Topological properties with WannierTools

Tutorial I: Topological insulators

Hands-on session

Wannier 2022 Summer School Trieste

Hands-on based on WannierTools v2.6.2

Useful information about WannierTools:
Documentation: www.wanniertools.com
Forum: www.wanniertools.org
Open source: https://github.com/quanshengwu/wannier_tools
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Tips: Open file.eps, file.pdf file in Linux, you can use command "evince". such as

```
$ evince file.eps
```

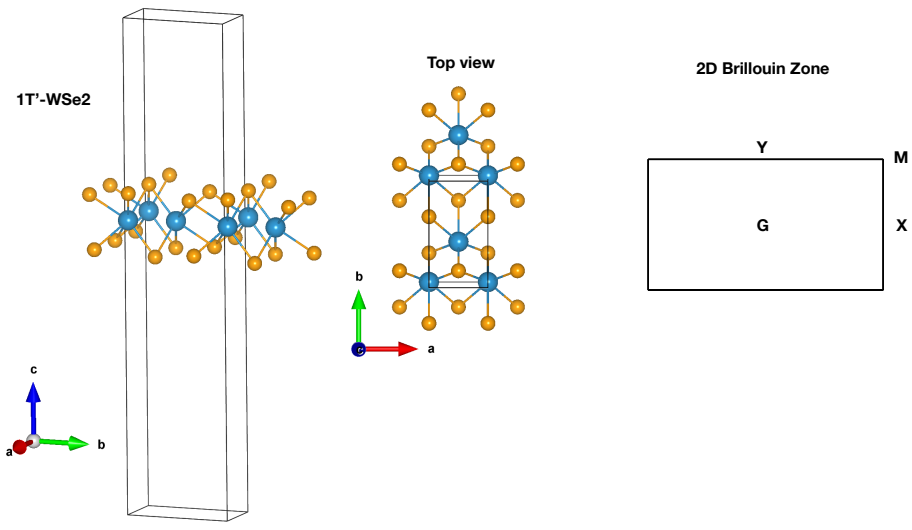
Open file.png file in Linux, you can use command "eog". such as

```
$ eog file.png
```

In this session we will study a 2D topological insulator WSe2 and a 3D topological insulator using WannierTools.

2D topological insulator 1T'-WSe_2

1T'-WSe_2 is predicted as a 2D topological insulator which is also called quantum spin hall (QSH) insulator. In our calculation, we treat it as a 3D material with a thick vacuum along z direction. There is no dispersion along z direction. So we only need to study properties on $k_z = 0$ plane. The crystal structure and Brillouin zone are shown in the following figure.



▶ **Preparation** First, please copy the tutorial input files of the exercise:

```
$ git clone https://github.com/wannier-developers/wannier-tutorials.git
$ cd wannier-tutorials/2022_05_Trieste/DAY4_WannierTools/ex1/topological_insulators/WSe2_1Tprime/
$ tar xzvf wannier90_hr.dat.tar.gz
```

The tight binding model *w*annier90_hr.dat and the input file of WannierTools *w*t.in are prepared. If you open and check the *wt.in* file, you will find that we are going to calculate the bulk band structure, surface state spectrum and Wannier charge center (WCC) at $k_z = 0$ plane.
Here we will not list all parameters we need to do all calculations. We only want to mention the parameters to generate the WCC in order to get the topological $\mathbb{Z}_2$ number.

```
--                                                                                    wt.in
&CONTROL
Wanniercenter_calc   = T
/

&SYSTEM
NumOccupied = 28    ! We assume the band below NumOccupied'th band are full occupied.
/

&PARAMETERS
Nk1 = 61            ! number k points
Nk2 = 101            ! number k points
/

KPLANE_BULK
 0.00  0.00  0.00   ! Starting point of the k-slice
 1.00  0.00  0.00   ! The first vector is used for integration.  k1
 0.00  0.50  0.00   ! the WCC is along this vector. k2
```

▶ Note: The third vector $\mathbf{k}_2$ in **KPLANE_BULK** card for $\mathbb{Z}_2$ calculation is only half of the reciprocal lattice vector which is different from that of Chern number calculation for Haldane model.
The hybrid WCCs are defined as

$$\bar{x}_n(\mathbf{k}_2) = \frac{a_1}{2\pi} \int d\mathbf{k}_1 \mathcal{A}_n(\mathbf{k}) \tag{1}$$

$$\mathcal{A}_n(\mathbf{k}) = i\langle u_{n\mathbf{k}} | \nabla_{\mathbf{k}} | u_{n\mathbf{k}} \rangle \tag{2}$$

$\mathbf{k}_1$ ($\mathbf{k}_2$) is the second (third) numeric line of **KPLANE_BULK** card.

