Article

Inhibited Aggregation of Lithium Salt in Spiro-OMeTAD for Perovskite Solar Cells

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Characterization

The crystallinity of perovskite film is measured and analyzed by an X-ray diffractometer (XRD, Rigaku, SmartLab3kW). The top-view images of films are scanned by scanning electron microscopy (SEM, JEOL JEM5610). The surface roughness of Spiro-OMeTAD film is characterized by atomic force microscopy (Hitachi AFM 5100 N). Steady-state photoluminescence (PL) spectra are measured by Raman spectrometer (LabRAM HR Evolution) with 532 nm laser unit, which HORIBA FRANCE SAS manufactures. Time-resolved photoluminescence (TRPL) is measured using a steady-state, transient fluorescence spectrometer (FLS1000, Edinburgh, England). The absorption spectra and (hv)2 versus photon energy of the Spiro-OMeTAD films are measured by UV–visible spectrophotometer. The device's current density–voltage (J-V) characteristic curves are tested and analyzed by the source meter (Keithley 2400). The solar energy quantum efficiency test system (SCS10-X 150A2400) analyzes the EQE of devices. Before the formal test, the standard single crystal silicon photovoltaic cell is used to calibrate the light intensity of each wavelength. EIS is performed using the Autolab PGSTAT204 electrochemical workstation manufactured by Metrohm.

