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**Sponsor:** National Natural Science Foundation of China (NSFC)

**Project title**: Research data supporting “Preferentially Coordinating Tin Ions to Suppress Composition Segregation for High-performance Tin-lead Mixed Perovskite Solar Cells”

The following files have been archived: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. |
| AFM-IR | This zip bundle includes the AFM-IR image files that was used to identify the distribution of organic dopant on the surface of the perovskite films. AFM-IR images were scanned with a nanoIR2 system (Anasys Instruments, Inc., Santa Barbara, CA, USA) in contact mode at ambient atmosphere. |
| 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 0.9 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 1100 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 additives 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. |
| ICP-MS | This zip bundle includes the ICP-MS data that determine the percentage of Sn element to the B-site cation in the mixed tin-lead perovskite. The perovskite solution samples were prepared as follows: First, perovskite powder was scraped down from the films and collected into a 4 ml vial. Then, the collected perovskite powder was digested with concentrated hydrochloric acid. Last, the resulting concentrated solution was diluted to around 10 ppm with 1%vol HCl solution. The standard solution of Sn and Pb was prepared to be 200 ppb, 400 ppb, 600 ppb, 800 ppb, 1000 ppb, 1500 ppb, and 2000 ppb. ICP-MS measurements were performed using an Agilent 7700X. |
| 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. The data were recorded from 0 V to 0.9 V, with a step size of 0.01 V. |
| NMR | This zip bundle includes the NMR data of the perovskite powder acquired from the perovskite films. These data provide information about the interaction between additives and perovskite components. Solution NMR measurements with DMSO-d6 as solution and its chemical shift as reference were conducted on a Bruker Avance 400 spectrometer (400M). |
| J-V | This zip bundle includes txt files recording the J-V curves 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. J-V curves were measured in reverse scan (from 0.9 V to -0.2 V) with a step size of 0.02 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 FLS1000 spectrofluorometer with a near IR detector, excited by a xenon lamp. |
| 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. |
| TEM-EDS | This zip bundle includes the SEM image of the perovskite films, providing compositional information of the perovskite films at the micro scale. Specifically, TEM-EDS was performed to analyze the elemental composition and reveal the homogeneity of Sn/Pb elemental distribution in mixed Sn-Pb perovskite films. TEM-EDS was performed using a Titan Themis G2 |
| TG | This zip bundle includes the thermogravimetry data (.xlsx) that was used to demonstrate that there is no decomposition happens in the mixtures of additive and perovskite components below 200°C. TG 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. The TRPL spectra were measured utilizing a FLS980E Fluorescence Spectrophotometer (United Kingdom), excited by a pulsed laser with a wavelength of 532 nm. |
| UPS&XPS | This zip bundle includes the UPS and XPS data of the perovskite films. The UPS data were applied to determine the work function and valence band of each layer of the PSCs. XPS data reveal the interaction between additive and the perovskite components. Both UPS and XPS data were measured using an Thermo Fisher Scientific ESCALAB Xi+ instrument. A non-monochromated HeI α photon source (hν = 21.22 eV) was applied for UPS measurements. Au is taken for calibration. XPS measurements were performed with pass energy of 30 eV and a step size of 0.1 eV. |
| 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. XRD measurements were performed using a Rigaku Smartlab diffractometer with Cu Kα1,2 radiation (λ = 1.541 Å, 9kW). The data were acquired from 10° < 2θ < 40° with Δθ=0.02°. |

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