

User guide of Wannier_tools

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1. Installaion

(a) Check out the repository by " git clone https://github.com/quanshengwu/wannier_tools.git" or download the zip file.

(b) cd wannier_tools/soc directory, Edit Makefile, Change the blas library " libs= " to your mkl library, you can use your own blas and lapack library. Then type make. The executive binary is copied to directory wannier_tools/bin

(c) add the wannier_tools/bin path to your PATH by "export PATH=yourdirecory/wannier_tools/bin:\$PATH"

(d) Look for more informations and examples on wiki https://github.com/quanshengwu/wannier_tools/wiki

2. The introduction of input file

Before execute wann_tools, you should edit the input file in the directory wannier_tools/example by your own necessary. Here we take Bi₂Se₃ as an example.

At present, The input file is not very flexible. It is a normal fortran free format file.

```
1| wannier90_hr.dat ! input file
2| output          ! output file's filename
3| T               ! BulkBand_calc
4| F               ! SlabBand_calc
5| F               ! WireBand_calc
6| T               ! SlabSS_calc
```

```

7| T          ! SlabArc_calc
8| F          ! SlabSpintexture_calc
9| T          ! wanniercenter_calc
10| F         ! berry
11| 100       ! Nk
12| 500       ! omega number
13| -0.60 0.50 ! omegamin omegamax
14| 0         ! E_arc
15| 10       ! nslab
16| 1        ! np
17| 18       ! NumOccupied
18| 18       ! ntotch
19| 2        ! soc
20| 0.001    ! eta
21| 4.4195   ! e-fermi
22| 0.0      ! surf_onsite
23| 0 0 0    ! Bx By Bz
24| -2.069 -3.583614 0.000000 ! crystal lattice information
25| 2.069 -3.583614 0.000000
26| 0.000 2.389075 9.546667
27| 5                ! number of atoms in unit cell
28| Direct          ! Direct or Cartesian coordinate
29| Bi 0.3990 0.3990 0.1970
30| Bi 0.6010 0.6010 0.3030
31| Se 0 0 0.5
32| Se 0.2060 0.2060 0.1180
33| Se 0.7940 0.7940 0.8820
34| 3 3 3 3 3 ! number of projectors
35| Bi px py pz ! projectors
36| Bi px py pz
37| Se px py pz
38| Se px py pz
39| Se px py pz
40| 5 ! number of k line only for bulk band
41| G 0.00000 0.00000 0.0000 X 0.50000 0.00000 0.5000 ! k
point path
42| X 0.50000 0.00000 0.5000 W 0.75000 0.25000 0.5000

```

```

43| W 0.75000 0.25000 0.5000 L 0.50000 0.50000 0.5000
44| L 0.50000 0.50000 0.5000 G 0.00000 0.00000 0.0000
45| G 0.00000 0.00000 0.0000 K 0.75000 0.37500 0.3750
46| 1 0 0 ! Umatrix for new lattice 001
47| 0 1 0
48| 0 0 1
49| 2 ! number of k line for 2D case
50| X 0.5 0.0 G 0.0 0.0 ! k path for 2D case
51| G 0.0 0.0 Y 0.5 0.0
52| -0.1 -0.1 ! Original point for 2D k plane
53| 0.2 0.0 ! The first vector to define 2D k plane
54| 0.0 0.2 ! The second vector to define 2D k plane for arc
plots
55| 0.0 0.0 0.00 ! Original point for 3D k plane
56| 0.0 1.00 0.00 ! The first vector to define 3d k space plane
57| 0.0 0.00 0.50 ! The second vector to define 3d k space plane

```

line 1 : wannier90_hr.dat ! input file

The file name of wannier90_hr.dat, which is generate from wannier90 package (<http://www.wannier.org>).

Currently, we support two formats, one is from wannier90. One is from Openmx, which rewrite wannier90_hr.dat.

line 2 : output ! output file

Filename for some outputs. You can check this file for running status.

From line 3-10 : give some control parameters for this program. The value should be F or T relate t False and True respectively.