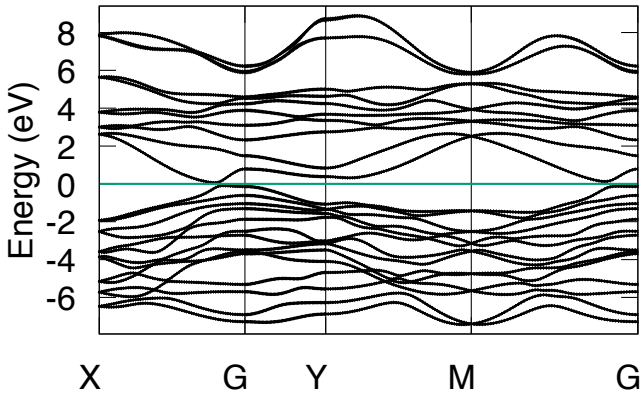
▶ **Run WannierTools:**

```
$ mpirun -np 2 wt.x &
```

▶ **Visualize the results using Gnuplot**
1). Now we can plot the band structure with

```
$ gnuplot bulkek.gnu
```

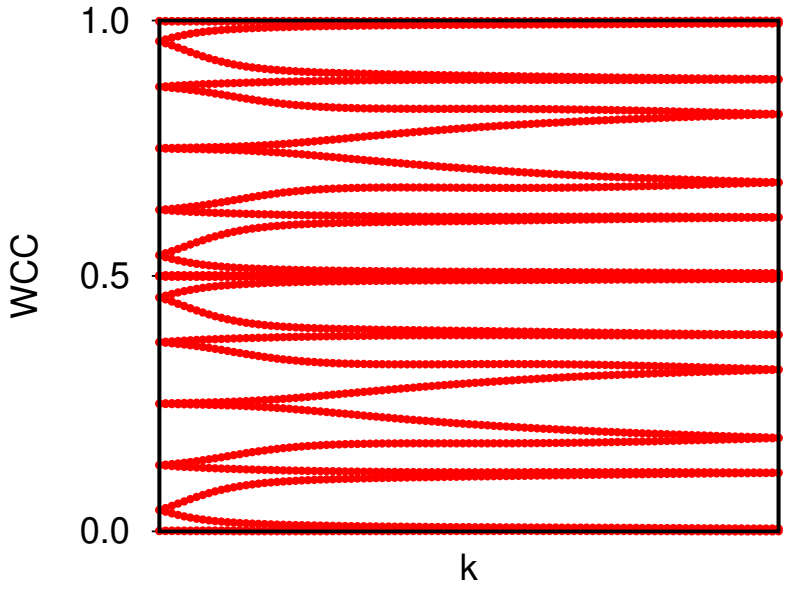
Two plots are named as bulkek.pdf, They should look like this:



The band structure of this phase shows that it is a insulator.
2). We can also plot the Wannier charge center (Wilson loop) to get the $\mathcal{Z}_2$ number.

```
$ gnuplot wcc.gnu
```

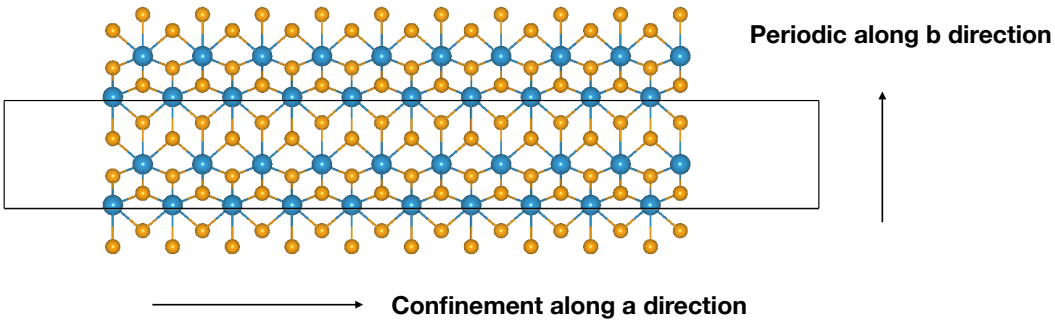
The plot are named as *w*cc.eps. It should look like this:



This WCC shows that $\mathcal{Z}_2 = 1$ since the crossing times between the WCCs and the line that you draw from the left to the right is odd.
4). Due to the bulk-edge correspondence, there is non-trivial edge states if we cut the edge along one direction. So now we want to plot the edge state spectrum. Here we cut the edge along **a** direction and leave **b** direction periodic. It means that the surface is defined by lattice vectors **b** and **c**. So the **SURFACE** card should look like this

```
SURFACE  ! define two vectors on the surface
0  1  0
0  0  1
```

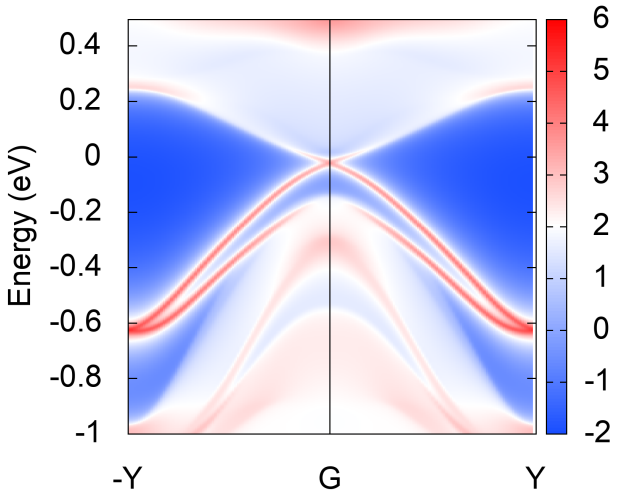
The sketch plot of the slab system can be obtained with visualize the file *P*OSCAR-slab in software VESTA.



This time we don't use the slab band structure functionality with SlabBand_calc=T, instead we use the surface green's function technique to calculate the surface state with a semi-infinite slab system. The surface state spectrum can be obtained with

```
$ gnuplot surfdos_l.gnu
$ gnuplot surfdos_r.gnu
```

We will get surfdos_l.png and surfdos_r.png. Both are the same since they have the same termination and should look like this:



This shows that the edge states are non-trivial since they connect valence band and conduction band together.

▶ **Exercises**

1. Try to increase Nk1, OmegaNum in the input file *wt*.in to calculate surface state spectrum using SlabSS_calc= T.
2. Increase the energy window of surface state spectrum which is controled by OmegaMin and OmegaMax in the **PARAMETERS** card.
3. Calculate surface state spectrum when confinement happens along **b** direction. Plot surface state spectrum for both dual surfaces.

3D topological insulator Bi_2Se_3

Bi_2Se_3 was theoretically predicted and experimental confirmed as a 3D TI. In this section, we are going to study its topological properties. The topological number and surface state spectrum will be studied.

▶ **Preparation** First, please copy the tutorial input files of the exercise:

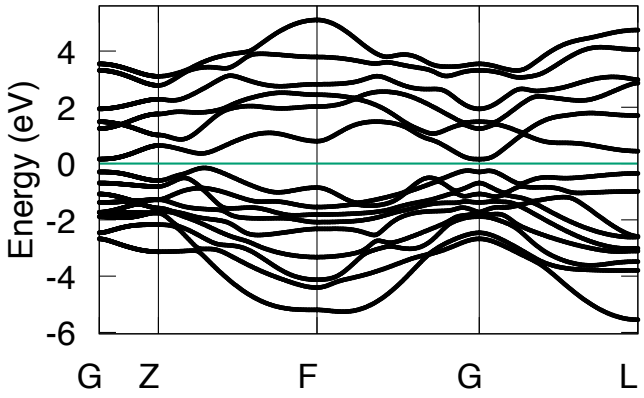
```
$ git clone https://github.com/wannier-developers/wannier-tutorials.git
$ cd wannier-tutorials/2022_05_Trieste/DAY4_WannierTools/ex1/topological_insulators/Bi2Se3
$ tar xzvf wannier90_hr.dat.tar.gz
```

