BoltzTraP2: A program for interpolating band structures and calculating semi-classical transport coefficients.

April 22, 2020

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3 BoltzTraP2

BoltzTraP2 is a modern implementation of the smoothed Fourier interpolation algorithm for electronic bands that formed the base of the original and widely used BoltzTraP code. One of the most typical uses of BoltzTraP is the calculation of thermoelectric transport coefficients as functions of temperature and chemical potential in the rigid-band picture. However, many other features are available, including 3D plots of Fermi surfaces based on the reconstructed bands. For more information, check out the BoltzTraP2 article.

4 Prerequisites

BoltzTraP2 is a Python module, with a small performance-critical portion written in C++ and Cython. BoltzTraP2's runtime requirements are **Python version 3.5 or**

higher, and the Python libraries NumPy, SciPy, matplotlib, spglib, NetCDF4 and ASE.

All of them can be easily obtained from the Python Package Index(PyPI), using tools such as pip. They may also be bundled with Python distributions aimed at scientists, like Anaconda, and with a number of Linux distributions. If pip is used to install BoltzTraP2, dependencies should be resolved automatically.

If available, BoltzTraP2 will also make use of pyFFTW (for faster Fourier transforms), colorama (to colorize some console output) and VTK (to generate 3D representations) . Those packages are not required, but they are recommended to be able to access the full functionality of BoltzTraP2.

Furthermore, compiling BoltzTraP2 from its sources requires a C++ compiler, and the development headers and libraries for Python. Cython is **not** required for a regular compilation.

5 Compiling and install BoltzTraP2

The easiest way to get BoltzTraP2 is to run:

```
pip3 install BoltzTraP2
```

This should take care of downloading and installing the dependencies as well.
Users installing from source must install the dependencies first and then run:

```
python setup.py install
```

from the source directory. For finer-grained control, please see the output of these commands:

```
python setup.py --help
python setup.py --help-commands
python setup.py install --help
```

The BoltzTraP2 installer supports

```
python setup.py develop
```

which install the module through a set of symbolic links to the source directory, allowing users to immediately tests the effects of their changes to the code.

6 Running the tests

BoltzTraP2 comes with a comprehensive set of unit and integration tests of its core functionality. To run those, install pytest (also available through pip), change to the source directory and use the command

```
pytest -v tests
```

7 Command lines help

```
btp2 -h
```

usage: btp2 [-h] [-v] [-n NWORKERS] [-V] command [options] ... ...

BoltzTraP2, a program for interpolating band structures and calculating semi- classical transport coefficients

optional arguments:

-h, –help show this help message and exit

-v, –verbose increase the verbosity level (default: 0)

-n NWORKERS, –nworkers NWORKERS number of processes to span for parallel operations (default: 1)

-V, –version print version information

available subcommands:

command [options] ...

interpolate	interpolate the DFT input and save the results
integrate	compute transport coefficients based on the interpolated bands
dope	compute transport coefficients for particular carrier concentrations
plotbands	create a plot of the interpolated band structure
plot	create a plot of the integration results
describe	provide basic information about a .bt2 or a .btj file
fermisurface	create an interactive visualization of the Fermi surface