

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

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## 1 Authors Copyright

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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:

```
1 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:

```
1 python setup.py install
```

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

```
1 python setup.py --help
2 python setup.py --help-commands
3 python setup.py install --help
```

The BoltzTraP2 installer supports

```
1 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

```
1 pytest -v tests
```

## 7 Command lines help

```
1 btp2 -h
```

**usage:** `bt2 [-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