Tutorial for KPROJ

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Procedures for doing band unfolding

Step 1: Do a standard VASP SCF calculation to get CHGCAR.

Step 2: Do a band calculation to get WAVECAR.

- The k-points in file KPOINTS now may be different from those we usually used for the supercell.
- If your system is large, you may split the band calculation into multiple calculations (see user_guide and examples defected_graphene and Ge_Al2O3).

Step 3: Do a ***KPROJ*** calculation.

- File INKPROJ is needed.
- For interfaces, you may set proper values for LZLAYER, zlay1, zlay2. For bulk, you can comment out LZLAYER, LXLAYER, LYLAYER.

Step 4: Preparing for plotting.

- Set the right E-fermi in the output file bs_projected.dat.
- If you have multiple bs_projected.dat for a large system, please merge them into one first (see user_guide).
- Run **futil** or the script **run_futil** to put the data on a grid for plotting.
- **futil** can be obtained by "make futil" under src.
- **run_futil** is script under the directory **utils**. Please copy it to your working directory.

Step 5: Do the plotting.

Regarding Step 2:
How to set the k-points for band unfolding?

- Using the transformation matrix between the primitive cell and the supercell

Basis vectors for the supercell $\begin{pmatrix} A_1 \\ A_2 \\ A_3 \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} & S_{13} \\ S_{21} & S_{22} & S_{23} \\ S_{31} & S_{23} & S_{33} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}$ Basis vectors for the primitive cell

- In reciprocal space

$$\begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} = S^T \begin{pmatrix} B_1 \\ B_2 \\ B_3 \end{pmatrix}$$

primitive cell supercell

S^T is the transpose of the matrix S

- Do a transformation for the k-points. Remember that we are trying to get the unfolded band structure for the primitive cell. So the k-points used for the band structure should be those in the BZ of the primitive cell. If these k-points are given in the direct coordinates (in the basis $\boldsymbol{b}_i$). We need to write them in the reciprocal basis of the supercell, i.e., $\boldsymbol{B}_i$.

$$\mathbf{(k'_x, k'_y, k'_z) = (k_x, k_y, k_z)S^T}$$

- Use (k'_x, k'_y, k'_z) for Step 2

Examples for getting the k-points

- Graphene in 5 x 5 supercell

$$S = \begin{matrix} 5 & 0 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 1 \end{matrix}$$

S^T: transpose of S

The *K* point in the 1st BZ of the primitive cell may be (1/3, 1/3, 0), which is in the reciprocal basis vectors of the primitive cell, i.e., $\boldsymbol{b}_i$.

We need to write it in the reciprocal basis vectors of the supercell, i.e., $\boldsymbol{B}_i$.

$$(k'_x, k'_y, k'_z) = (k_x, k_y, k_z)S^T = (5/3, 5/3, 0)$$

For the *M* point (0, 0.5, 0), it is (0, 2.5, 0)

KPOINTS direct coordinates

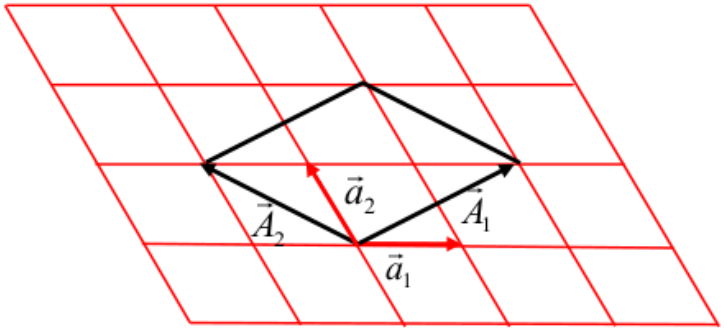
```
0.00000000000000 2.50000000000000 0.00000000000000 1   M
0.00000000000000 0.00000000000000 0.00000000000000 1   Γ

0.00000000000000 0.00000000000000 0.00000000000000 1   Γ
1.66666666666667 1.66666666666667 0.00000000000000 1   K
```

