

symmFS计算并绘制费米面

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，来加密k-mesh
INCAR:

ISTART = 0

ICHARG = 11; LCHARG=. FALSE.

ISYM=2 (use symmetry)

(Check if "irot" is present in the OUTCAR file.)

KPOINTS:

K-Spacing Value

0

Gamma (Γ -centered mesh)

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Step 3 运行symmFS程序，生成bands.fermi.bxsf文件
读入CONTCAR OUTCAR KPOINTS EIGENVAL

Step 4 读bands.fermi.bxsf，运行xcrysden绘制费米面

Example Cu

bands.fermi.bxsf is generated.

#commands

```
$ cp INCAR.scf INCAR
```

```
$ cp KPOINTS.scf KPOINTS
```

```
$ vasp_std > vasp.out.scf  
(sbatch sub-vasp.slurm)
```

```
$ cp INCAR.nscf INCAR
```

```
$ cp KPOINTS.nscf KPOINTS
```

```
$ vasp_std > vasp.out.nscf  
(sbatch sub-vasp.slurm)
```

```
$ gfortran symmFS.f90 -o symmFS
```

```
$ ./symmFS.sh
```

#plot

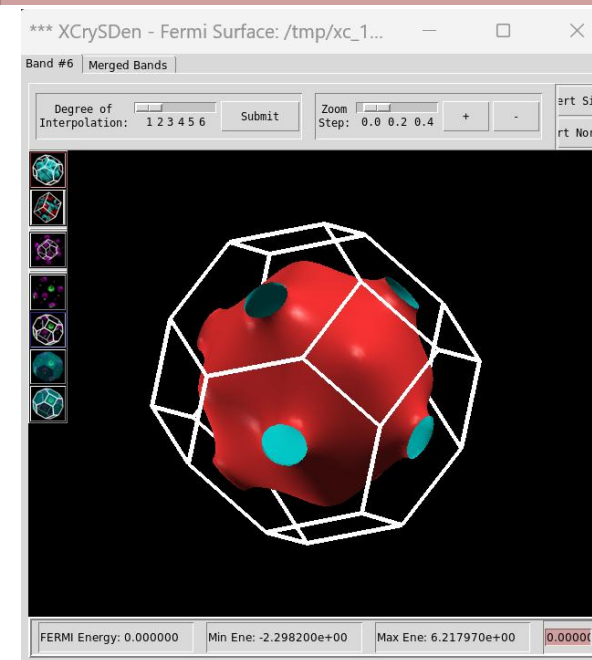
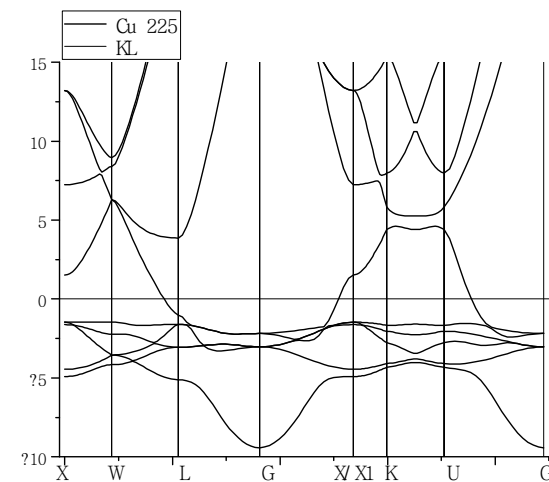
```
$ xcrysden --bxsf bands.fermi.bxsf
```

