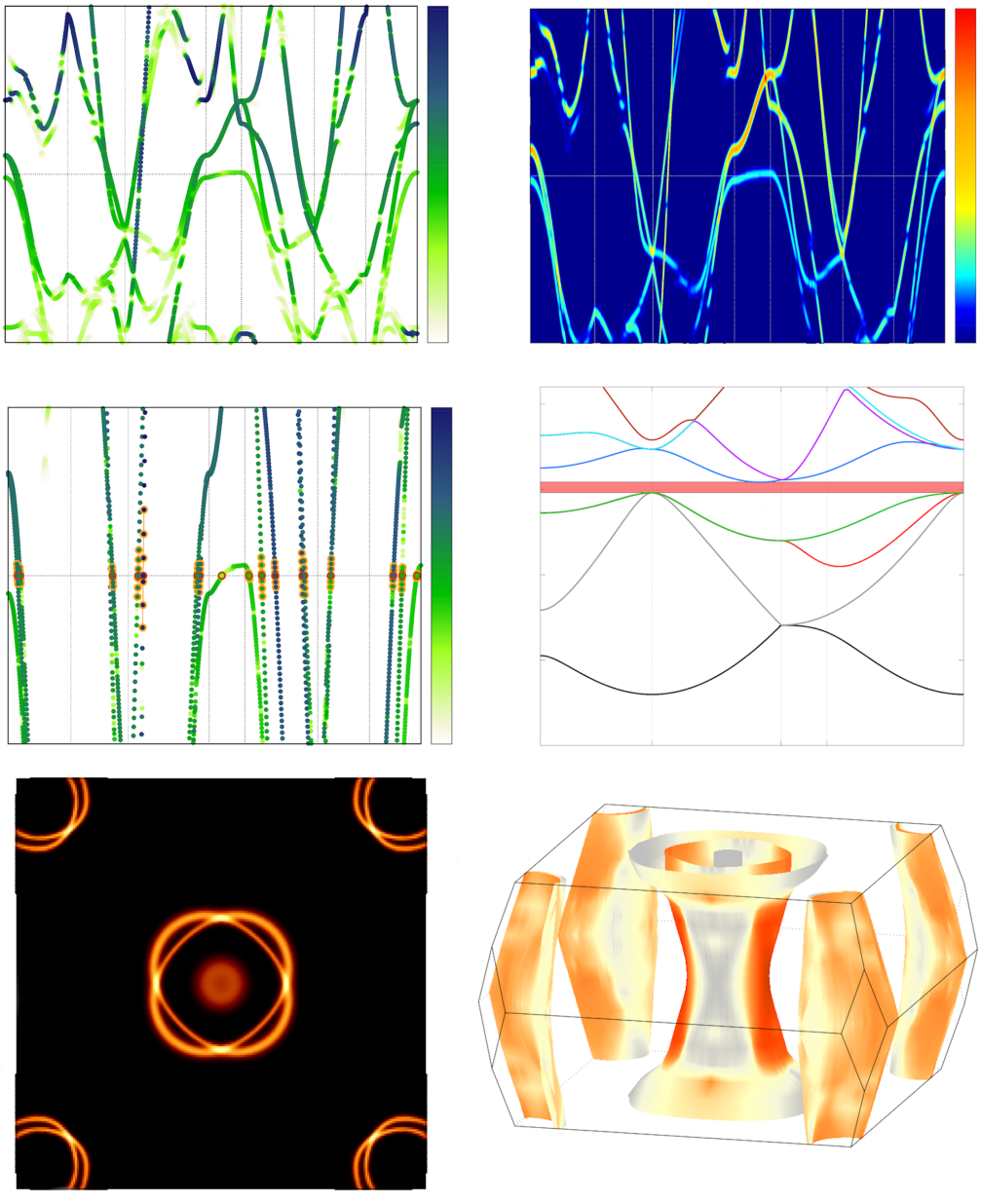
Manual for the **bands4vasp** post-processing package

May 31, 2021



Contents

1 About bands4vasp

The bands4vasp post-processing package is exclusively build for the analysis and visualisation of band structure and especially unfolding calculations from VASP. Bands4vasp is visualizing the band structure or the effective band structure (EBS) of static calculations, it can calculate the spectral function of this band structure or of the associated Fermi surface. Bands4vasp can also visualize the nlm- and site projected wave function character of each orbital and it provides a plot with the bandindex colour-coded band structure. But the core part of bands4vasp is an algorithm which automatically determines the Fermi vectors of the calculated structure. Because of the huge variety of band structures, this algorithm doesn't find allways all Fermi vectors on the first run. For such cases bands4vasp provides several parameters which helps to identify all bands and facilitate thereby the calculation of all Fermi vectors. There is a Fermi surface mode, which automatically project this Fermi vectors onto the surface, where the VASP calculations were done. There are also some pre-processing routines, for preparing the VASP files for this kind of Fermi surface calculation. Bands4vasp is written in FORTRAN, it uses Gnuplot for the visualisation and a Bash-environment brings all together.