Flag option	Function	Output	Tested
	Band structure for	bulkek.dat,	

BulkBand_calc	bulk	bulkek.gnu	yes
SlabBand_calc	Band structure for slab system	slabek.dat,slabek.gnu	yes
WireBand_calc	Band structure for ribbon system	ribbonek.dat,ribbonek.gnu	yes
SlabSS_calc	Surface spectrum $A(k,E)$ along a k line and energy interval	dos.dat_l, dos.dat_r surfdos_l.gnu,surfdos_r.gnu	yes
SlabArc_calc	Surface spectrum $A(k_1,k_2,E_0)$ for a fixed energy E_0	arc.dat_l, arc.dat_r arc_l.gnu,arc_r.gnu	yes
SlabSpintexture_calc	calculate spin texture for slab system	spindos.dat	No
wanniercenter_calc	calculate wannier centers for slabs	wcc.dat, wcc.gnu	yes
berry_calc	calculate berry phase along one k line		No

For Bulkband calculation, you should specify number of k lines and the special klines in line 41-45 (these line number is relatively). The output for this subroutine are bulkek.dat and bulkek.gnu. You can run "gnuplot bulkek.gnu", or "xmgrace bulkek.dat" to get bandstructure plot.

For Slab band calculation, you only need to change Nk in line 11 to get more points for k line.

The output for this subroutine are slabek.dat and slabek.gnu. You can run "gnuplot slabek.gnu", or "xmgrace slabek.dat" to get bandstructure plot. If you use gnuplot, you should check the png files.

The procedure for ribbon band calculation is similar to slab band calculation. the data is different by the names.

For surface state calculation, the output files are dos.dat_l, dos.dat_r, surfdos_l.gnu, surfdos_r.gnu. dos.dat_l and dos.dat_r are the spectrum weight for each k point and each energy, related to the top and bottom surface state respectively. You can run "gnuplot surfdos_l.gnu" to get surfdos_l.png.

For Fermi arc calculation, basically, the principle for this calculation is similar to surface state calculation. The difference is to get spectrum $A(k, \omega)$ for a fixed energy ω but (k_x, k_y) in 2D in this calculation, while get get spectrum $A(k, \omega)$ for some special k lines and an energy interval for the surface state calculation.

SlabSpintexture_calc and wanniercenter_calc are not tested yet.

line 11 : 40 ! Nk

Number of k points for any necessary subroutines, like bulk, slab, ribbon band structure calculation

line 12 : 500 ! omega number

Number of energies when calculate surface state, this value determines

the resolution of the surface state pictures. If it's large, the calculation will be slow linearly scaling.

You can set it to be 200 at first, if the resolution of the picture is not enough, then increase it.

line 13 : -2.00 2.00 ! omegamin omegamax

Energy interval for surface state calculation.

line 14 : 0 ! E_arc

Energy at which the fermi arc is calculated.

line 15 : 10 ! nslab

Number of slabs for slab band. If you calculate the band structure for nanoribbon, it represent the thickness of one direction. The thickness for the other direction is Np.
see Np.

line 16 : 1 ! Np

Number of principle layers for calculating surface state and fermi arc. If your wannier function is not enough localized. For instance, there are big hoppings beyond the home unit cell. Then we should set this value to 2 or 3 or 4. In principle, you should check the convergency of the surface state by increasing this value. The computation will be cubically grows as a functional of Np. at the beginning, you can set Np=1.

If you calculate band structure for nanoribbon, then this value is the thickness of another direction of nanoribbon. See slab.

line 17 : 18 ! NumOccupied

This value is not valid at present, leave it alone. However, don't delete this line.

line 18 : 18 ! Ntotch

number of electrons, if you want to determine the fermi level, this value will work.

line 19 : 1 ! soc

The flag for soc, if there is no spin-orbital included in your wannier90_hr.dat, then set it to be zero. else, set it to be 1.

line 20 : 0.001 ! eta

Broadening of green's function when calculate the surface states. If you don't know what it is, leave it unchanged.

line 21 : 4.4195 ! e-fermi in eV

Fermi level of your wannier90_hr.dat.

line 22-24 :

-2.069 -3.583614 0.000000 ! crystal lattice information
2.069 -3.583614 0.000000
0.000 2.389075 9.546667

Three lattice vectors coordinates.

line 25- 33 :

5 ! number of atoms for projectors
Direct ! Direct or Cartesian coordinate
Bi 0.3990 0.3990 0.1970
Bi 0.6010 0.6010 0.8030
Se 0 0 0
Se 0.2060 0.2060 0.6180
Se 0.7940 0.7940 2.3820

Set the number of atoms in your wannier90_hr.dat when you constructed it. Notice, this is the atoms that has projectors

contribution to Wannier functions, not the whole atoms in the unit cell.