√3 x √3 supercell of graphene

- The **transform matrix *S*** between the primitive cell and supercell:

$$\begin{pmatrix} \vec{A}_1 \\ \vec{A}_2 \\ \vec{A}_3 \end{pmatrix} = \begin{pmatrix} 2 & 1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \vec{a}_1 \\ \vec{a}_2 \\ \vec{a}_3 \end{pmatrix}$$



- High symmetry points for KPOINTS for the band unfolding:

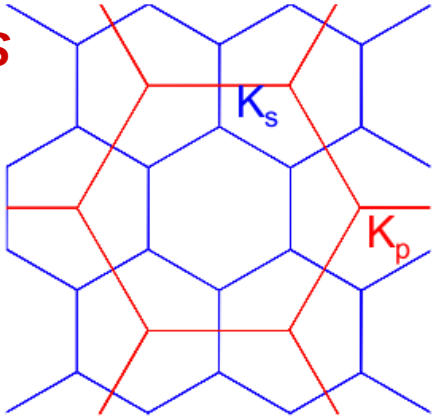
$(k'_x, k'_y, k'_z) = (k_x, k_y, k_z)\mathbf{S}^T$ ← **transpose of *S***

M: (0.5, 0.5, 0)
Γ: (0, 0, 0)
K: (1, 0, 0)

M: (0, 0.5, 0)
Γ: (0, 0, 0)
K: (1/3, 1/3, 0)

↓

File KPOINTS

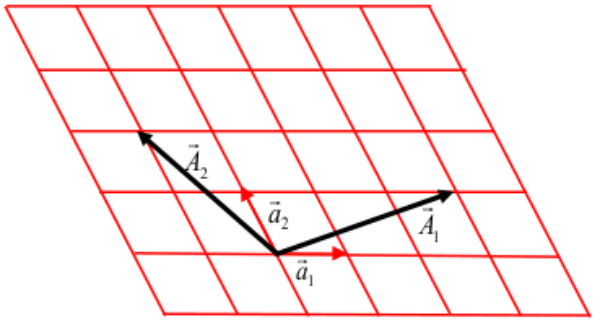


Brilloin zones

√7 x √7 supercell of graphene

- The **transform matrix *S*** between the primitive cell and supercell:

$$\begin{pmatrix} \vec{A}_1 \\ \vec{A}_2 \\ \vec{A}_3 \end{pmatrix} = \begin{pmatrix} 3 & 1 & 0 \\ -1 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \vec{a}_1 \\ \vec{a}_2 \\ \vec{a}_3 \end{pmatrix}$$



- High symmetry points for KPOINTS for the band unfolding:

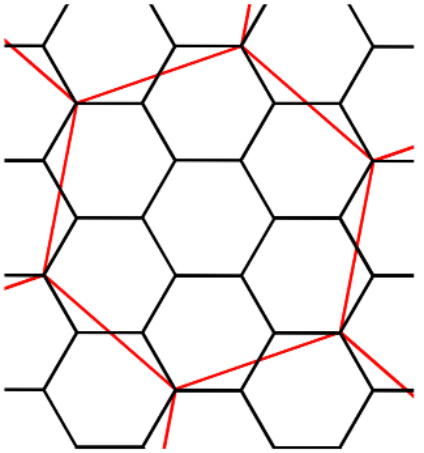
$(k'_x, k'_y, k'_z) = (k_x, k_y, k_z)S^T$ ← **transpose of *S***

M: (0.5, 1.0, 0)
Γ: (0, 0, 0)
K: (4/3, 1/3, 0)

M: (0, 0.5, 0)
Γ: (0, 0, 0)
K: (1/3, 1/3, 0)

↓

File KPOINTS



Brilloin zones

- For large systems, please read user_guide for more details regarding setting up KPOINTS.