2 The Algorithm

First bands4vasp reads in all data inbetween a given energy interval and a Bloch character (if present) bigger than the given threshold. These values can be defined in the INPAR file (see section INPAR - The bands4vasp input file). The next step is to evaluate the spectral function (1) and write it in *banddata.specfun.dat*, if **SPECFUN** is activated in INPAR.

$$A(\boldsymbol{k}, E) = \sum_m P_{\boldsymbol{K}m}(\boldsymbol{k})\delta(E_m - E) \tag{1}$$

If this is done, it compresses the data depending on the given parameters in the INPAR file. For a specific state n with the energy E_n the algorythm picks all states inbetween the energy interval $[E_n - EDIF; E_n + EDIF]$ and they will be compressed to a new weighted averaged state (2), than the procedure starts again with the next energy state. Let $\{E\}_{i=1,\ldots,d}$ be a set of energy states inbetween the interval $[E_1 - EDIF; E_1 + EDIF]$.

$$\tilde{E} = \frac{\sum_i P_i \cdot E_i}{\sum_i P_i} \tag{2}$$

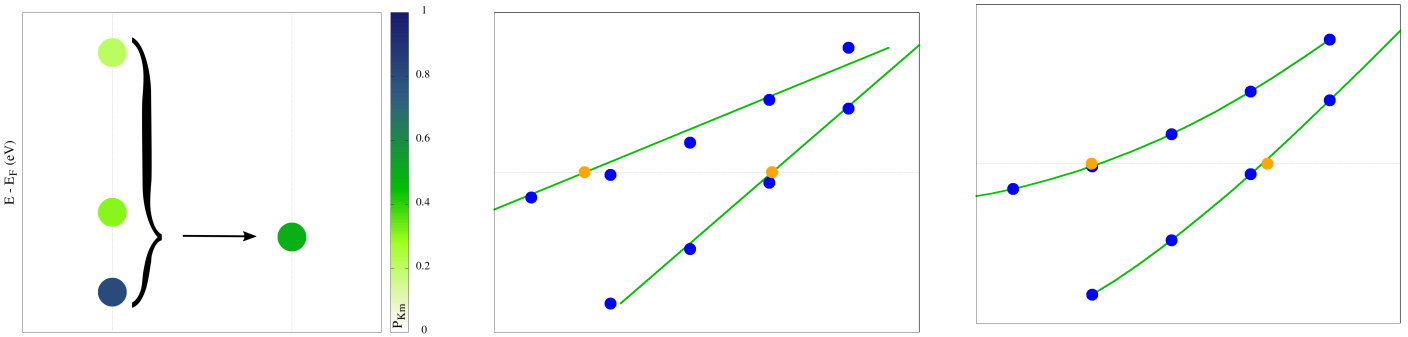
Where $\tilde{E}$ is the weighted averaged energy of the band center of mass, E_i is the energy and P_i the Bloch character of state i. Also the orbital- and Bloch character have to be weighted with the following relations:

$$\tilde{P} = \frac{\sum_i P_i(E_\Delta - \mid \tilde{E} - E_i \mid)}{\sum_i (E_\Delta - \mid \tilde{E} - E_i \mid)} \tag{3}$$

$$\tilde{Oc} = \frac{\sum_i Oc_i(E_\Delta - \mid \tilde{E} - E_i \mid)}{\sum_i (E_\Delta - \mid \tilde{E} - E_i \mid)} \tag{4}$$