Set the coordinate system type, Direct or Cartesian. Direct means the coordinates based on primitive unit cell.

Set the name and coordinate of each atoms. this coordinate is based on the three lattice vectors. It's easy to find it for through the wannier90.win.

line 34- 39 :

```
3 3 3 3 3      ! number of projectors
Bi px py pz
Bi px py pz
Se px py pz
Se px py pz
Se px py pz
```

Number of projectors for each atom when you construct your wannier functions. And the name of projectors.

line 40- 45 :

```
5      ! number of k line\\
G 0.00000 0.00000 0.0000 X 0.50000 0.00000 0.5000 ! k point path\\
X 0.50000 0.00000 0.5000 W 0.75000 0.25000 0.5000\\
W 0.75000 0.25000 0.5000 L 0.50000 0.50000 0.5000\\
L 0.50000 0.50000 0.5000 G 0.00000 0.00000 0.0000\\
G 0.00000 0.00000 0.0000 K 0.75000 0.37500 0.3750
```

Number of high-symmetric k point lines. Look the format carefully.

This k lines are in unit of the reciprocal lattice built by the lattice vector given in line 24-26

line 46-48 :

```
1 0 0 ! Umatrix for new lattice a11, a12, a13\\
0 1 0 ! a21 a22 a23\\
0 0 1 ! a31 a32 a33
```


These three lines are very important for slabs and ribbon calculation. It defines the surface we needed. Basically, you should know of which surface you want to get the surface, and of which direction you want to simulate the ribbon. So we need to define the new lattice vector system like this, choose two vectors on the surface we want to study, and choose another vector which is not in this plane. The volume of the cell constructed by these three vectors should be the same of the previous one. And the orientation should be the same by checking $\mathbf{R}_1 \cdot (\mathbf{R}_2 \times \mathbf{R}_3) = \mathbf{R}_1 \cdot (\mathbf{R}_2 \times \mathbf{R}_3)$. The relations between old and new basis are

$$\begin{aligned} \mathbf{R}_1' &= a_{11} \mathbf{R}_1 + a_{12} \mathbf{R}_2 + a_{13} \mathbf{R}_3 \\ \mathbf{R}_2' &= a_{21} \mathbf{R}_1 + a_{22} \mathbf{R}_2 + a_{23} \mathbf{R}_3 \\ \mathbf{R}_3' &= a_{31} \mathbf{R}_1 + a_{32} \mathbf{R}_2 + a_{33} \mathbf{R}_3 \end{aligned}$$

The slab calculations are base on the surface constructed by vector $\mathbf{R}_1', \mathbf{R}_2'$. The ribbon is along \mathbf{R}_3' direction, two surfaces are constructed by vector $\mathbf{R}_1', \mathbf{R}_3'$ and $\mathbf{R}_2', \mathbf{R}_3'$ respectively.

line 49-51 :

```
2      ! number of k line for 2D case
X 0.5 0.0 G 0.0 0.0 ! k path for 2D case
G 0.0 0.0 Y 0.5 0.0
```

Number of high-symmetric k point lines for 2D system, such as the surface state spectrum or the band structure for slab system . Look the format carefully. This k lines are in unit of the reciprocal lattice built by the lattice vector for 2D system given in line 46-48. Number of k points along each line is Nk , which is set in line 11.

line 52-54 :

```
-0.1 -0.1      ! Original point for 2D k plane
0.2  0.0      ! The first vector to define 2D k plane
0.0  0.2      ! The second vector to define 2D k plane for arc plots
```

Define a 2D k space plane for arc plots. Line 52 is the start point of

the plane. Line 53 and Line 54 are the two vectors define the plane.

line 55-57 :

