1. Overview

This online repository includes additional data to accompany the article:

> First-principles modelling of the thermoelectric properties of n-type $CaTiO_3$, $SrTiO_3$ and $BaTiO_3$
>
> A. Z. Khan, J. M. Flitcroft and J. M. Skelton
>
> *Materials Advances* **5**, 652–664 (**2024**), DOI: 10.1039/d3ma00624g

This paper is open-access and freely available to download or read online from the DOI link given in the reference above.

2. Summary of Data

2.1 Overview

This repository contains data for each of the three systems investigated in this article, *viz.* the *Pnma* phase of $CaTiO_3$, *I*4/*mcm* $SrTiO_3$ and *R*3*m* $BaTiO_3$.

For each structure, there are four types of data: (1) an optimised structure; (2) a lattice-dynamics calculation to evaluate phonon spectra and lattice thermal conductivities; (3) an electrical-transport calculation to determine the Seebeck coefficients, electrical conductivity and electronic thermal conductivity; and (4) a calculation combining the data to predict the thermoelectric figure of merit ZT.

The following three subsections provide a brief overview of the content and format of the files included for the four types of calculation.

2.2 Optimised crystal structures

Structures are provided in the `CONTCAR` files in the folders for each material. These are in the plain-text `POSCAR` format used by Vienna *Ab initio* Simulation Package (VASP) code, a description of which can be found in the online manual/Wiki.[1]

2.3 Harmonic lattice-dynamics calculations

Data for the lattice-dynamics calculations are provided in `Phono_3_py` subfolder in the parent folders for each system.

The lattice-dynamics and thermal-conductivity calculations were conducted using the Phonopy and Phono3py codes,[2,3] which use a mix of plain-text, YAML, HDF5 and PDF files. We assume those using the data in this repository are familiar with Phono(3)py. The Phonopy and Phono3py input and output files included in the repository are briefly summarised in the following two tables, and further information can be found in the online documentation for the two codes.[2,3]

For convenience, thermal-conductivity curves extracted from the main Phono3py output files, and analyses using the constant relaxation-time approximation (CRTA) method described in the text, are provided as CSV files that can be easily loaded into spreadsheet software such as Excel for visualisation and/or read into scripts/programs for further processing.

File	Format	Description
`phonopy_disp.yaml`	YAML	Metadata from the Phonopy setup.
`FORCE_SETS`	Text	Sets of atomic forces used to calculate the second-order force constants.
`BORN`	Text	Phonopy `BORN` file containing the high frequency dielectric constant $\boldsymbol{\varepsilon}_\infty$ and atomic Born effective-charge tensors $\boldsymbol{Z}^*$.
`projected_dos.dat`	Text	Atom-projected phonon density of states $g(f)$ (PDoS) calculated using the tetrahedron method.
`band.yaml`	YAML	Phonon dispersions curves.
`band.conf`	Text	Configuration file used to generate the `band_dos.pdf` file.
`band_dos.pdf`	PDF	Plot of the phonon dispersion and PDoS.

File/Folder	Format	Description
`phono3py_disp.yaml`	YAML	Metadata from the Phono3py setup.

`FORCES_FC3`
`fc2.hdf5`
`fc3.hdf5`
`fc2.phono3py.hdf5`
	Text/HDF5	Sets of atomic forces and calculated 2nd-/3rd-order force constants. Two sets of 2nd-order FCs are provided: one from the Phonopy calculation (`fc2.hdf5`), and one from the Phono3py calculation (`fc2.phono3py.hdf5`). The former is used in the post-processing to obtain the thermal conductivity.

`kappa-m*.hdf5`	HDF5	Main output file from the thermal-conductivity calculations.
`kappa-m*.csv` `kappa-m*-CRTA.csv`	CSV	Thermal-conductivity curve $\boldsymbol{\kappa}_{\text{latt}}(T)$ and analysis using the CRTA model described in the text.

2.4 AMSET calculations

Data for the electrical-transport calculations are provided in the `AMSET` subfolders in the parent folders for each system.

These calculations were performed using the AMSET code,[4] which uses a mix of XML, HDF5 and YAML files. We again assume those using the data in this repository are familiar with AMSET. The

AMSET input files included in the repository are briefly summarised in the following table, and further information can be found in the AMSET online documentation.[4]

Note that the doping levels and temperatures in the AMSET `settings.yaml` files are indicative, do not cover the entire range of parameters studied in the calculations, and can be changed as needed.

File	Format	Description
`vasprun.xml`	XML	`vasprun.xml` file containing electronic band energies from the dense uniform band structure calculation.
`deformation.h5`	HDF5	Band deformation potentials.
`wavefuncation.h5`	HDF5	Wavefunction extracted from the VASP `WAVECAR` file produced during the dense uniform band structure calculation.
`settings.yaml`	YAML	Calculation settings, including materials parameters, for the AMSET runs.

2.5 ZT calculations

The thermoelectric figure of merit is obtained by combining data from the lattice thermal-conductivity and electrical-transport calculations.

For each of the systems for which these calculations were performed, we provide a CSV-format file, `ZT.csv`, in each of the folders, which provides the ZT and associated properties as a function of extrinsic carrier concentration ("doping level") n and temperature T for n-type (electron) doping.

We also provide a YAML file, `ZT-Paper.yaml`, summarising the selected ZT and properties reported in the paper.

3. References

1. https://www.vasp.at/wiki/index.php/The_VASP_Manual
2. https://phonopy.github.io/phonopy
3. https://phonopy.github.io/phono3py
4. https://hackingmaterials.lbl.gov/amset