$$E_\Delta = max(\{E\}_i) - min(\{E\}_i) \tag{5}$$

Here E_Δ is the maximal energy interval of all the energy states which will be compressed to one band center of mass. These compression of the eigenstates is schematically shown in the sketch 1a).
At this point bands4vasp writes the raw data and as well the processed data in the files:
Bandstructure, *EBSbloch*, *EBSorbit*, and *Bandindexplot*.
If **ROOTSCALC** is set to true (default), bands4vasp scans the bands for roots, which are associated with Fermi vectors. To find the Fermi roots there are many different parameters to distinguish the bands and indentify the states which belong to the same band. How to use these paramters is described in section 3.3. Once it founds a band crossing the Fermi level, the intersection point is either calculated with linear regression (**LPOLY**=.FALSE.) or with polynomial interpolation (**LPOLY**=.TRUE.) and the regula falsi method. The linear regression yield to reliable results for localy straight bands and the roots can be calculated exactly with an analytical algorithm [see figure 1 b)]. The polynomial interpolation is a good choice, if the bands are very sinuous around Fermi. The degree of the polynomial is given by the number of points which are included in the calculation $\Rightarrow\ 2 \cdot NPOINTS - 1$. If you set for example **NPOINTS**=3, there will be 3 points on each side of Fermi level or 6 in total. This will lead



a) weighted average of the eigenstates **b)** roots calculation with linear regression **c)** roots calculation with polynomial interpolation and the regula falsi method

Figure 1: Schematic representations of the methods used for the automatic calculation of the Fermi vector

to a polynomial of degree 5. To calculate the roots, bands4vasp uses the regula falsi method [see figure 1 c)]. This is in comparison to the exact analytical solution of the linear regression a disadvantage. Nevertheless it always depends on the shape of the bands and the number of included points near the Fermi level, which method is the best choice, but the most reliable method is the linear regression with a small amount of considered points and therefore it is the default method. The orbital- and Bloch characters are averaged with the same principle as discribed for the compression [see Eq. (2),(3),(4)]. These calculated Fermi roots are transformed to a 3-dimensional Fermi vector and written in the *FERMIROOTS.dat* file.

Bands4vasp comes with the possibility for an automatic determination of the Fermi surface. If Fermi surface mode is activated with −−fermi option , it will first figure out the orthonormal basis vectors of the surface, where the calcualations were done. The basis set is used for the transformation of the Fermi vectors into terms of the surface. Now it checks if the points of symmetry (**SYMPOINT1**/**SYMPOINT2**) are defined in INPAR and are part of that surface. After all coordinates are transformed into terms of the surface and reflected, if the point(s) of symmetry are set, all data are written in the file *Fermisurface.dat* and as well the data of the Fermi surface spectral function in the file *Fermisurface.specfun.dat*, if activated.
In the case that no Fermi roots were found, bands4vasp calculates the energy gap around the Fermi level. This is done by taking the energy distance from the lowest energy over the Fermi level to the highest energy under Fermi. In that case the files *Fermisurface.dat* and *Fermisurface.specfun.dat* and as well the *Fermisurface** image are not created.

3 In- and output files

3.1 VASP-files (input)

There are 3 typs of files bands4vasp is able to read:

- The **PRJCAR** file for unfolding calculations in VASP.
- The **PROCAR** file for nlm- and site projected wave function character of each eigenvalue.
- The **PROCAR.prim** file, analogous to PROCAR, but for unfolding calculations.

Additionally bands4vasp needs the Fermi energy and the lattice of the structure. The Fermi energy can be defined either in the INPAR file or extract from a OUTCAR file. For unfolding calculations the lattice is extracted from PRJCAR file. If it is not an unfolding calculation the lattice will extracted from the POSCAR file.

3.2 bands4vasp output files

Bands4vasp provides a lot of different information, which are derived from VASP files.

Datafiles - The datafiles are stored in './bands4vasp_data/', except *FERMIROOTS.dat*.

- *FERMIROOTS.dat* contains all information of the evaluated Fermi vectors and some calculation specific information. This file is stored in the execution directory.
- *banddata.dat* contains the raw data of the whole band structure.
- *banddata.slim.dat* contains the processed data of the band structure.
- *banddata.specfun.dat* contains all information of the spectral function from the band structure.
- *Fermisurface.dat* contains all information of the evaluated Fermi surface.
- *Fermisurface.spec.dat* contains all information of the evaluated Fermi surface spectral function.
- *autognuplot_bands4vasp.gnu* is the gnuplot file for generating all images.

Images - The images are stored in './bands4vasp_img/', except the image of interest.