0.0 0.0 0.00 ! Original point for 3D k plane

0.0 1.00 0.00 ! The first vector to define 3d k space plane

0.0 0.00 0.50 ! The second vector to define 3d k space plane

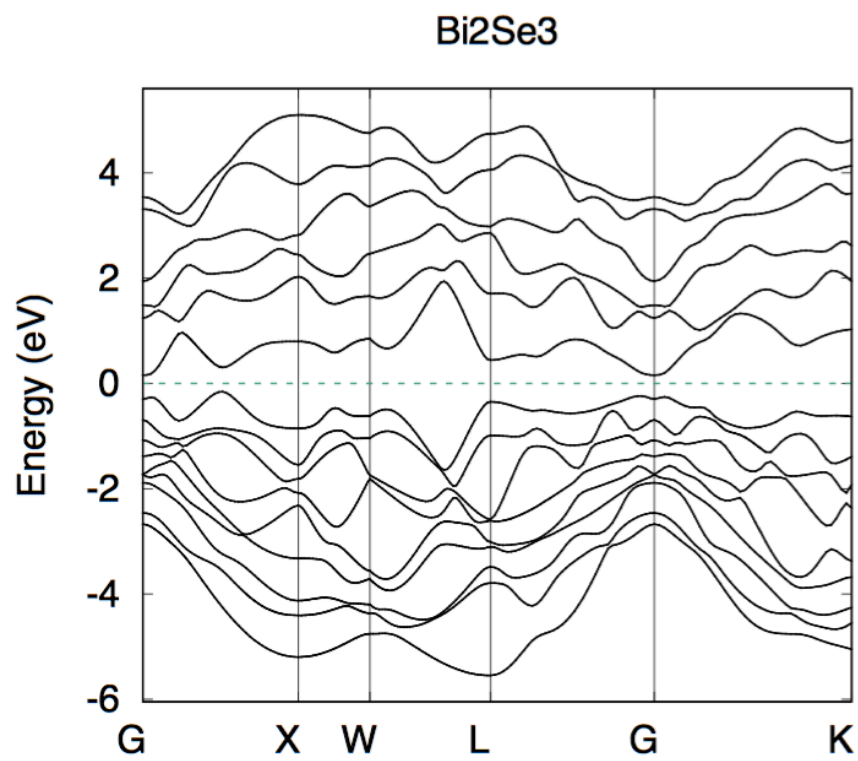
The same set as line 52-54, but for 3D case. We can use these two vectors to calculate the band gap of a plane in 3D BZ, then we can check whether there are Weyl points in that plane. Notice that these vectors is in unit of reciprocal vectors.

If you want to calculate Wannier charge center, which is sometimes called Wilson loop, you should notice that the first vector in line 56 is the integration direction, the difference between two vectors should be in one primitive reciprocal lattice vector. Such as 0.0 0.0 0.0 1.0 0.0 0.0. After the calculation, you can get the Wannier charge center along the second k line.

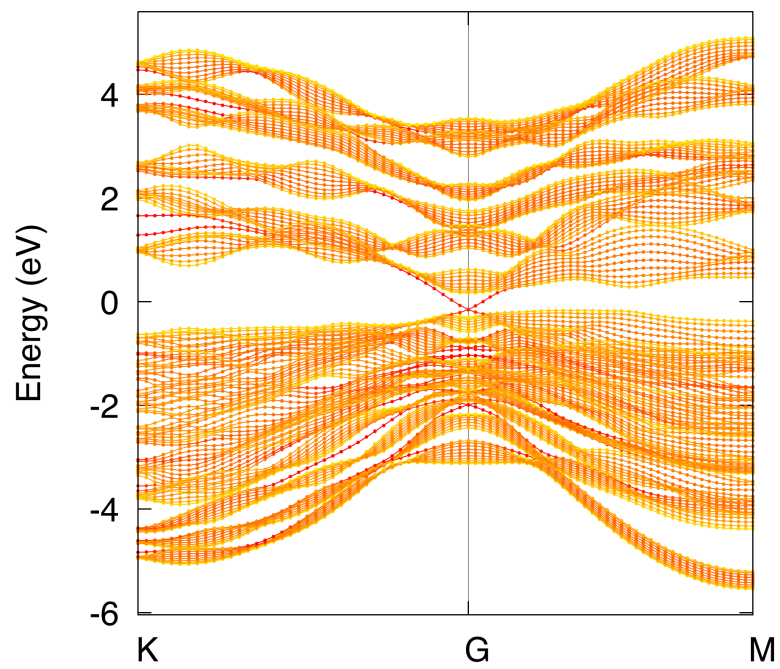
Examples (Bi₂Se₃)

The wannier90_hr.dat is compressed as Bi₂Se₃_hr.tar.gz in examples/ folder. You can decompressed by a command “tar xzvf Bi₂Se₃_hr.tar.gz”. The input.dat file can also be found in that folder.