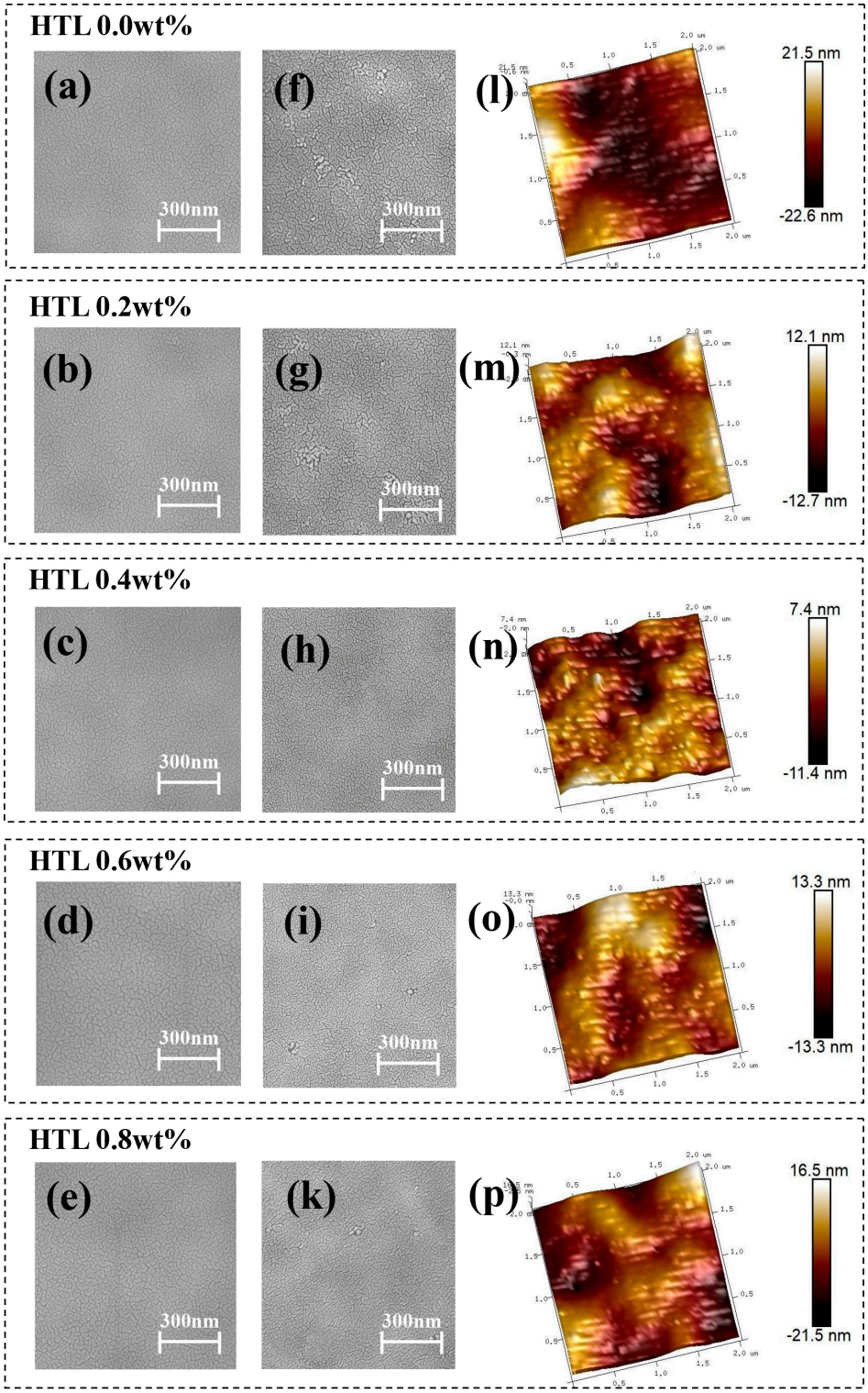

Figure S1. (a–e) Top-view SEM images of fresh Spiro-OMeTAD film (HTL 0.0wt%, HTL 0.2wt%, HTL 0.4wt%, HTL 0.6wt% and HTL 0.8wt%) after spin coating. (f–k) Top view SEM image of the corresponding Spiro-OMeTAD film after being oxidized in air for 8 hours. (l–p) Top view 3D AFM image of the corresponding Spiro-OMeTAD film after oxidation in air for 8 hours.

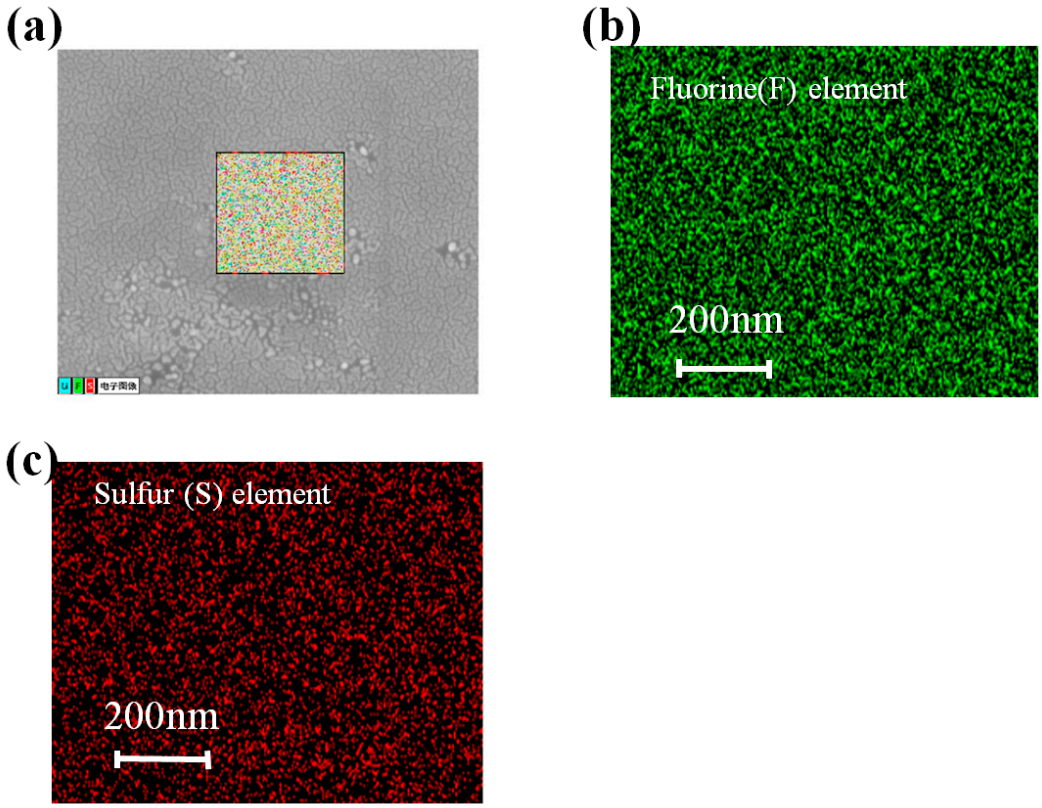

Figure S2. (a) Elementary characterization of HTL 0.0wt%; (b–c) EDS mapping of S and F elements in HTL 0.0wt%.

