Use VASP4FS to calculate the Fermi surfaces (FS)

所需程序：VASP4FS，XCrySDden

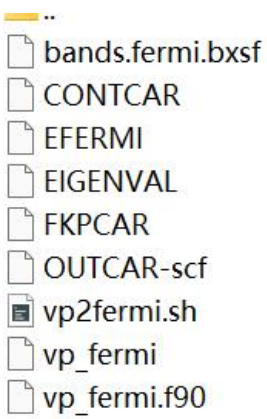
1）首先进行scf计算，得到CONTCAR，EIGENVAL，OUTCAR—scf文件。

2）将INCAR中的IBRION设为8，运行vasp_FS程序，得到简约布里渊区和全布里渊区的对应关系，存储在文件FKPCAR中。

3）运行脚本 vp2fermi.sh
$$ bash vp2fermi.sh

4）得到三维费米面文件bands.fermi.bxsf，可用xcrysden查看
$$ xcrysden ——bxsf bands.fermi.bxsf

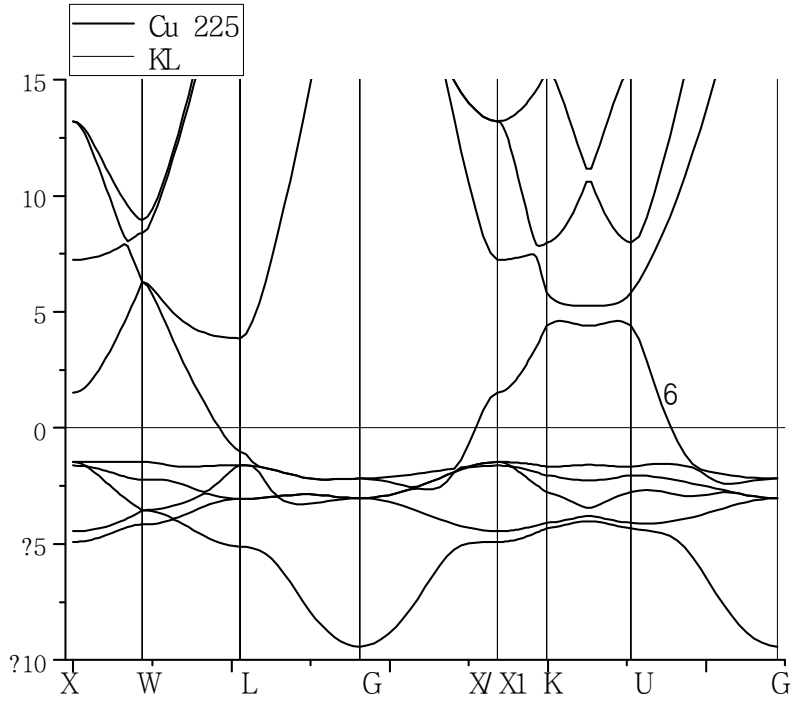
所需文件：

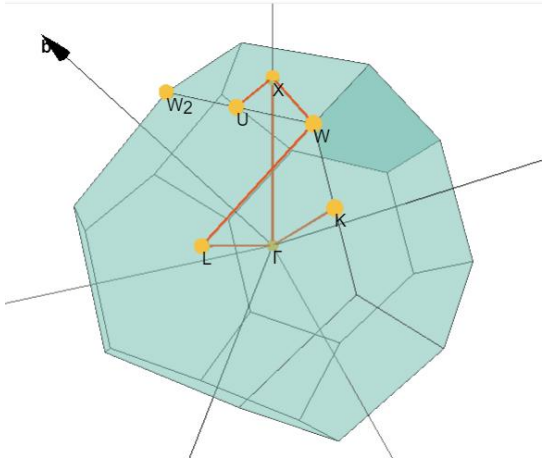


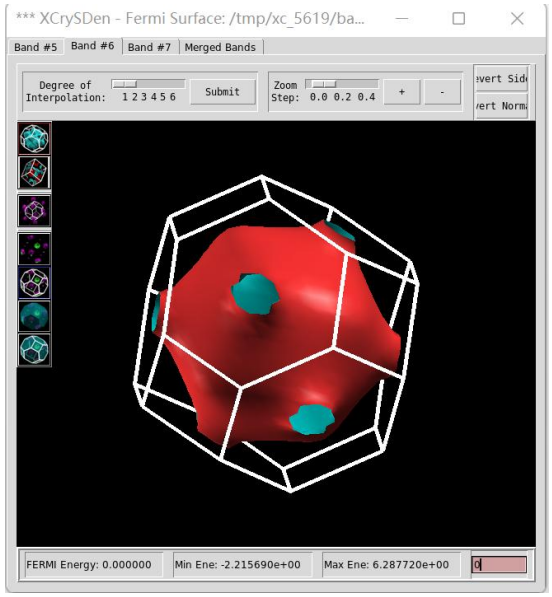
vp2fermi.sh：

```
#!/bin/bash
outfile=OUTCAR-scf
infile=INCAR
if [ -a $outfile ]; then
    echo "The" $outfile "exists, we use it to get the Fermi level,"
    echo "the RWIGS tag and the number of spins."
    efermi=$(grep "E-fermi" $outfile | tail -1 | awk '{print $3}')
    echo "Fermi level:" $efermi
    echo "$efermi : Fermi level "> EFERMI
    ISPIN=$(grep "ISPIN" $outfile | tail -1 | awk '{print $3}')
    echo "ISPIN: " $ISPIN
    echo "$ISPIN      : IPSIN" >> EFERMI
fi

./vp_fermi
```