- *Bandsturcture.** shows the bands inbetween the energy interval defined by **EDELTA1**.
- *EBSbloch.** shows the bands inbetween the energy interval defined by **EDELTA1**/**EDELTA2** with respect to Bloch character.
- *EBSorbit.** shows the bands inbetween the energy interval defined by **EDELTA1** with respect to orbital character and if present a variable pointsize proportional to the Bloch character.
- *Bandstructure.spec./EBSbloch.spec.* shows the spectral function inbetween the energy interval defined by **EDELTA1** with respect to Bloch character.
- *Bandindexplot* shows the bandstructure with colour-coded bandindex occuring in the VASP files.
- *Fermisurface.spec.* shows the Fermi surface spectral function.
- *Fermisurface* shows the derived Fermi surface from the Fermi vectors.
- *Fermisurface_bloch* shows the derived Fermi surface with the calculated avaraged Bloch characters.
- *Fermisurface_orbit* shows the derived Fermi surface with the calculated avaraged orbital characters.

For spin polarized calculations the extansion .spin1. and .spin2. are added to the filenames.

**These images have also a processed version including technical details (for example, the interpolation calculated to determine the Fermi wave vectors). This is indicated by the extension .processed.*

3.3 INPAR - The bands4vasp input file

bands4vasp can be controlled by a variety of parameters, these parameters need to be stored in a file called INPAR. If you run bands4vasp and no INPAR file is present in the execution directory, bands4vasp will take the default values. The INPAR file with the default values is stored in the installation directory of bands4vasp. For a better overview of the parameters which are used for the calculation, bands4vasp prints them in the OUTPAR file in the execution directory. Some parameters have only an effect, if a specific VASP filetype was chosen. This will be shown by the following 3 signs:

- • for PRJCAR files
- ◦ for PROCAR files
- ⊙ for PROCAR.prim files

General control parameters

- • ◦ ⊙ **EFERMI** - sets the source for the Fermi energy, default is from ./OUTCAR. It is possible to set a directory which includes the OUTCAR file (e.g. /home/calculation/), to set the Fermi energy explicitly (e.g. 0.4), or by setting the keyword 'bands' to take the Fermi energy from the OUTCAR files of each banddata respectively.

- • ◦ ⊙ **EDELTA1** - energy interval for the raw data plots *EBSbloch*, *EBSorbit*, *EBSbloch.spec*, *Bandstructure.spec* and *Bandindexplot*. If one value is given, the interval will be symmetric around the Fermi level, or one can set the two values individually seperated by a blank.

- • ◦ ⊙ **EDELTA2** - energy interval for the processed images, with the same functionality as EDELTA1, with the different that only energy states in this interval are taken account for calculating the Fermi vectors.

- •⊙ **EDIF** - Energy diffusion from the unfolding calculation. EDIF defines the maximal energy difference for one k-point, inbetween this interval all energy states will merged and represented in the processed data as one state, as explained in section 2.

- • ◦ ⊙ **EGAP** - defines the maximal energy difference of energy states from proximate k-points. Proximate energy states with a energy difference less than this value are considered to belong to the same band. This is used for the Fermi vector calculation.

- •⊙ **BAVERAGE** - If BAVERAGE is set to .TRUE. the weighted average of the Bloch character is calculated and represented in the processed data, else the values will summed up.

- ◦⊙ **OAVERAGE** - If OAVERAGE is set to .TRUE. the weighted average of the orbital character is calculated and represented in the processed data, else the values were summed up.

- •⊙ **BLOCH_THRESHOLD** - sets the minimal Bloch character value. Energy states with a Bloch character less than BLOCH_THRESHOLD will rejected. For unfolding calculations it is recommended to set it to a small value.

- •⊙ **DBLOCH** - defines the maximal Bloch character difference for proximate energy states to belong to the same band. This is used for the Fermi vector calculation.

- ◦⊙ **ODISTINCT** - defines the maximal orbital character difference for proximate energy states of each orbital to belong to the same band. This is used for the Fermi vector calculation.

- • ◦ ⊙ **GRADIENTD** - sets the maximal gradient deviation.

- • ◦ ⊙ **NPOINTS** - defines the number of energy states above and below the Fermi level, which will be included in the Fermi vector calculation.

- • ◦ ⊙ **LPOLY** - If LPOLY is set to .TRUE. a polynomial interpolation with the degree 2·NPOINTS will be used for calculating the Fermi vector. If it is set to .FALSE. (default), the coordinates of the Fermi vectors are calculated by linear regression.