▶ **Run WannierTools:**

```
$ mpirun -np 2 wt.x &
```

▶ **Visualize the results using Gnuplot**
▶ **1). Like always, we plot the bulk band structure first.**

```
$ gnuplot bulkek.gnu
```



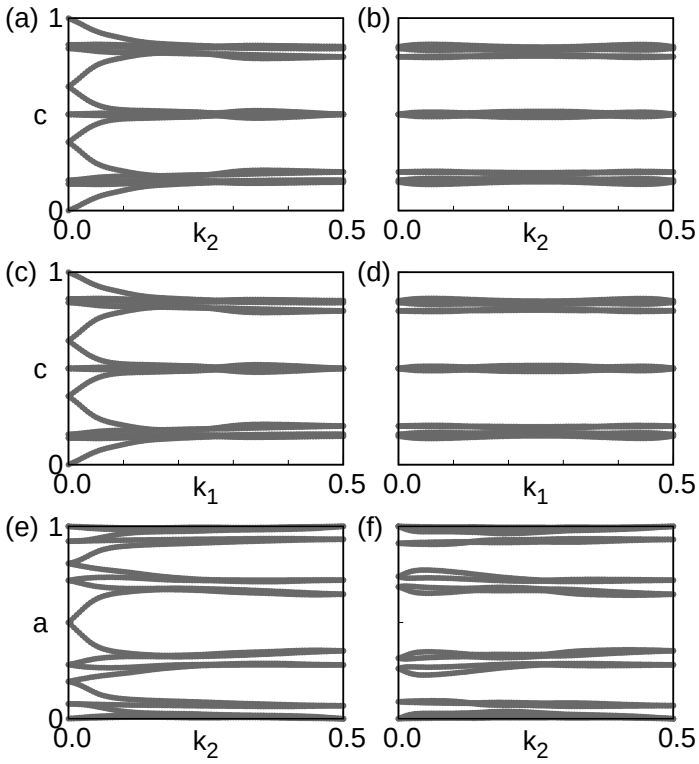
The bulk band structure shows that it's insulator (Here, "insulator" means there is gap at every k point).

▶ **2). Let's check the topological number.**

Bi2Se3 is a nonmagnetic material. The time reversal symmetry is preserved. Since it's a 3D material, we have to calculate the WCCs in six time reversal invariant planes $\mathbf{k}_1 = 0, 1$, $\mathbf{k}_2 = 0, 1$ and $\mathbf{k}_3 = 0, 1$. WannierTools has one function to calculate them all by setting *Z*2_3D_calc=T. The WCCs plot *w*anniercenter3D_Z2.eps can be obtained by running

```
$ gnuplot wanniercenter3D_Z2.gnu-tutorial
```

It should look like this



According to the WCCs rule, the $\mathcal{Z}_2$ number for panel a, c and e is 1, panel b, d and f is 0. This can also be read directly from WT.out by

```
$ sed -n '/# z2 number/,/Time/p' WT.out
```

It shows as

```
 # z2 number for 6 planes
 k1=0.0, k2-k3 plane:            1
 k1=0.5, k2-k3 plane:            0
 k2=0.0, k1-k3 plane:            1
 k2=0.5, k1-k3 plane:            0
 k3=0.0, k1-k2 plane:            1
 k3=0.5, k1-k2 plane:            0
 Time cost for Z2_calc is about          62.250 s
```

The $\mathcal{Z}_2$ number of a 3D insulator is consistent with four numbers $(\nu_0;\nu_1\nu_2\nu_3)$. $\nu_0 = \mathcal{Z}_2(k_i = 0) + \mathcal{Z}_2(k_i = 0.5)$ tells whether it's a strong ($\nu_0 = 1$) or weak ($\nu_0 = 0$) topological insulator. $\nu_1 = \mathcal{Z}_2(k_1 = 0.5), \nu_2 = \mathcal{Z}_2(k_2 = 0.5), \nu_3 = \mathcal{Z}_2(k_3 = 0.5)$ are called weak topological invariants (Ref:Phys. Rev. B 76, 045302 (2007)). Eventually, the $\mathcal{Z}_2$ number of Bi_2Se_3 is (1;000) which indicates Bi_2Se_3 is a strong topological insulator. That's means there is topological protected surface states in any termination.