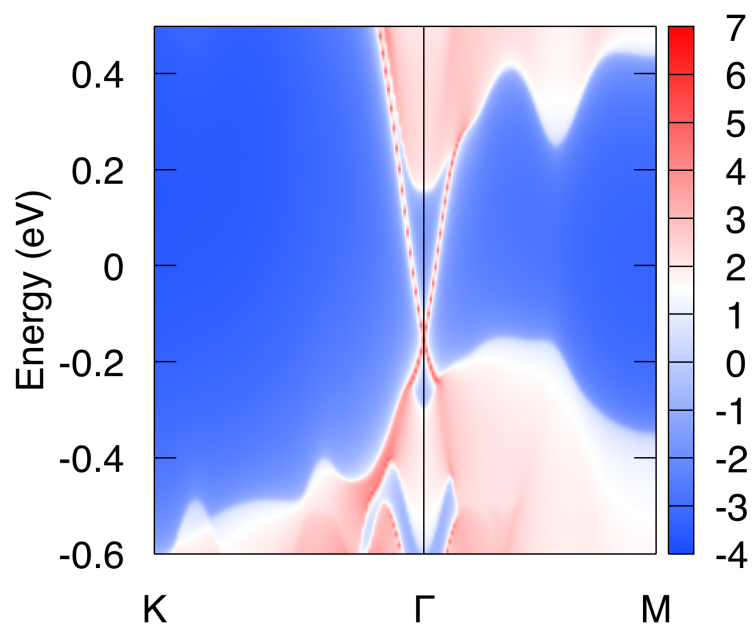
(1). Bulk band structure



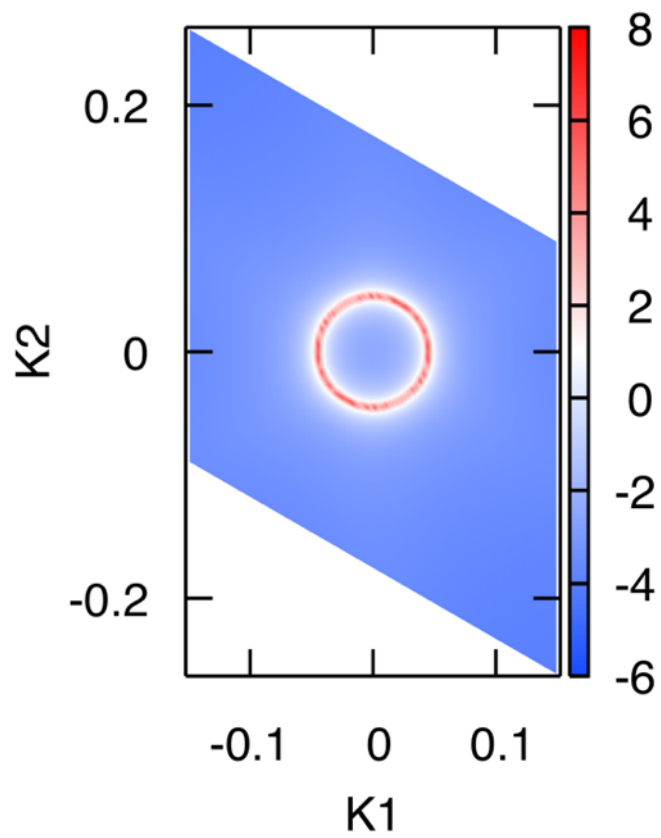
(2). (001) oriented slabs.



(3). (001) surface state



(4). (001) surface spectrum for a fixed energy $E=0\text{eV}$



4. License and agreement.

If you use our code, please cite this website "Q.S Wu S.N Zhang, https://github.com/quanshengwu/wannier_tools". If you have good ideas to improve this code, do not hesitate to contact me. Your contribution will be recorded.

5. Enjoy and good luck.