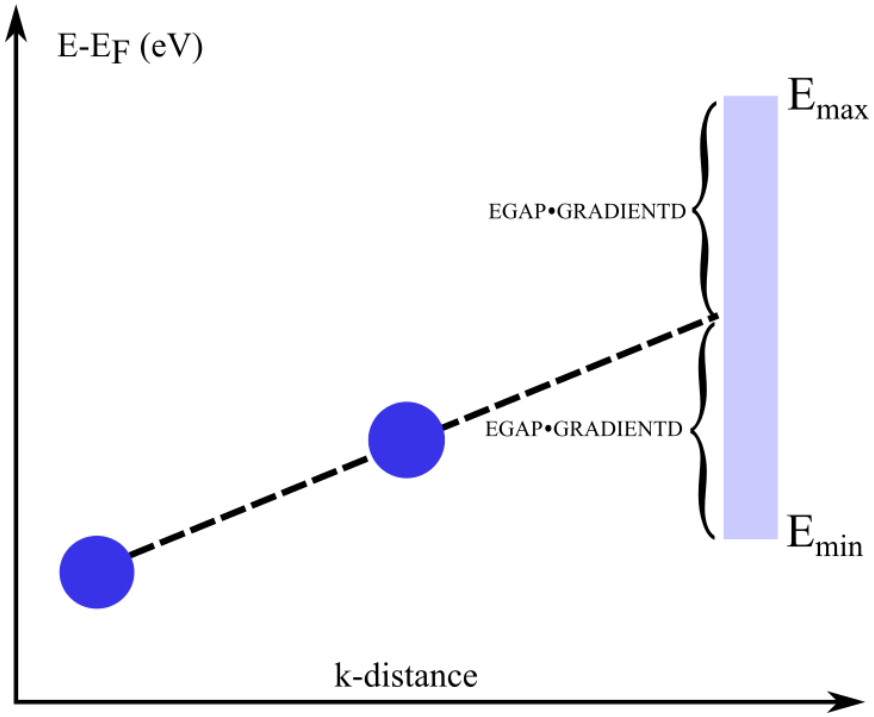


Figure 2: Sketch for demonstration of the meaning from **GRADIENTD**

• ○ ⊙ **REGULAPREC** - sets the accuracy for the Regula falsi method, which is used for the polynomial interpolation.

○⊙ **PLOTORB** - sets the orbital number for the orbital plots in order of appearence in PROCAR[.prim] file. If it's set to 0 (default) all orbitals will be considerd and visualized in *EBSorbit_ALL*. For any negative value bands4vasp calculates the total amount of all orbitals (*EBSorbit_tot*).

• ○ ⊙ **BNDDIFF** - If BNDDIFF is set to .TRUE. (default) bands4vasp considers bandcrossing from bands with different bandindices for the Fermi vector calculations. If set to .FALSE., only bands with the same bandindex are considered as one band. In most of the cases it is the best to set it .TRUE. for unfolded bands and .FALSE. for non-unfolded bands, but one can always take a look at the Bandindexplot to be sure.

• **KAPPANORM** - If KAPPANORM is set to .TRUE. the Bloch character for each band and K-point from the super cell will be normalized respectively. This works only with PRJCAR files.

○⊙ **SELECTION** - select a specific ion and the associated orbital characters in order of appearence in PROCAR[.prim] file. By giving two numbers seperated by a minus 'n-m', bands4vasp will take ion n up to m and sum the orbital characters together. If the value is 0 (default) all ions are considered.

• ○ ⊙ **SKIPKPOINT** - if SKIPKPOINT is set to one integer n, the first n k-points will be ignored. By setting two numbers seperated by a minus 'n-m', bands4vasp will ignore k-points n up to m.

• ○ ⊙ **ROOTSCALC** - if ROOTSCALC is set to .FALSE. no Fermi vectors will be calculated.

The following parameters are for ALL filetypes.

Fermisurface

The parameters in the following section are only considered if a fermisurface calculation is done, by passing the option −−fermi (see also section 4.2).

▷ **SYMPOINT1/SYMPOINT2** - These are the symmetry points for the resulting *Fermisurface** plots. If *SYMPOINT1* is set to a 3d-vector, where the values have to be seperated by one space

("SYMPOINT1 = 0.0 0.0 0.0"), the calculated Fermi vectors will be copied to the rotaded positions at rotation angles $[90°; 180°; 270°]$. If *SYMPOINT2* is set to a vector as well, the Fermi vectors will axial reflected with the mirror axis defined by *SYMPOINT1* and *SYMPOINT2*. The symmetry points will only be accept, if they are on the Fermi surface.