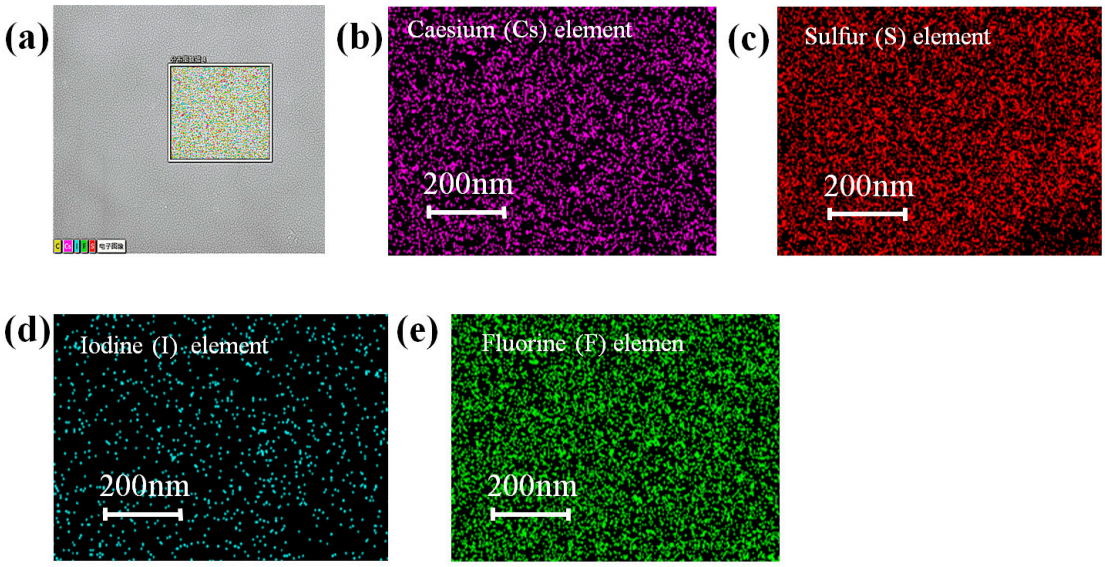

Figure S3. (a) Elementary characterization of HTL 0.4wt%; (b–e) EDS mapping of Cs, S, I and F elements in HTL 0.4wt%.

