

Vasp2mat计算Wilson loop

Step 1 运行vasp自洽计算，得到自洽的CHGCAR

Step 2 读CHGCAR，运行vasp非自洽计算，
得到固定 $k_a=0$ ，沿 k_b 方向(loop方向)周期离散 k 点的WAVECAR
INCAR:

ISTART = 0

ICHARG = 11

LWAVE=.TRUE. ; LCHARG=.FALSE.

KPOINTS:

k-points

30

Line-mode

rec

0.0 0.0 0.0

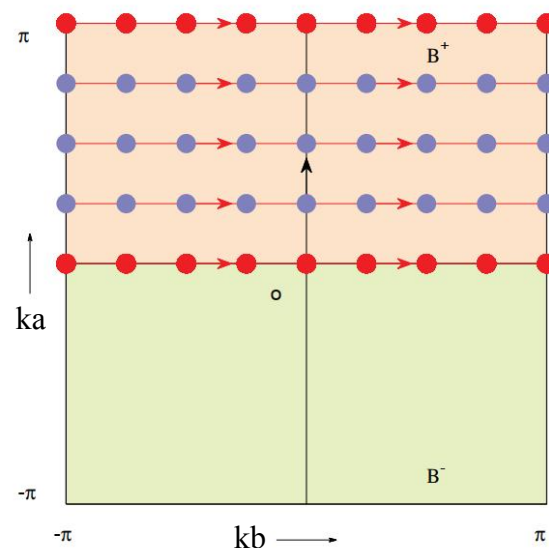
0.0 1.0 0.0

Step 3

运行vasp2mat，读WAVECAR，计算Wannier charge center (WCC)
输出到MAT_Berry_K.m文件

Step 4 (可选)

变化 k_a ，进行非自洽计算，运行vasp2mat



INCAR: ISTART = 1 ICHARG = 0

INCAR.mat :

&vmat_para

print_only_diagonal = .true.

vmat = 14

vmat_name = 'Berry_K'

bstart=25, bend=32 #band range

/

EX_graphene

Calculate the berry phase for a loop around the K point

#commands

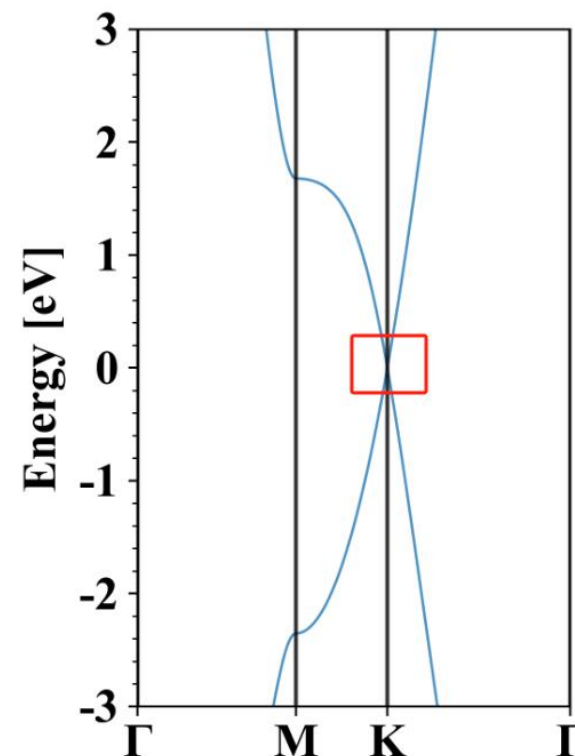
```
$ cp INCAR.scf INCAR
$ cp KPOINTS.scf KPOINTS
$ vasp_std > vasp.out_scf
(sbash sub-vasp.slurm)
```

```
$ cp INCAR.nscf INCAR
$ cp KPOINTS.nscf KPOINTS
$ vasp_std > vasp.out_nscf
(sbash sub-vasp.slurm)
```

```
$ cp INCAR.mat2 INCAR
$ vasp2mat > out_vasp2mat
(sbash sub-vasp.slurm)
```

```
MAT_Berry_K.m
1  % vmat
2  %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
3  % k = 0.29616611 0.32214380 0.00000000 in b_i
4  % B1 = 1.34718398 0.77779703 0.00000000 in bohr^-1
5  % B2 = 0.00000000 1.55559407 0.00000000 in bohr^-1
6  % B3 = 0.00000000 0.00000000 0.20780742 in bohr^-1
7  % Number of k-points along the wilson loop: 80
8  % On bands : 1 2 3 4
9  % Berry's phase in 2pi
10 Berry_K(1:4, 1:2)=[
11     1 (-0.00015 +0.99984i)
12     2 (+0.00015 +0.99984i)
13     3 (+0.00000 +0.99985i)
14     4 (+0.50000 +0.91555i)
15 ];
16 % trace = ( +0.50000 +0.00000i)
17 -WCC
```

berry phase = π



EX_BiH-wcc

considering spin-orbit coupling(SOC),
loop along kb direction to get Wannier charge center (WCC), WCC evolves along the ka direction.

```
#commands
$ cp INCAR.scf INCAR
$ cp KPOINTS.scf KPOINTS
$ vasp_ncl > vasp.out_scf
(sbatch sub-vasp.slurm)

$ ./loop_run.sh

$ python get_wcc.py

$ gnuplot wcc_plot.gnuplot
```

```
loop_run [7].sh
1  #!/bin/bash
2  for ((i=0;i<=10;i+=1))
3  do
4    k1=$(printf "%.10f" $(echo "scale=10;(0.0+0.5*1/10*$i)/1"|bc))
5
6
7  if [ ! -d "ka$i" ]; then
8    echo ka$i
9    mkdir ka$i
10   cp INCAR.nscf INCAR.mat INCAR.mat2 POSCAR POTCAR CHGCAR ka$i/
11   cd ka$i
12
13   cat > KPOINTS << eof
14   k-points along high symmetry lines
15   25
16   Line-mode
17   rec
18   $k1 0.0 0.0
19   $k1 1.0 0.0
20   eof
21
22   qsub ../loop_vasp.pbs >jobid
23   cd ../
24   fi
25 done
```

