

Data set about *Metastable Oxygen-Induced Light-Enhanced Doping in Mixed Sn-Pb Halide Perovskites*

Title: Metastable Oxygen-Induced Light-Enhanced Doping in Mixed Sn-Pb Halide Perovskites

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Description: Data for SSMC and TRMC results, XRD, UV-Vis-NIR spectroscopy and XPS results in the main manuscript and Supporting Information published with DOI: 10.1021/jacs.4c08924. The raw data were collected in the years 2023-2024, using various structural, compositional, and opto-electronic characterization methods on solution-based spin-coated mixed tin-lead (Sn-Pb) perovskite thin films. All measurements were conducted at room temperature, after varying exposure to oxygen and/or light, or after rest in nitrogen, to study the metastable oxygen-induced light-enhanced doping 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.

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

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 different types of exposure, *i.e.* treatments, applied to the samples present the following naming convention:

- For short exposure to: only oxygen ("oxy"), only light ("light"), simultaneously oxygen and light ("oxylight"), resting in nitrogen ("restN2").
- For long exposure to: only oxygen ("longoxy") or simultaneously oxygen and light ("longoxylight").

The X-ray Diffraction (XRD) and GIXRD (grazing incidence XRD) data present the following naming convention: XRD_Sn*fraction*_treatment*_Fig*X*.

The X-ray Photoelectron Spectroscopy (XPS) data present the following naming convention: XPS_*elementorbitals*_name*_Sn*fraction*_treatment*_Fig*X*.

The *name* describes the peak fitting or depth profiling derived from the XPS results. If no *name* is indicated, the data shows the as-measured surface XPS peaks.

The UV-Vis-NIR spectroscopy data present the following naming convention: UV-Vis_Sn*fraction*_treatment*_Fig*X*.

The Steady State Microwave Conductance (SSMC) data present the following naming convention: SSMC_Sn*fraction*_treatment*_Fig*X* when a mixture of cesium and formamidinium are present in the perovskite composition. Alternatively, SSMC_MASn*fraction*_treatment*_Fig*X* when methylammonium is present in the perovskite composition.

The SSMC data involving the deposition of a Al₂O₃ layer by ALD present the following naming convention: SSMC_ALDSn*fraction*_treatment*_Fig*X*.

The analysis of the SSMC data present the following naming convention: Changeindarkconductivity_Sn*fraction*_treatment*_Fig*X*.

The Time-resolved Microwave Conductivity (TRMC) data present the following naming convention: TRMC_Sn*fraction*_treatment*_Fig*X*.

The data about the LED light used for light exposure present the following naming convention: LEDTRMC_Fig*X*.

The data about the effect of laser light under N₂ or O₂ present the following naming convention: SSMC_Sn*fraction*_effectlaserN2orOxy_Fig*X*.

The data about the effect of resting in N₂ for a long time present the following naming convention: SSMC+TRMC_Sn*fraction*_effectlongrestN2_Fig*X*.

Important symbols and abbreviations:

- O₂ = molecular oxygen
- N₂ = molecular nitrogen
- SnO_x = tin(II) oxide and tin(IV) oxide species
- SnF₂ = tin(II) fluoride
- Al₂O₃ = aluminum(III) oxide

- x = tin fraction (-)

- 2θ = diffraction angle (°)
- a = cubic lattice parameter (nm)
- FWHM = full-width half-maximum of the XRD peaks (°)
- d₀₀₁ = interplanar distance of the (001) crystal atomic planes (nm)
- F_A = fraction of absorbed light (absorptance) (-)
- E_g = bandgap energy (eV)
- α = absorption coefficient (cm⁻¹)
- λ = photon wavelength (nm)
- E_{ph} (or hν) = photon energy (eV)
- G = conductance (S)
- β = microwave cell form factor (-)
- e = elementary charge (C)
- I₀ = laser light intensity (cm⁻²)
- K = microwave cell sensitivity factor (-)
- σ_{dark} = dark conductivity (S m⁻¹)
- p₀ = dark holes concentration (cm⁻³)
- Σμ = carrier mobilities sum (cm² V⁻¹ s⁻¹)
- E_b = binding energy (eV)
- t_{etch} = etching time for XPS depth profiling (s)

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