

Data set about *Quantitative Analysis of the Doping and Defect Density in Mixed Sn-Pb Perovskites Mediated by SnF₂*

Title: *Quantitative Analysis of the Doping and Defect Density in Mixed Sn-Pb Perovskites Mediated by SnF₂*

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Description: Data for SSMC and TRMC results, UV-Vis-NIR spectroscopy, XRD, XPS and SEM results and analysis in the main manuscript and Supporting Information published with DOI: 10.1021/acs.chemmater.5c00816.

The raw data were collected in the years 2024-2025, using various structural, compositional, and optoelectronic characterization methods on solution-based spin-coated mixed tin-lead (Sn-Pb) perovskite thin films with varying concentration of tin fluoride (SnF₂) additive, combined with absorption spectroscopy analysis on perovskite precursors solutions. All measurements were conducted at room temperature, to study the effect of tin oxidation (SnI₂ precursor oxidation) and SnF₂ additive on the doping, crystal defect density and charge carrier transport properties in the layers. More specifically, all SSMC and TRMC measurements were conducted under nitrogen. The xy data obtained from X-ray diffraction (XRD), UV-Vis-NIR spectroscopy, and X-ray photoelectron spectroscopy (XPS) were imported into Igor Pro (Wavemetrics). In Igor Pro, these xy data are stored as "waves," corresponding to the values on the x and y axes in the plots. Data for Steady State Microwave Conductance (SSMC) and Time-Resolved Microwave Conductivity (TRMC) were collected directly as waves in Igor Pro on the computers connected to the respective microwave-based setups. Igor Pro was used to generate all data plots. The SEM micrographs were directly saved as .tiff files from the SEM software and converted in .png afterwards.

The SSMC results were simulated by COMSOL (finite element method analysis on the microwave cavity cell, for more details see the M.Sc. thesis by Koning, S. J, provided below and as a .pdf in the dataset) to obtain the dark conductivity. The TRMC results were simulated by SIMsalabim (drift-diffusion simulations, for more details see the URL about SIMsalabim provided below) to obtain the parameters governing the charge carrier dynamics.

For further information on file formats and naming, the units and abbreviations used for all measured values and labels, and instructions for opening or modifying Igor Pro files, please refer to the README.pdf included in the dataset. It is strongly recommended to consult the corresponding publication for guidance on the files in these datasets, as each file name includes a reference to its associated figure. The main manuscript and Supporting Information of the publication contains details about the characterization instruments and additional data processing specifics.

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Format: Igorfile/pxp; image/png

The Igor files were produced by for Igor Pro 9 by Wavemetrics. This software needs to be used to open the .pxp files, using Igor Pro Demo (valid for 30 days) or the version with license. Alternatively, an open-source reader like Python can be used, installing the *igor* or *pyigor* package:

Bash

```
pip install igor
```

Python

```
from igor.binarywave import load
data = load("file.pxp")
print(data)
```

Bash

```
pip install pyigor
```

Python

```
from pyigor import load
data = load("file.pxp")
print(data.keys())
```

Naming convention:

The X-ray Diffraction (XRD) data present the following naming convention:

XRD_*name*_0daysagedSnI2_Fig*X*.

The *name* is specified for the the lattice parameter and FWHM data derived from the XRD peaks.

The X-ray Photoelectron Spectroscopy (XPS) data present the following naming convention: XPS_*elementorbitals*_*name*_0daysagedSnI2_*X*SnF2_Fig*X*.

The *name* describes the peak fitting, depth profiling or Wagner plots derived from the XPS results.

The XPS data for the reference compounds samples present the following naming convention: XPS_*elementorbitals*_ref*compound*_Fig*X*.

The UV-Vis-NIR spectroscopy data present the following naming convention: UV-Vis_0daysagedSnI2_Fig*X*.

The absorption spectroscopy in solution present a slightly different naming convention, namely: Abs in solution_*name*_Fig*X*. The *name* always refers to the compound(s) analyzed in solution.

The Steady State Microwave Conductance (SSMC) data present the following naming convention: SSMC_*X*daysagedSnI2_Fig*X* or SSMC_slightlyagedSnI2_Fig*X*.

The Time-resolved Microwave Conductivity (TRMC) data present the following naming convention: TRMC_*open or cavity*cell_0daysagedSnI2_fit*X*SnF2_Fig*X*.

The data obtained by SSMC and TRMC simulations present the following naming convention: the or *name*_0daysagedSnI2_Fig*X*. The *name* describes the specific data (dark conductivity, dark free holes concentration, trap density, etc.) derived from the SSMC and TRMC simulations.

The Scanning Electron Microscopy (SEM) images present the following naming convention: SEM_0daysagedSnI2_*X*SnF2_Fig*X*.

Important symbols and abbreviations:

- SnI₂ = tin(II) iodide
- SnI₄ = tin(IV) iodide
- SnO_x = tin(II) oxide and tin(IV) oxide species
- SnO = tin(II) oxide
- SnO₂ = tin(IV) oxide
- SnF₂ = tin(II) fluoride
- SnF₄ = tin(IV) fluoride

- 2θ = diffraction angle (°)
- a = cubic lattice parameter (nm)
- FWHM = full-width half-maximum of the XRD peaks (°)
- $O.D.$ = optical density (absorbance) (-)
- F_A = fraction of absorbed light (absorptance) (-)
- E_g = bandgap energy (eV)
- α = absorption coefficient (cm⁻¹)
- E_{ph} (or $h\nu$) = photon energy (eV)
- G = conductance (S)
- β = microwave cell form factor (-)
- e = elementary charge (C)
- I_0 = laser light intensity (cm⁻²)
- σ_{dark} = dark conductivity (S m⁻¹)
- p_0 = dark holes concentration (cm⁻³)
- N_T = trap state (defect) density (cm⁻³)
- $N_{T,bulk}$ = trap state (defect) density in the bulk (cm⁻³)
- $N_{T,surf}$ = trap state (defect) density at the surface (cm⁻²)
- k_2 = band-to-band recombination rate constant (cm³ s⁻¹)
- $\Sigma\mu$ = carrier mobilities sum (cm² V⁻¹ s⁻¹)
- $\tau_{1/2,TRMC}$ = carrier lifetimes (ns)
- E_b = binding energy (eV)
- E_{kin} = kinetic energy (eV)
- t_{etch} = etching time for XPS depth profiling (s)
- α' = Modified Auger parameter (eV)

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