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**Project title**: Towards Air-processed Highly Oriented Pure α-FAPbI3 Perovskite High Performance Inverted Perovskite Solar Cells Through Adoption of a Coordinator Replenishment Strategy

The following files have been archived:

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| **File name** | **File description (Short description of content, sample size, format, any linking between different types of data, i.e. survey and interviews/focus groups)** |
| AFM | This zip bundle includes the AFM image files that reveal the morphology and roughness of the perovskite films. These AFM images with a 5\*5 μm scope at a resolution of 256\*256 data points were scanned using a MFP-3D-Stand Alone instrument (Asylum Research Abingdon-on-Thames, UK) under contact mode. |
| Dark J-V | This zip bundle includes the txt files of J-V curve scanning of the perovskite solar cells under a dark environment. These files were performed to compare the defect density in the PSCs. The measurements were performed using a Keithley 2400 instrument in an ambient and dark environment (~20 ºC and ~60% RH). |
| DSC | This zip bundle includes the differential scanning calorimetry (DSC) data (.xlsx) that provide information of the interaction between coordinator with perovskite components. DSC measurements were performed under N2-gas atmosphere with a TGA/DSC1 instrument (METTLER TOLEDO) at a heating rate of 2 K·min-1, beginning at 30 °C and ending at 400 °C. |
| EIS | This zip bundle includes the electrochemical impedance data (.csv) of the PSCs that compare the recombination resistance and electron transferring resistance of the solar cells. EIS measurements were conducted using a Zahner Zennium electrochemical workstation. EIS measurements were employed under a bias of 0.75 V, scanned from 1MHz to 1 Hz. |
| EQE | This zip bundle includes the external quantum efficiency data (.txt), which compares the integrated current density of the PSCs. EQE measurements were conducted with an Enli-Tech (Taiwan) instrument. The EQE scanning range from 300 nm to 900 nm. The light intensity for EQE measurements was calibrated using a standard single-crystal silicon solar cell. |
| FTIR | This zip bundle includes the FTIR data (.dpt) that provide information about the interaction between coordinators and perovskite components. The data was recorded using a Bruker Vertex v70 with transmission mode. The measurement was carried out at a range of 400 - 4000 nm-1, with a wavenumber length size of 4 nm-1. |
| GIWAXS | This zip bundle includes the in-situ GIWAXS data measured during the annealing process of the perovskite films. These data provide information about the crystallinity, orientation, and the crystallization dynamic of the perovskite films. GIWAXS and in-situ GIWAXS experiments were performed at the BL14B1 beamline of Shanghai Synchrotron Radiation Facility (SSRF), Shanghai, China. The measurement was conducted using a Mar 225 detector under a beam energy of 10 keV (λ = 1.24 Å). The grazing-incidence angles were 0.5°. |
| Mott Schottky | This zip bundle includes the Mott Schottky data (.csv) that determines the built-in potential (Vbi) and the trap density of the PSCs, which is helpful in studying the charge transport and recombination dynamics in the PSCs. MS measurements were conducted using a Zahner Zennium electrochemical workstation. In Chapter 4, MS plots were recorded from 0 V to 1.2 V, with a step size of 0.01 V. While in Chapters 5-6, they were recorded from 0 V to 0.9 V, with a step size of 0.01 V. |
| NMR | This zip bundle includes the 1H NMR data of the perovskite powder acquired from the perovskite films. These data provide information about the ratio of MA cation that remained in the perovskite films after annealing. Solution NMR measurements with DMSO-d6 as solution and its chemical shift as reference were conducted on a Bruker Avance 400 spectrometer (400M). |
| Performance | This zip bundle includes txt files recording the J-V curves and statistical distribution of the performance of PSCs. J-V measurements were performed with a Keithley 2400 instrument in an ambient environment (~20 ºC and ~60% RH). An Oriel Sol3A solar simulator was employed to produce 1-sun light illumination (AM 1.5G, 100 mW·cm-2), which was calibrated using a standard KG-5 Si diode. The devices for J-V measurements were covered with a shadow mask during the measurements to control the active area to be 0.08 cm2. The measurements were conducted with unencapsulated devices. The devices were soaked in light for around 3 min before J-V scanning. J-V curves were measured both in reverse scan (from 1.2 V to -0.2 V) and forward scan (from -0.2 V to 1.2 V) with a step size of 0.01 V. |
