HybriD^3 File Format Description: Band Structure

1 Overview

HybriD^3 is designed to include computationally predicted energy band structures $\varepsilon_n(\boldsymbol{k})$ (where n is the band index and $\boldsymbol{k}$ denotes the crystal momentum) for each compound included.

The level of theory should be appropriate for the quantitative computation of energy band structure. At a minimum, we require the HSE06 hybrid density functional. Additionally, spin-orbit coupling should be included in all submitted energy band structures. In order to upload electron band structures, we currently require the following two sets of input data:

1.1 Definition of the band structure path in reciprocal space

The absolute reciprocal-space locations of the $\boldsymbol{k}$-points chosen for the band structure require:

i. A file `geometry.in` that contains a definition of the real-space unit cell (which can be used to define the reciprocal-space unit cell). The format of the file `geometry.in` as currently supported by HybriD^3 can be found here.

ii. A file `control.in` that includes a definition of the $\boldsymbol{k}$-path segments chosen for each provided energy band, in units of the reciprocal-space lattice vectors. A typical file `control.in` defining 10 individual $\boldsymbol{k}$-path segments would look as follows:

```
...
output band  0.00000 0.00000 0.00000  0.50000 0.00000 0.50000   21 G X
output band  0.50000 0.00000 0.50000  0.50000 0.25000 0.75000   21 X W
output band  0.50000 0.25000 0.75000  0.37500 0.37500 0.75000   21 W K
output band  0.37500 0.37500 0.75000  0.00000 0.00000 0.00000   21 K G
output band  0.00000 0.00000 0.00000  0.50000 0.50000 0.50000   21 G L
output band  0.50000 0.50000 0.50000  0.62500 0.25000 0.62500   21 L U
output band  0.62500 0.25000 0.62500  0.50000 0.25000 0.75000   21 U W
output band  0.50000 0.25000 0.75000  0.50000 0.50000 0.50000   21 W L
output band  0.50000 0.50000 0.50000  0.37500 0.37500 0.75000   21 L K
output band  0.62500 0.25000 0.62500  0.50000 0.00000 0.50000   21 U X
...
```

All other lines in `control.in` will simply be ignored.

Each line beginning with `output band` specifies a linear segment in $\boldsymbol{k}$-space.

The first group of three numbers indicates the starting point of the $\boldsymbol{k}$-space segment in fractional coordinates of the reciprocal-space unit vectors.

The second group of three numbers indicates the end point of the $\boldsymbol{k}$-space segment in fractional coordinates of the reciprocal-space unit vectors.

1.2 Files including the energy band structure corresponding to each k-path segment defined in `control.in`

For each $\boldsymbol{k}$-space segment defined in `control.in`, we require a separate file `bandxxxx.out` that contains the actual energy band structure information, where `xxxx` is a placeholder for four separate integer numbers. The actual files are thus called `band1001.out`, `band1002.out`, and so on.

The initial number `1` denotes the spin channel. In the case of spin-polarized systems, a second set of files `band2001.out`, `band2002.out`, etc. might be required for the spin-down channel. In spin-orbit coupled band structures as required in HybriD^3, however, spin is no longer a good quantum number and thus, only the initial number `1` is supported in HybriD^3.

The following three numbers can run from `001` to `999` and denote the ordering of the `output band` lines in `control.in`.

2 Format of a `bandxxxx.out` file

A `band1xxx.out` file might look like this:

```
...
1 0.0000000 0.0000000 0.0000000 1.00000 -97689.70082 1.00000 -97689.70082...
2 0.0250000 0.0000000 0.0250000 1.00000 -97689.70082 1.00000 -97689.70082...
...
```

Each row represents a $\boldsymbol{k}$-point. The first four columns represent the $\boldsymbol{k}$-point number and its reciprocal-space coordinates in units of the reciprocal-space lattice vectors, respectively.

Each following pair of two columns represent the electron occupancy number $f_n(\boldsymbol{k})$ and the energy level $\varepsilon_n(\boldsymbol{k})$. The first pair of numbers corresponds to band n=1, the second pair of numbers corresponds to pair n=2, and so on, in a single long line for each $\boldsymbol{k}$-point.