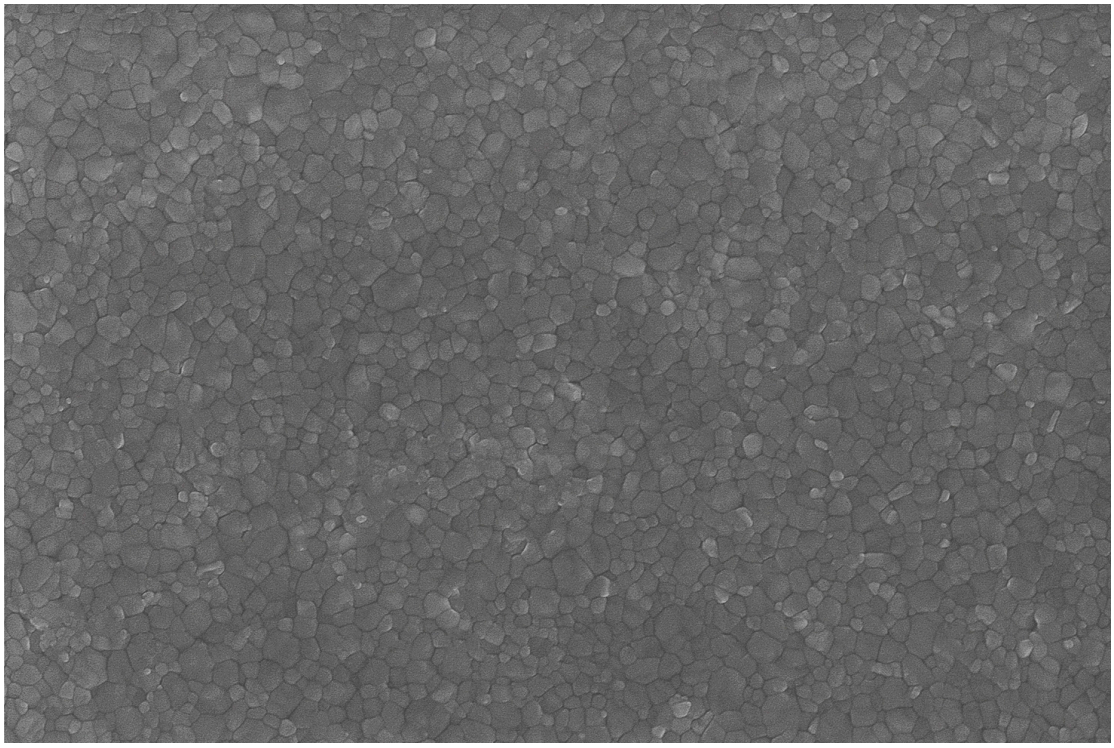

Figure S4. Top-view SEM image of the perovskite film.

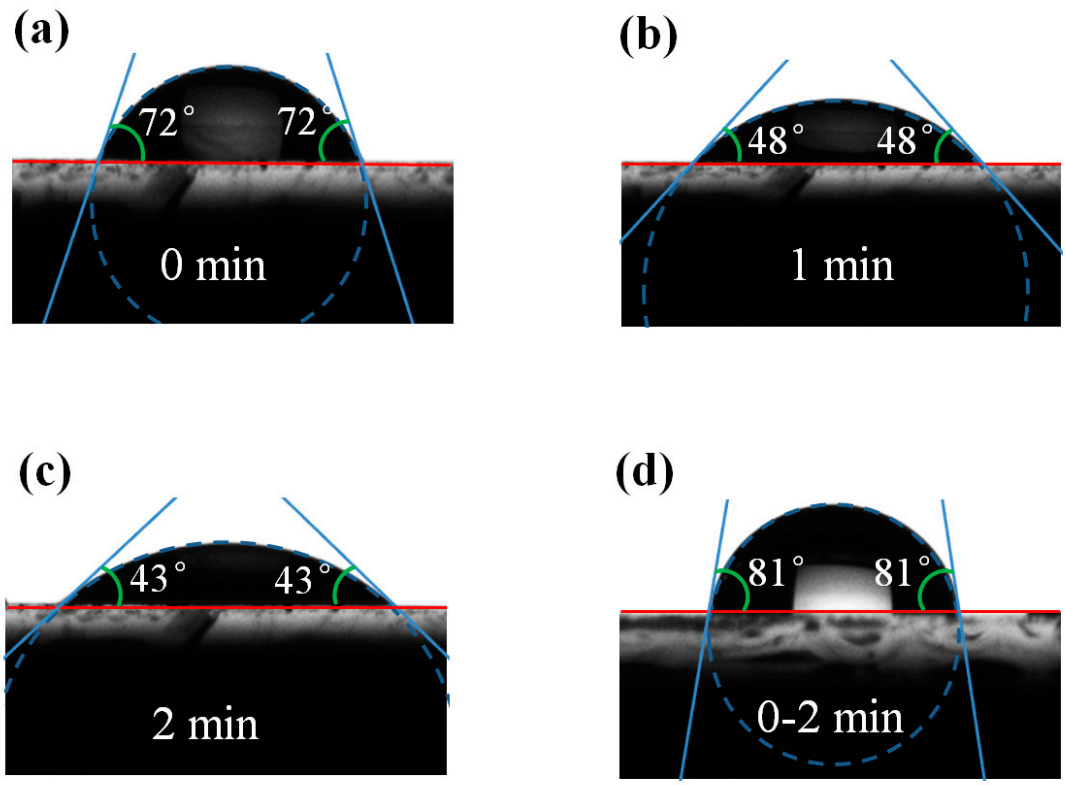

Figure S5. Water contact angles of ITO/SnO2/perovskite/HTL 0.0wt% (a–c) and ITO/SnO2/perovskite/HTL 0.4wt% (d).