Step 3: KPROJ calculation

Files used by KPROJ

INKRPOJ	in	input parameters
WAVECAR	in	the wavefunctions from vasp calculations
OUTKPROJ	out	general outputs
bs_projected.dat	out	weights from k-projection band unfolding, used for plotting

INKPROJ

```
! LZLAYER = .TRUE.
! zlay1  = 0.0
! zlay2  = 1.00

! LXLAYER = .TRUE.
! xlay1  = 0.0
! xlay2  = 1.00

LSORBIT = F

MAT_P2S= 2  1  0 \
        -1  1  0 \
         0  0  1
```

This example is for band unfolding for a √3 x √3 supercell of graphene, not for any heterostructure. So, layer projection is not needed. These settings can be safely commented out.
The same results can be obtained if we set LZLAYER =T and zlay1 = 0, zlay2 = 1 ..., which means integration over the whole space. But, it takes longer than the way of simply commenting them out.

Run KPROJ by $PATH_TO_KPROJ/KPROJ

Step 4: Preparing for plotting

- Modifying file ***bs_projected.dat***, giving the right E_F.

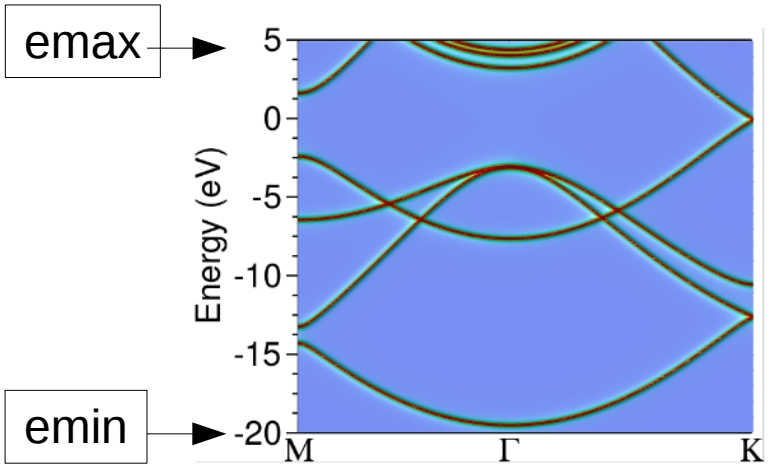
Replacing it by the one from the SCF calculation.

```
321  1            1.3539      ! NKPTS, jspins, ef (eV)
3  ! number of segments; positions:
    2.676543    3.345679    4.504656
```

- Run script ***run_futils*** (making it before the first using, i.e., make futils under src)

A sample of run_futils is given under the directory **utils**

```
#!/bin/bash
$PATH_TO_KPROJ/futils <<!
emin = -20
emax =  5
de = 0.01
dele=0.02
x
!
```