▶ 3). Let's study surface state properties.

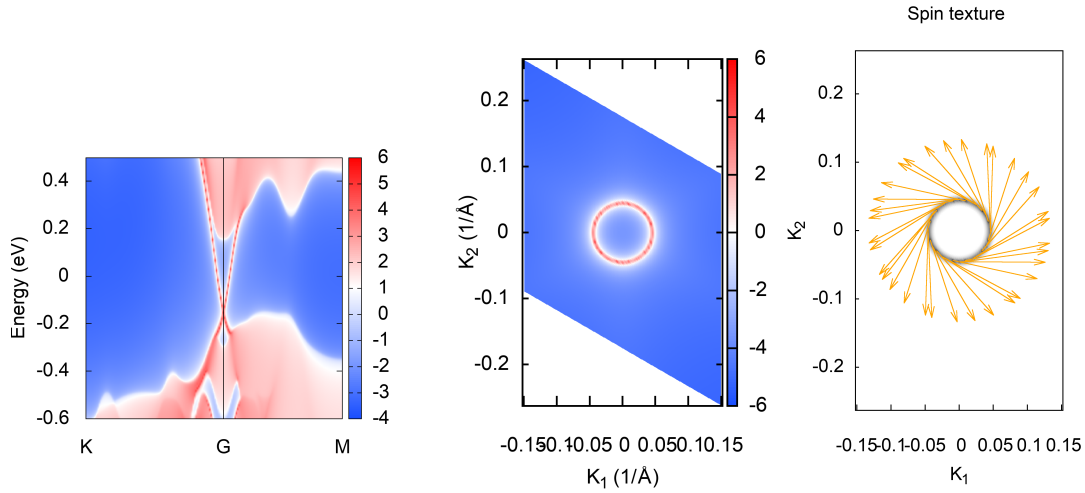
In this tutorial, we study the (001) surface which is a cleavage surface. The **SURFACE** card is defined as

```
SURFACE  ! define two vectors on the surface
1   0   0
0   1   0
```

The first and the second lattice vectors are in the (001) surface when we set our initial crystal structure. So, it becomes very easy to set the SURFACE card.
Now, let's plot the surface state spectrum

```
$ gnuplot surfdos_l.gnu
$ gnuplot arc_l.gnu
$ gnuplot spintext_l.gnu
```

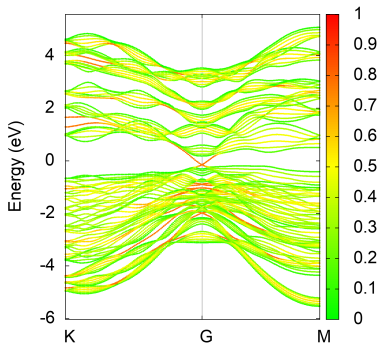
Three figures called surfdos_l.png, arc_l.png, and spintext_l.png are shown as



The left panel surfdos_l.png shows the spectrum along a given kpath defined by KPATH_SLAB and a given energy interval defined by OmegaMin and OmegaMax.
The middle panel arc_l.png is a iso-energy plot with a given energy defined by E_arc parameter.
The right panel spintexture.png shows the spin texture in a given KPLANE_SLAB and E_arc.
There is another way to study the surface states. That's to calculate the slab band structure with given slab thickness controlled by a parameter **Nslab**.

```
$ gnuplot slabek.gnu
```

The file slabek.png would be generated which looks like this:



1. Study the surface state for another surface defined by the second and the third lattice vector.
2. Change E_arc parameter to recalculate surface state spetrum with SlabArc_calc=T.
3. Calculate slab band structures for different slab thickness by changing Nslab from 1 to 6.