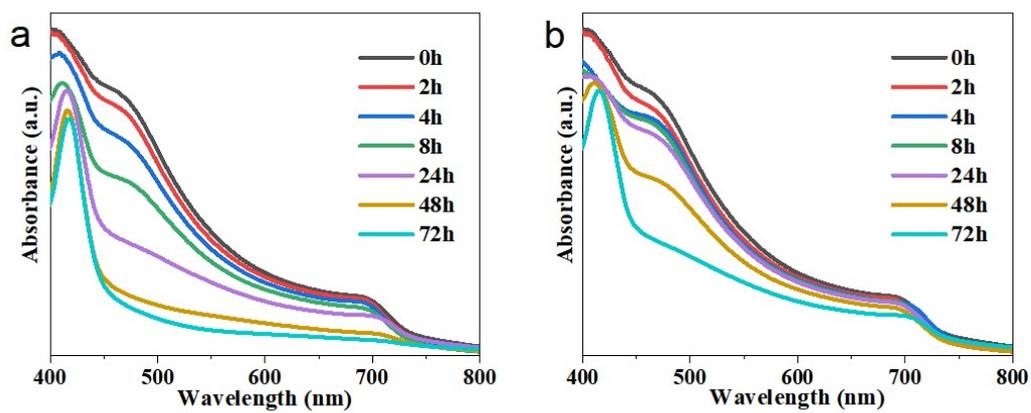


Fig. S11. The evolution of the UV-vis spectra of the films during aging for 72 hours. (a) the CsPbI₃ and (b) the 0.2PAN-CsPbI₃ (at the ambient conditions with 30±5% RH and at 25°C).

Table S1. TRPL characteristic values of the CsPbI₃ and the 0.2PAN-CsPbI₃ perovskites.

Samples	τ_1 (ns)	A_1	τ_2 (ns)	A_2	τ_{ave} (ns)
CsPbI ₃	2.91	2173.32	6.43	168.36	3.42
0.2PAN-CsPbI ₃	5.43	3005.63	12.72	332.08	6.93

Note: $\tau_{ave} = (A_1 * \tau_1^2 + A_2 * \tau_2^2) / (A_1 * \tau_1 + A_2 * \tau_2)$