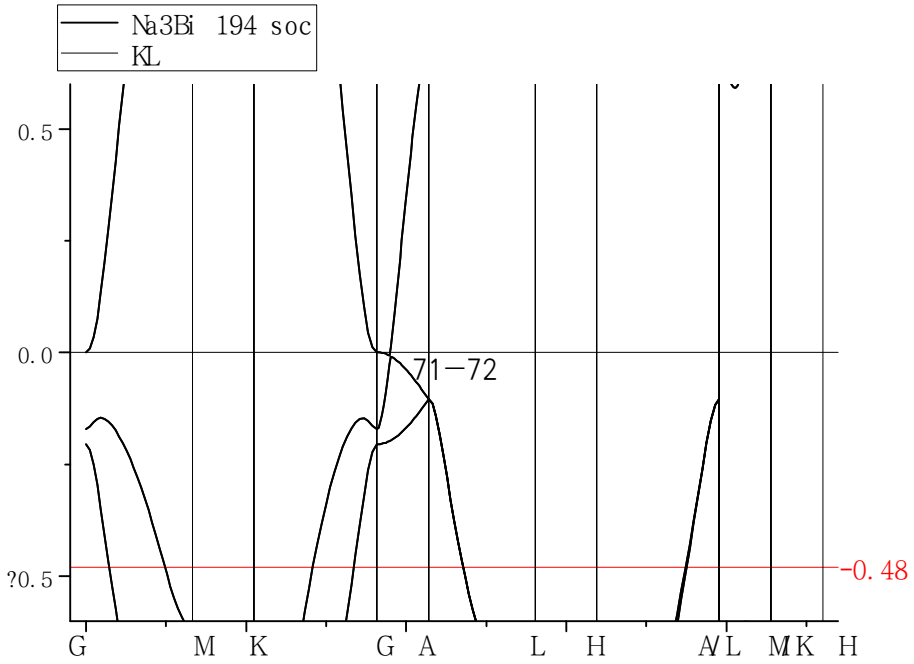


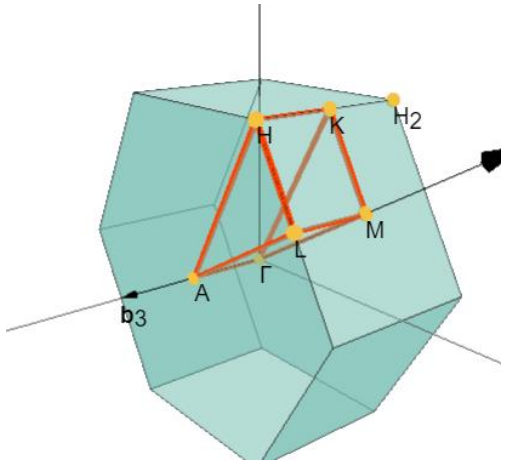




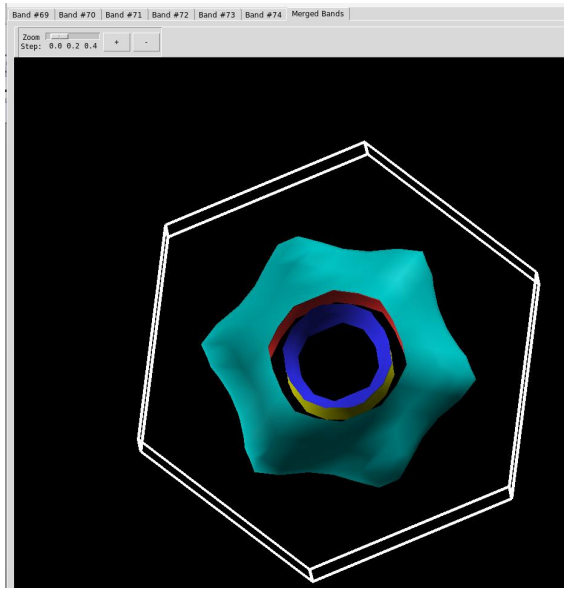

```
The OUTCAR-scf exists, we use it to get the Fermi level,
the RWIGS tag and the number of spins.
Fermi level: 7.7165
ISPIN:  1
  Primitive Cell
 pa_xyz=     0.00000000       1.79950000       1.79950000
 pb_xyz=     1.79950000       0.00000000       1.79950000
 pc_xyz=     1.79950000       1.79950000       0.00000000
          1   11.6542826997500
  Primitive Riciprocal 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
 writing FS3D.dat!!!
ibktn,nconb,gap:  140    6    7   12.117267   12.980952    0.863685
ibktn,nconb,gap:  145    6    7   14.004224   14.004394    0.000170
```

```
vp_fermi [2].f90
187             EXIT
188           ENDIF
189         ENDDO
190       ENDIF
191       do irow=1,nrow
192       write(myout,"(A6,I5)")   ' BAND:',irow
193       write(myout,"(6e13.6)")   (fdata(1,irow,KBZFS(jcol))-Efermi,jcol=1,NKFS)
194        IF(irow==nconb) THEN
195           t=1.d0