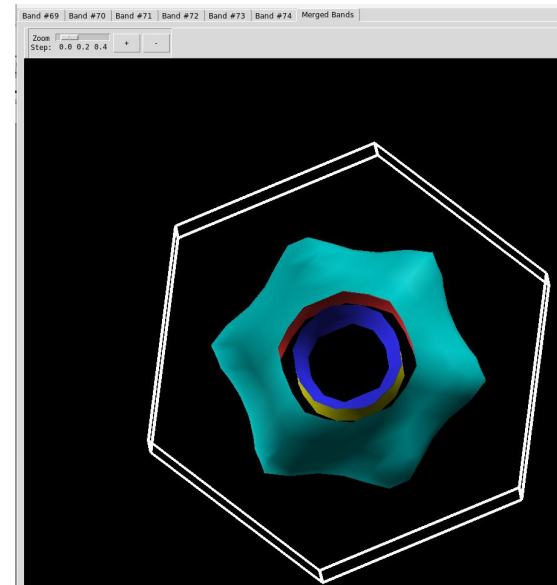
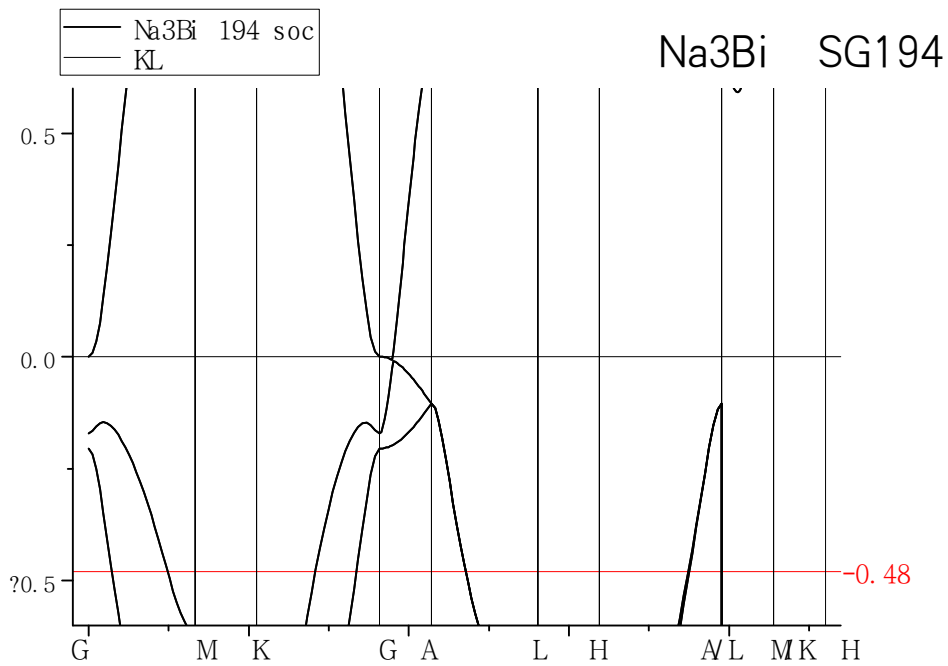
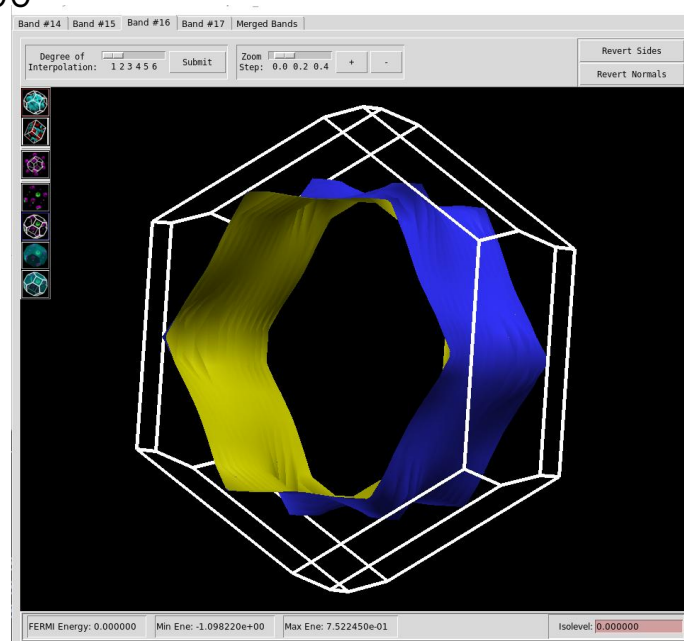
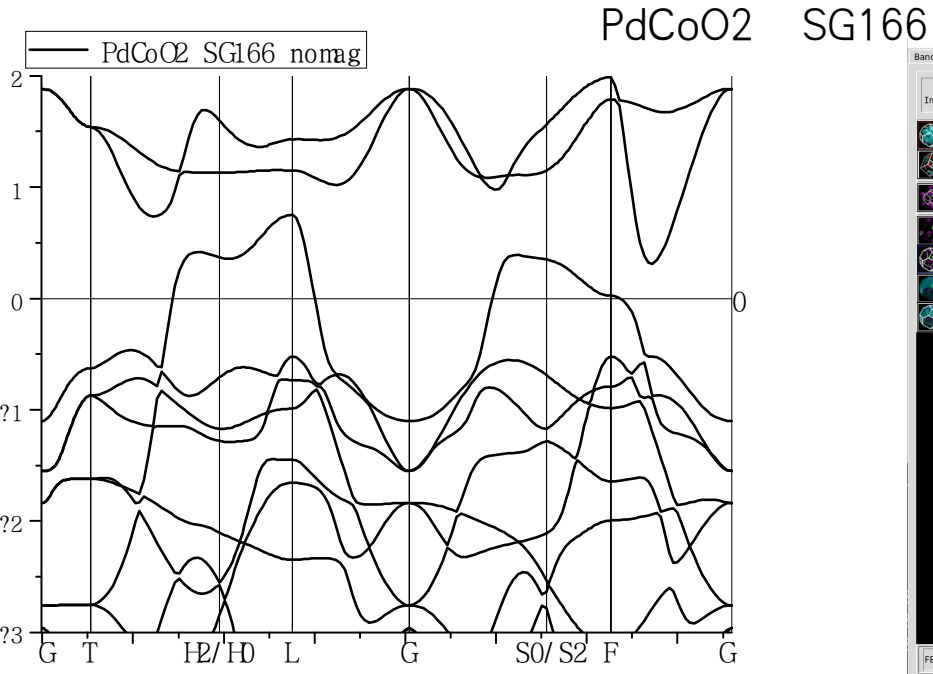
1) ./symmFS.sh