| PL | This zip bundle includes the steady-state PL data of the perovskite films, which compare the trap density at grain boundary and surface of the perovskite films. TRPL measurements were performed using an FLS980 spectrofluorometer with a standard detector, excited by a pulsed laser with a wavelength of 405 nm. |
| SCLC | This zip bundle includes the space charge limited current data of the PSCs, which were collected to acquire the voltage of the trap filling limit, and thus calculate the trap density of the perovskite films. SCLC measurements was performed on both electron-only devices with a structure of ITO/SnO2/Perovskite/PCBM/BCP/Ag and hole-only devices with a structure of ITO/NiOx:2PACz/Perovskite/Spiro-OMeTAD/Au. The measurements were carried out using a Keithley 2400 instrument in an ambient and dark environment (~20 ºC and ~60% RH). |
| SEM | This zip bundle includes the SEM image of the perovskite films, providing information about their surface and cross-sectional morphology. SEM images were measured using a HITACHI SU8230 instrument in a secondary electron mode. Electron beams with 3-5 kV accelerated voltage were used, accompanied by an in-lens detector. |
| Stability | This zip bundle includes the J-V curves (.txt) that recorded the performance of the PSCs at a serious of storage time points and the maximum power point tracking data (.mdb) that continuously tracked the performance-decay of the PSCs. The MPPT measurements were performed under continuous LED light illumination in an ambient environment (~20 ºC and ~60% RH). The maximum power point (MPP) was measured every 17 s. |
| TAS | This zip bundle includes the transient absorption data that reflects the carrier density and carrier lifetime in the perovskite films. Perovskite films for TAS measurements were deposited on quartz glass. TA spectra were measured using a pump–probe spectrometer (TA-100, Time-tech spectra) and were illuminated on the top surface with a 400 nm pump. |
| TGA | This zip bundle includes the thermogravimetry data (.xlsx) that used for studying the strength of chemical interaction between the additives and the perovskite components. TGA was performed under N2-gas atmosphere with a TGA/DSC1 instrument (METTLER TOLEDO) at a heating rate of 2 K·min-1, beginning at 30 °C and ending at 400 °C. |
| TPV&TPC | This zip bundle includes the transient photovoltage (TPV) and transient photocurrent (TPC) data of the PSCs. These data provide direct information about carrier lifetime and charge extraction time in the PSCs. Both TPV and TPC measurements were conducted using a platform built by Time Tech Spectra Co. LTD. |
| TRPL | This zip bundle includes the time-resolved photoluminescence data (.csv) of the perovskite films that evaluated the lifetime of their excited state, which is the key to determine the quality of the perovskite films. TRPL measurements were performed using an FLS980 spectrofluorometer with a standard detector, excited by a pulsed laser with a wavelength of 405 nm. |
| UV-vis | This zip bundle includes the ultraviolet-visible (UV-vis) absorption data of the perovskite films that compared their light-absorbing ability and determined their absorption edge of the solar light spectrum. UV-vis absorption measurements were conducted with a Lambda 950 spectrometer, measured over a range of 1100 nm-400 nm with a step size of 1 nm. |
| Voc-Light intensity | This zip bundle includes the records of PSCs’ Voc when they were exposed to different light intensities. These light-dependent open-circuit voltage data were measured to determine the ideal factor of the PSCs and thus calculated the trap density inside the PSCs. Light-dependent Voc data were measured by scanning J-V curves under various light intensity, ranging from 100 mW·cm-2  to 0.1 mW·cm-2. The measurements were performed using a Keithley 2400 instrument in an ambient environment (~20 ºC and ~60% RH). |
| XRD | This zip bundle includes the X-ray diffraction data of the perovskite films, which were collected to identify the impurities, crystallinity, and orientation of the perovskite films. They were also used for the analysis of lattice strain in α-FAPbI3 perovskite films according to the Williamson-Hall method. XRD measurements were performed using a Bruker D8 Advance ECO diffractometer with Cu Kα1,2 radiation (λ = 1.541 Å, 1kW). Diffraction patterns were measured within an angular range of 5° < 2θ < 45° with a step size of Δθ = 0.02°. |

**Publications**: (based on this data, if any)