- ▷ **SYMREC** - if SYMREC is set to .TRUE., the coordinates for SYMPOINT1 and SYMPOINT2 are treated in reciprocal coordinates (default). If SYMREC is set to .FALSE., bands4vasp consideres cartesion coordinates.
- ▷ **FSURCART** - if FSURCART is set to .TRUE., the cartesian distances of the surface are shown in the images, else it will show the k-vectors (default).
- ▷ **FGRID** -An integer value gives the density of a grid for the Fermi surface plots. If set to 0 (default) no grid will be shown.

Spectral function

- ▷ **SPECFUN** - if SPECFUN is set to .TRUE., the spectral function of the bandstructure/fermisurface is calculated and visualized (default = .FALSE.).
- ▷ **SIGMA** - sets the smearing of the deltafunction, which is used for the spectral function (see equation 1).
- ▷ **SPECDELTA** - The smaller this value (in eV), the higher is the number of energy states of a k-point included in the evaluation of the spectral function. Hence a smaller value results in a higher resolution, more computing time and larger **.specfun** files (see section 3.2).
- ▷ **SLIMSPEC** - if SLIMSPEC is set to .TRUE., only data with a Bloch character greater than 0 will be written without an interpolation.

Plot specific otpions

- ▷ **MAKEPLOTS** - if MAKEPLOTS is set to .FALSE. no plots will be created.
- ▷ **FILEFORMAT** - bands4vasp supports a choice of different file format of the plots. Possible formats are: png, pngcairo, pdf, eps (default).
- ▷ **BANDINDEXPLOT** - if set to .TRUE. the Bandindexplot will be created (see section 3.2).
- ▷ **LEAVEPLOTDATA** - if set to .FALSE. the directory './bands4vasp_data/' will be removed after bands4vasp is finished.

Visual parameters

- ▷ **PATHPOINTS** -sets the letters for each pathpoint seperated by a blank. A '/' infrot of a letter print the greek letter. For example PATHPOINTS=/G M X Y
- ▷ **LFITPOINTS** - if set to .TRUE. the fitpoints from the linear regression/polynomial interpolation are shown in the plots. By default they are only shown in the processed versions of the plots.
- ▷ **LLINES** - if set to .TRUE. the graph from the linear regression/polynomial interpolation are shown in the plots. By default they are only shown in the processed versions of the plots.
- ▷ **LROOTS** - if set to .TRUE. the Fermi roots from the linear regression/polynomial interpolation are shown in the plots. By default they are only shown in the processed versions of the plots. If there are no Fermi roots found, the energy interval of the band gap is show in the plots, only if LROOTS is not set to .FALSE..

▷ **PSFAC** - this factor changes the pointssize in the plots.
⇒ $pointsize = original\_pointsize \times PSFAC$

▷ **BCOLOURS** - is defined by two gnuplot colors seperated by a blank. The colors define the color palette for the Bloch plots. For a list of all accesable colornames open the terminal and enter:
$gnuplot -e 'show palette colornames'

▷ **OCOLOURS** - same as BCOLOURS, but for the orbital plots.

▷ **BACKCOLOUR** - sets the background color of all plots, except the spectral function plots.

4 Getting Started

For the installation *bands4vasp_v< version >.tar.gz* and *install.sh* are needed and can be downloaded here. The installation starts with an execution of the *install.sh* file.

```
$ source ./install.sh
```

4.1 Usage

```
$ b4vasp [OPTION] ... [file]
```

To start a calculation there have to be the following files:

- PROCAR.prim, PROCAR or PRJCAR :: For the data of the bandstructure.
- PRJCAR or POSCAR :: For the information of the lattice. When analysing unfolding calculations it is necessary to have at least one PRJCAR file.
- OUTCAR :: If the Fermi energy is not given in the INPAR file, bands4vasp takes it from OUTCAR.

