1. Overview

This online repository provides additional data to accompany the paper:

Thermodynamics, Electronic Structure, and Vibrational Properties of $Sn_n(S_{1-x}Se_x)_m$ Solid Solutions for Energy Applications

D. S. D. Gunn, J. M. Skelton, S. Metz and S. C. Parker

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2. Summary of Data

2.1 Raw Data

A complete set of raw data for each of the ~5,000 structures in the four solid solution models is provided in four subfolders named as follows: *Pnma* Sn(S,Se) - `SnE-Pnma`, rocksalt Sn(S,Se) - `SnE-RS`, $Sn(S,Se)_2$ - `SnE2` and $Sn_2(S,Se)_3$ - `Sn2E3`. The following table summarises the raw data provided in each folder, and a description of the file formats can be found in Section 3.

File/Folder	Format	Description
`Structures.tar.gz`	`TAR/GZip (POSCAR)`	Optimised structures
`TotalEnergies.csv`	`CSV`	Total energies E_0 and degeneracies g
`Bandgaps.csv`	`CSV`	Bandgaps E_g
`CoreLevels.tar.gz`	`Tar/GZip (CSV)`	Core-level eigenvalues
`PartialDoS.tar.gz`	`Tar/GZip (CSV)`	Partial electronic density of states (PDoS) curves $n(E)$
`DielectricFunctions.tar.gz`	`Tar/GZip (CSV)`	Dielectric functions $\varepsilon(E) = \varepsilon_{\mathrm{Re}}(E) + i\varepsilon_{\mathrm{Im}}(E)$
`LatticeDynamics`	`Various (Phonopy)`	Lattice-dynamics calculations on selected structures

2.2 Processed Data

We have also provided the majority of the processed data discussed in the manuscript and supporting information. The following table summarises the data provided, and a description of the file formats can again be found in Section 3.

File/Folder	Format	Description
`MixingEnergy.csv`	`CSV`	Calculated mixing free energy G_{mix} and enthalpy H_{mix} as a function of composition and temperature
`OccurrenceProbabilities-900K.csv`	`CSV`	Calculated occurrence probabilities P_n for each structure in each composition at 900 K
`PartialDoS-Averaged-900K.csv`	`CSV`	Averaged Partial electronic density of states (PDoS) curves $n(E)$ for each composition for a 900 K formation temperature
`DielectricFunctions-Averaged-900K.csv`	`CSV`	Averaged dielectric functions $\varepsilon(E) = \varepsilon_{\mathrm{Re}}(E) + i\varepsilon_{\mathrm{Im}}(E)$ for each composition for a 900 K formation temperature
`PairDistributionFunctions-Averaged-900K.csv`	`CSV`	Averaged pair-distribution functions (PDF; $g(r)$) for each composition for a 900 K formation temperature
`StructureFingerpring-Averaged-900K.csv`	`CSV`	Structural similarity distance matrices for the structures in each composition calculated using the fingerprinting method described in the paper, and calculated distances to the weighted "centre of mass" for a 900 K formation temperature

2.3 Example input files

Example input files for the Vienna *Ab initio* Simulation Package (VASP) code used in this work are provided in the `ExampleInputFiles` folder. Each file is named according to the scheme `<file_type>_<system(s)>[_<calculation_type>`. The following table provides a brief summary of the file and calculation types:

File Type	Calculation Type	Description
`INCAR`	`Opt`	Geometry optimisations and total-energy calculations
	`DoS`	Bandgaps, partial density of states (PDoS) curves and dielectric functions
	`NSCF-HSE06-*`	Non-self-consistent electronic-structure calculations using HSE 06; two files are provided for the initial self-consistent calculation of the wavefunctions (`a`) and subsequent non-self-consistent recalculation of the band energies using HSE 06 (`b`).
	`Phonon`	Single-point force evaluations for the lattice-dynamics calculations
`KPOINTS`	–	Monkhorst-Pack *k*-point meshes used for geometry optimisations and total-energy calculations
	`DoS`	Γ-centred MP *k*-point meshes used for electronic-structure calculations
	`Phonon`	*k*-point meshes used for the phonon supercells

3. Data Formats

For ease of downloading, large sets of files (e.g. optimised structures, DoS/dielectric function calculations) are stored in GZip-compressed TAR archives. These can be unpacked using the `tar` utility on Mac or Linux, or using the free `PeaZip` software on Windows.[1] Within the archives, files are organised into folders by composition (e.g. `001_Sn16Sn16`, `002_Sn15Se1Sn16`, `...`, `017_Se16Sn16`), and each file is prefixed with a unique identifier consisting of the spacegroup number and an incrementing structure number (e.g. `SG-062_0001`). These identifiers are common across all sets of data for a given solid-solution model.

Optimised structures are provided in the plain-text `POSCAR` format used by the Vienna *Ab initio* Simulation Package (VASP) code, a description of which can be found in the online manual/Wiki.[2] Lattice-dynamics calculations are provided as folders of input and output files for the Phonopy code in plain-text, YAML or PDF format. The folders are named by composition, spacegroup and structure number (e.g. `009_SG-164_0001`). Information on the content and format of the Phonopy files can be found in the online documentation.[3] All other data is provided in plain-text comma-separated values (CSV) files, which can be loaded into spreadsheet software such as Excel for visualisation or read into scripts/programs for further processing.

The sample input files provided are for the VASP code, and details of the formats can be found in the online manual.[2]

3. References

1. http://www.peazip.org/ (accessed 29/05/2019)

2. https://cms.mpi.univie.ac.at/wiki/index.php/The_VASP_Manual (accessed 29/05/2019)

3. https://atztogo.github.io/phonopy/ (accessed 29/05/2019)