Example Cu

2) xcrysden --bxsf bands.fermi.bxsf

```
[pub123@alpha100 calculation-result]$ ./symmFS.sh
The OUTCAR exists, we use it to get the Fermi level,
the RWIGS tag and the number of spins.
Fermi level: 7.7788
ISPIN: 1
LNONC: F
kmesh: 40 40 40
Primitive Cell
pa_xyz= 0.00000000 1.79950000 1.79950000
pb_xyz= 1.79950000 0.00000000 1.79950000
pc_xyz= 1.79950000 1.79950000 0.00000000
Primitive Rciprocal Cell
pra_xyz= -1.74581420 1.74581420 1.74581420
prb_xyz= 1.74581420 -1.74581420 1.74581420
prc_xyz= 1.74581420 1.74581420 -1.74581420
48 : the number of symmetries
1661 : the number of IBZ k-points
64000 : the number of FBZ k-points
40 40 40 : kmesh
7972879728
!!! ISPIN=1 or 2 (colliner), Warning: time-reversal symmetry was used !!!
writing bands.fermi.bxsf!!!
ibktn,nconb,gap: 370 6 7 11.914004 12.825613 0.911609
ibktn,nconb,gap: 384 6 7 12.423078 12.823048 0.399970
ibktn,nconb,gap: 739 6 7 12.592469 12.761841 0.169372
ibktn,nconb,gap: 1232 6 7 12.743964 12.878151 0.134187
ibktn,nconb,gap: 1507 6 7 13.042350 13.095356 0.053006
ibktn,nconb,gap: 1661 6 7 14.002746 14.002883 0.000137
[pub123@alpha100 calculation-result]$
```





E_f = -0.48