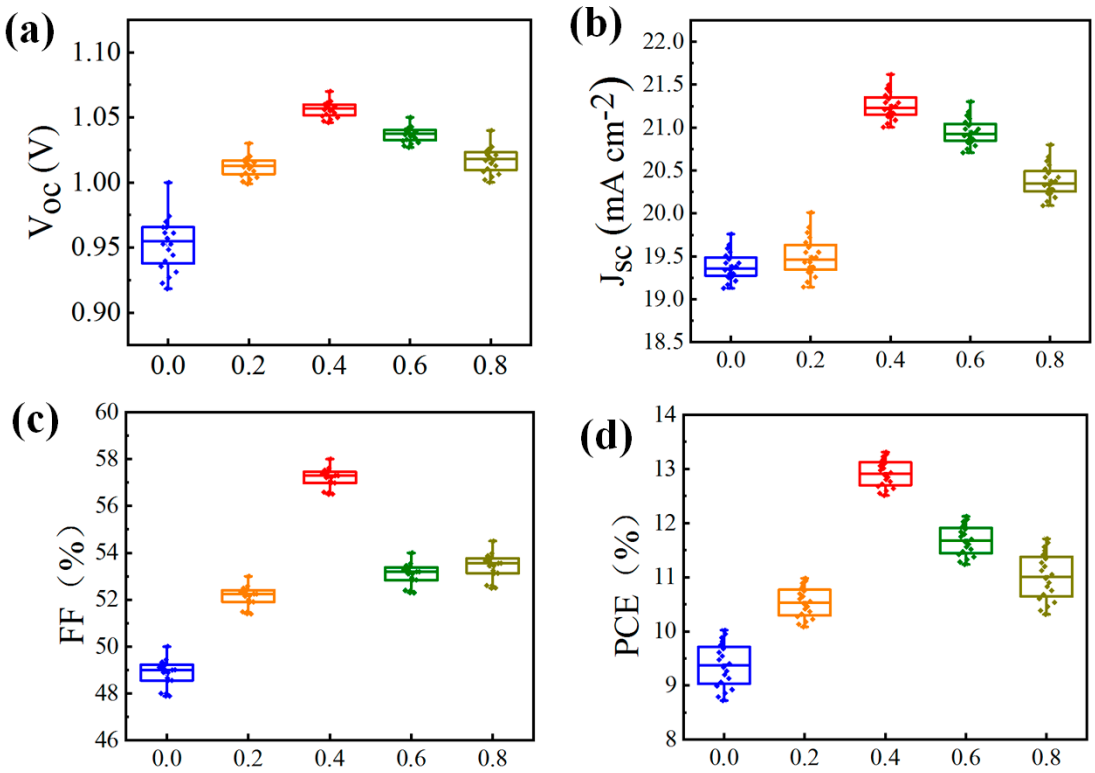

Figure S6. At five concentrations of 0.0, 0.2, 0.4, 0.6 and 0.8 wt% (mass ratio, CsI/TBP). The statistical distribution of Voc (a), Jsc (b), FF (c) and PCE (d) photovoltaic parameters of 20 PSCs samples under the same test conditions.

Table S1. AFM data of Spiro-OMeTAD doped with different mass ratio of CsI.

Roughness	0.0 wt%	0.2 wt%	0.4 wt%	0.6 wt%	0.8 wt%
Rq (nm)	6.19	3.75	2.21	4.43	5.03
Ra (nm)	5.13	3.03	1.77	3.58	3.97

Table S2. TRPL data of ITO/Perovskite, ITO/Perovskite/HTL 0.0wt% and ITO/ Perovskite/HTL 0.4wt%.

Samples	A_1 (%)	τ_1 (ns)	A_2 (%)	τ_2 (ns)
ITO/Perovskite	72.68	38.54	86.24	17.74
ITO/Perovskite/HTL 0.0wt%	57.46	16.96	43.26	32.04
ITO/Perovskite/HTL 0.4wt%	51.09	10.26	39.97	24.31