There are 3 different ways of using bands4vasp:

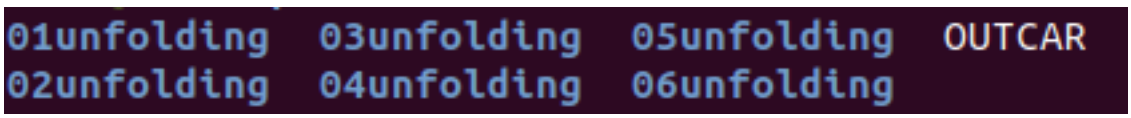
- **Single path** calculations can be done in the directory of the VASP files by entering the command 'b4vasp',

  ```
  $ cd [folder-path]
  $ b4vasp
  ```

  or one can pass the directory.

  ```
  $ b4vasp [folder-path]
  ```

- **Multi path** calculations are possible if there are numbered folders including the VASP files from the band calculation. To pass this kind of structure a %-sign represents the number in the foldername.


  ```
  $ b4vasp %unfolding
  ```

  This will pass all directories with numbers from 1-1000 (also with leading zeros) and the name 'unfolding' $\Rightarrow$ $1unfolding$, $01unfolding$, $001unfolding$, $2unfolding$, ...

- **Fermisurface** calculations need the same structure as the multi path calculations and additionally with option flag –fermi.

  ```
  $ b4vasp --fermi %unfolding
  ```

  To get a reasonable result, the line calculations performed with VASP need to be on one plane, but the geometrical arrangement of the lines is not important.

4.2 Options

Beside the −−fermi option is also the option -rs [−−readsave]. The -rs option reads the raw data obtained from a previous execution of bands4vasp (avoiding to read VASP files, which could be time consuming), thus, it is useful for testing, visualization purposes and adjustment of the parameters to get all Fermi vectors. It can be used in the following way:

- First run a calculation in the normal mode.

```
$ b4vasp %unfolding
```

- Now one can modify the INPAR file and run the calculation again, but this time without a path specification, with the optional –fermi option and the option -rs.

```
$ b4vasp −−fermi -rs
```

CAUTION: There are some parameter, which can not be reset in the −−readsave mode. EDELTA1 and EDELTA2 can only set to intervals which are included in the original EDELTA1 interval. SKIPKPOINT, SELECTION, EFERMI, KAPPANORM and BLOCH_THRESHOLD don't have any influence on the −−readsave mode.

There aro also some pre-processing options available. For all the following pre-processing procedures there has to be a folder, which includes all files for the VASP calculation. The section in the KPOINTS file, where one specifies the coordinates of the k-points, is replaced by the flag '#makepath', followed by coordinates depending on the type of sampling. The entries above the '#makepath' flag are copied in every KPOINTS file followed by the calcuclated coordinates. A KPOINTS file for a radial sampling with the first line from center (0, 0, 0) to (0.5, 0, 0) and the last line from (0, 0, 0) to (0, 0.5, 0) in reciprocal coordinates is shown below:

```
automatic radial sampling of k-points
100
p
line
rec
#makepath
0 0 0
0.5 0 0
0 0.5 0
```

More information about unfolding method with vasp or the KPOINTS file can be found on the vasp wiki page. There are 3 typs of sampling methods:

- **−−pre-lines $1 $2** :: prepares a structure of line calculations for each pair of k-points in KPOINTS file after the flag '#makepath'. The following two informations need to be passed:
  $1 ⇒ The directory for the prepared VASP files $2 ⇒ The name for the new created multi-directory

- **−−pre-circles $1 $2 $3** :: prepares radial centered sampling. The specification of the radial sampling is done by three coordinates defined in the KPOINTS file, after the flag '#makepath': The first coordinate is the center of the circle. The second coordinate defines the first line of the sampling, starting from the center. The third coordinate defines the last line of the sampling. The sampling is done in a mathematical positiv sense. The following 3 informations need to be passed:
  $1 ⇒ directory for the prepared VASP files $2 ⇒ number of equidistant points on the circle $3 ⇒ name of the new created multidirectory

- $--$**pre-surface $1 $2 $3** :: prepares a equidistant sampling within a rectangle defined by the coordinates given in the KPOINTS file after the flag '#makepath': The first coordinate is the corner of the rectangle where the calculation starts. The second coordinate defines with the first one, the direction and the length of the line calculations. With the third coordinate the rectangle is defined and as well the translation direction of the line sampling. The following 3 informations need to be passed:
  $1 ⇒ directory for the prepared VASP files $2 ⇒ number of equidistant lines on the surface $3 ⇒ name of the new created multidirectory

With the options $--help$ and $--info$ the most important informations about bands4vasp is printed.