Data set about *Quantifying the Phonon-Induced Contribution to the Urbach Energy in Mixed Sn-Pb Perovskites*

Title: Quantifying the Phonon-Induced Contribution to the Urbach Energy in Mixed Sn-Pb Perovskites
Date: 30/10/2025
Author: Jasmeen Nespoli
Description: Data for the XRD, XPS, UV-Vis-NIR spectroscopy, TRMC, carrier mobilities, Urbach energy and data extracted from the literature in the main manuscript and Supporting Information to be submitted in the next future, now comprised in Ch. 4 of my PhD thesis (the corresponding DOI will be provided as soon as possible).
The raw data were collected in the years 2024-2025, using various structural and optoelectronic characterization methods on solution-based spin-coated mixed tin-lead (Sn-Pb) perovskite thin films with varying Sn/Pb ratio to study the Urbach tails and Urbach energy of the layers. The measurements were conducted with varying temperatures, to understand the stability window of the perovskite alpha-phase and separate the contributions of the static component and dynamic phonon-induced component to the Urbach energy. More specifically, all TRMC measurements were conducted under nitrogen. The xy data obtained from X-ray diffraction (XRD) and UV-Vis-NIR spectroscopy 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 manuscript once it is published (the corresponding DOI will be provided as soon as possible) 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 (the corresponding DOI will be provided as soon as possible) contains details about the characterization instruments and additional data processing specifics, comprising the process of calculation of the Urbach energy values from the TRMC data.

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 *pygor* 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 temperature-dependent X-ray Diffraction (XRD) data present the following naming convention: XRDvsT_(*XXX*)peak_Fig*X* for specific XRD peaks where XXX are the corresponding Miller indices or XRDvsT_patterns_Fig*X* for the full XRD patterns for all perovskite compositions.

The temperature-dependent UV-Vis-NIR spectroscopy data present the following naming convention: UV-Vis_Sn*fraction*_RT_effecttinfraction_Fig*X* for the fraction of absorbed light (absorptance) data at room temperature and UV-Vis_Sn*fraction*_effecttemperature_Fig*X* for the temperature-dependent absorbance data for all perovskite compositions.

The temperature-dependent Time-resolved Microwave Conductivity (TRMC) data for laser excitations above the bandgap present the following naming convention: TRMC_Sn*fraction*_effecttemperature_Fig*X*.
The room temperature TRMC data for laser excitations above and below the bandgap present the following naming convention: TRMC_Sn*fraction*_RT_effectexcwavelength_Fig*X*.
The room temperature absorption data derived from the TRMC results present the following naming convention: Abscoeff_RT_effecttinfraction_Fig*X*.
The temperature-dependent absorption data derived from the TRMC results present the following naming convention: Abscoeff_effecttemperature_Fig*X* or FA_effecttemperature_Fig*X*.
The temperature-dependent carrier mobilities and Urbach energies+fit derived from the TRMC results present the following naming convention: MobilityvsT_Fig*X* and EUvsT+fit_Fig*X*.

The comparison with room temperature or temperature-dependent Urbach energies in the literature present the following naming convention: *name*_comparisonliterature_Fig*X*.

Important symbols and abbreviations:

-SnF2 = tin(II) fluoride

- x = tin fraction (-)
- T = temperature (K)

- 2θ = diffraction angle (°)
- F_A = fraction of absorbed light (absorptance) (-)
- $F\_{R,corr}$ = fraction of reflected light (reflectance) corrected for the reflection of the quartz substrate (-)
- A = absorbance (also called optical density) (-)
- E_g = bandgap energy (eV)
- α_{ph} = absorption coefficient (cm^-1)
- λ = photon wavelength (nm)
- E_{ph} (or hv) = photon energy (eV)
- G = conductance (S)
- β = microwave cell form factor (-)
- e = elementary charge (C)
- I_0 = laser light intensity (cm^-2)
- $\Sigma\mu$ = carrier mobilities sum (cm^2 V^-1 s^-1)
- E_U = Urbach energy (eV)
- θ_E = Einstein phonon temperature (eV)
- k_B = Boltzmann constant (eV K^-1)

Contact information:
Jasmeen Nespoli (PhD candidate)
nespolijasmeen@gmail.com
OR
Tom J. Savenije (promotor)
T.J.Savenije@tudelft.nl