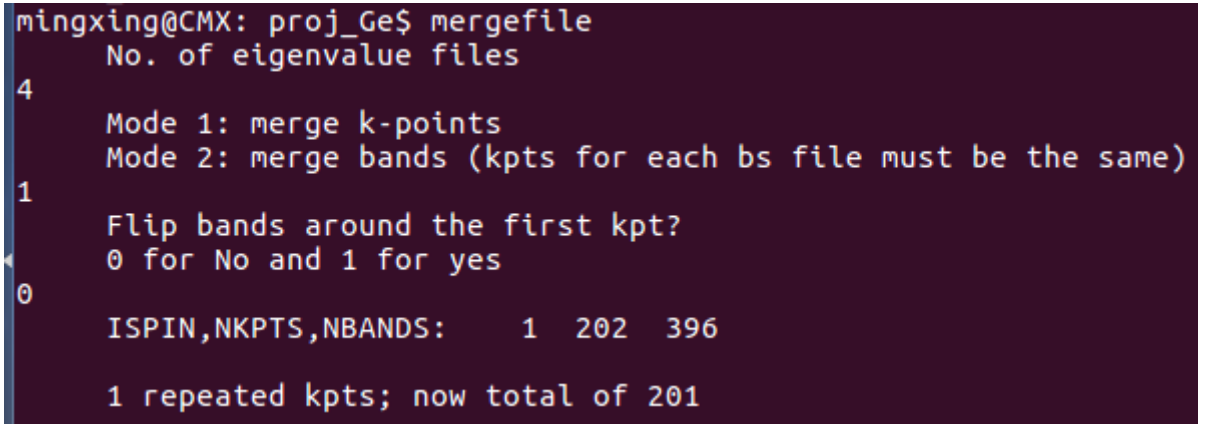


de: energy interval for the grid between emin and emax
dele: broadening factor, usually 2*de
Please play with these parameters to have a feeling to obtain a nice plot.

Large systems

If you have multiple bs_projecte.dat, please merge them into one first.

- You need copy them to a new working directory and rename them like bs_projecte.dat_1, bs_projecte.dat_2, …
- User program mergefile to do that. You can get it by "make mergefile" under src.
- An example is given under Ge_Al2O3.
  - I split the calculation into four sub-calculations. Two are for the k-path along M-Gamma and the others are for the k-path along Gamma-K.
  - After KPROJ, each calculation gives me one bs_projected.dat.
  - Then I make a new working directory merge_bs. After that, I did the copy "cp MG/CAL1/bs_projected.dat merge_bs/bs_projected.dat_1" and "cp MG/CAL2/bs_projected.dat merge_bs/bs_projected.dat_2", ...
  - Then, I merge them into one bs_projected.dat (see the picture below).
  - E-fermi has to be set correctly (Using the one from the scf calculation).



Outputs of run_futils

Nonmagnetic/SOC calculations:

band_kproj_1.dat
plotbnds.gnu — For gnuplot

plot_bands_1.dat
plot_bands_1.general — For opendx

bsplot.agr — For xmgrace

magnetic calculations:

band_kproj_1.dat — spin up
band_kproj_2.dat — spin down
band_kproj_tot.dat — total
plotbnds.gnu
For gnuplot

plot_bands_1.dat
plot_bands_1.general — spin up

plot_bands_2.dat
plot_bands_2.general — spin down

For opendx

Step 4: plot using gnuplot

plotbnds.gnu looks like

```
set cbrange [0: 99.19]

# tics pointing out
set tics out

# hide tics on x
unset xtics
set ytics font "Helvetica,32" nomirror # hide tics on the oppo
#set ytics   -0.600   1.000   0.400 font "Helvetica,32" nomir

# set tics width
set border lw 2
set ylabel offset -5.5,0
set ylabel "E (eV)" font "Helvetica,32"
set tmargin 1
set bmargin 1

#set label "{/Symbol G}"   font "Helvetica,32" at 0.50,-15.3
set label "K" font "Helvetica,32" at  -0.07909,  -0.65000
set label "K" font "Helvetica,32" at   0.25594,  -0.65000
set label "K" font "Helvetica,32" at   1.42762,  -0.65000
set label "K" font "Helvetica,32" at   2.25612,  -0.65000
set label "K" font "Helvetica,32" at   3.08463,  -0.65000

splot  "band_kproj_1.dat"
```

You may modify this value to make a nice plot.

Give the name of the high symmetry k-points. For example, if it is expected to be M, change “K” to “M”.
If it is Γ, then change “K” to “{\Symbol G}”

Give the desired spin states

```
set term postscript enhanced color
#set term png truecolor transparent
set output "plotbnds_up.eps"
#set output "plotbnds_up.png"
```

Name of the file for your plot

On the terminal, running “gnuplot plotbnds.gnu” will give a *.eps file.

Problems

- When MAT_P2S is not complete.
- When using LSORBIT = T for calculations without SOC included or using LSORBIT = F for SOC calculations.
- When WAVECAR is too large. In this case, splitting the band calculation into several sub-calculations.