

Supplementary Material: High-throughput study of the anomalous Hall effect

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I. DATABASE DESCRIPTION

We provide detailed results of our calculations in the supplementary files 'database.json' and 'database.csv'. The content of these files are identical, the only difference is formatting. The csv file can be directly loaded into spreadsheet applications such as Microsoft Excel or LibreOffice Calc, whereas the json file is more suited for usage with various programming languages. Here we give a description of the data structure. Using python and the pandas library, the database can be loaded as

```
import pandas
df = pandas.read_json('database.json')
```

The rows of this database are the individual calculations and the columns are various properties of the calculations. The rows are labeled by an integer index. In the json file each calculation is grouped together by the index.

The columns are:

- **formula** - The chemical formula.
- **id** - the Materials Project id
- **X** - This is a nested array containing the full calculation of the conductivity and the AHE for the 250x250x250 k-mesh. In python the array can be transformed to a numpy array:

```
import numpy as np
X_np = np.array(X)
```

The first dimension of the array corresponds to the type of response: 0 is the ordinary conductivity, 1 is the AHE. The second dimension corresponds to the Γ value (0 is the lowest Γ value, 4 the largest) and the last 2 dimensions give the response tensor. Thus when using the numpy array one can obtain for example the AHE response tensor σ_{ij}^{AHE} for $\Gamma = 1$ meV as $X_{\text{np}}[1,2,:,:]$.

- **h** - The Hall vector given in the global coordinate system for $\Gamma = 0.1$ meV in the units of S/cm.
- **norm_h** - The magnitude of the Hall vector.
- **Hall_angle** - The Hall angle
- **magnetic_moments** - The magnetic moments for all atoms in the primitive unit cell.
- **spacegroup** - The non-magnetic spacegroup number.
- **fplo_spacegroup** - This is the spacegroup used for the fplo calculation. It is a non-magnetic spacegroup, which is obtained by setting all atoms with distinct magnetic moments to chemically non-equivalent atoms.
- **n_ms** - Number of mirror symmetries in the non-magnetic spacegroup.
- **n_syms** - Total number of symmetries in the non-magnetic spacegroup.
- **total_magnetization** - The magnetic moment density, i.e., the total magnetic moment divided by the unit cell volume.

- **average_magnetization** - The sum of absolute magnetic moments for each atom divided by the unit cell volume.
- **V** - The primitive unit cell volume.
- **maxZ** - The largest atomic number of the material.
- **error_wanband** - The median relative error between the bands obtained from the DFT Hamiltonian and the Wannier Hamiltonian.
- **gamma_convergence** - The Γ convergence is the relative difference between the xy component of AHE for $\Gamma = 0.1$ meV and $\Gamma = 0.5$ meV. This is an estimate of how close is the lowest Γ AHE to the intrinsic value.
- **k_convergence** - The convergence in the number of k-points for the linear response calculation defined as the relative difference between calculations using $250 \times 250 \times 250$ and $125 \times 125 \times 125$ k-meshes for $\Gamma = 0.1$ meV and the xy component of AHE.
- **cond_xx** - The xx component of the conductivity for $\Gamma = 10$ meV and $250 \times 250 \times 250$ k-mesh.
- **structure_conv** - The structure in the conventional Bravais lattice system, exactly how it is used in the input to the FPLO. This defined the orientation of the structure with respect to the global coordinate system. This is given as a dictionary, which is human readable and can be directly loaded into pymatgen:

```
from pymatgen.core import Structure
struct = Structure.from_dict(struct_dict)
```

The structure also includes the magnetic moments (given in the global coordinate system).

- **structure_prim** - Same as `structure_conv`, but for the primitive unit cell.
- **kubo_formula** - This denotes which Kubo formula was used for the calculation of AHE. 1 denotes Eq. (2), 2 denotes the alternative Kubo formula that was used in case there were issues with formula 1. Vast majority of calculations use formula 1.

II. ROTATIONS DATABASE DESCRIPTION

The database 'database_rotations.json' contains the results for the materials for which the magnetization rotation was studied. The database contains columns 'formula', 'id' and 'spacegroup' which have the same meaning as in the main database. In addition, it contains the column 'symmetry_type', which gives the symmetry type as given in the main text. Each row contains results for the magnetization rotation for one material. We have considered 5 magnetization directions defined as

$$[0, \cos(\varphi), \sin(\varphi)], \quad \varphi = 0, \frac{\pi}{8}, \frac{\pi}{4}, \frac{3\pi}{8}, \frac{\pi}{2}. \quad (1)$$

The Hall vectors for these magnetization directions are given in columns q0 - q4. These are values for $\Gamma = 0.1$ meV and $250 \times 250 \times 250$ k-mesh. In column 'magnetic_moments' we give the magnetic moments for all magnetization directions. The first dimension of this array is the magnetization direction and the second are the magnetic moments for all atoms in the unit cell.