196         do jcol=1,ncol
197         IF( fdata(1,irow,jcol)- fdata(1,irow-1,jcol) .lt. t+0.1d-4  ) THEN
198           t= fdata(1,irow,jcol)- fdata(1,irow-1,jcol)
199           write(*,"(A,3I5,3F12.6)")'ibktn,nconb,gap:',jcol,nconb-1,nconb,fdata(1,irow-1,jcol),fdata(1,irow,jcol),t
200         ENDIF
201         enddo
202        ENDIF
203       enddo
204       if( ISPIN == 2)  then
205       do irow=1,nrow
206       write(myout,"(A6,I5)")   ' BAND:',irow+nrow
207       write(myout,"(6e13.6)")   (fdata(2,irow,KBZFS(jcol))-Efermi,jcol=1,NKFS)
208       enddo
209       endif
210
211       write(myout,*)  'END_BANDGRID_3D'
212       write(myout,*)  'END_BLOCK_BANDGRID_3D'
213
214       close(myout)
215
216       deallocate(NIBZK,fdata,NCHTS,KBZFS)
Fortran free form source file   length : 5,866   lines : 220   Ln : 199   Col : 51   Sel : 3 | 1   Unix (LF)   UTF-8
```





−0.48



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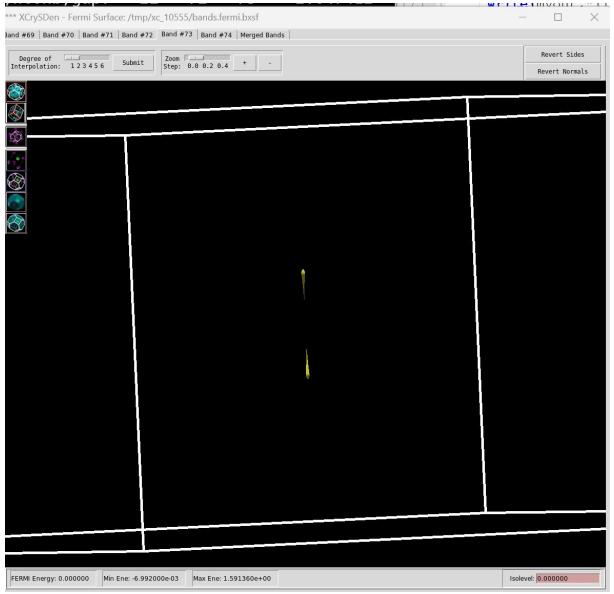
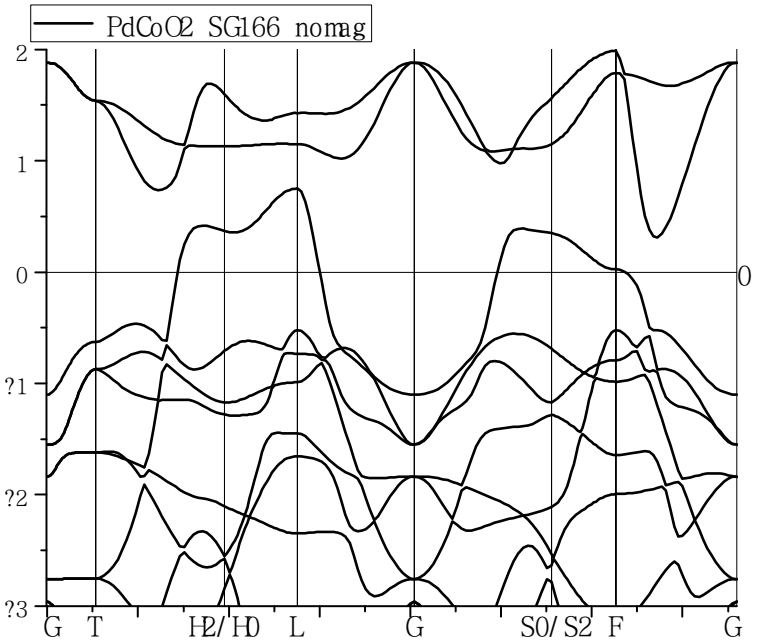
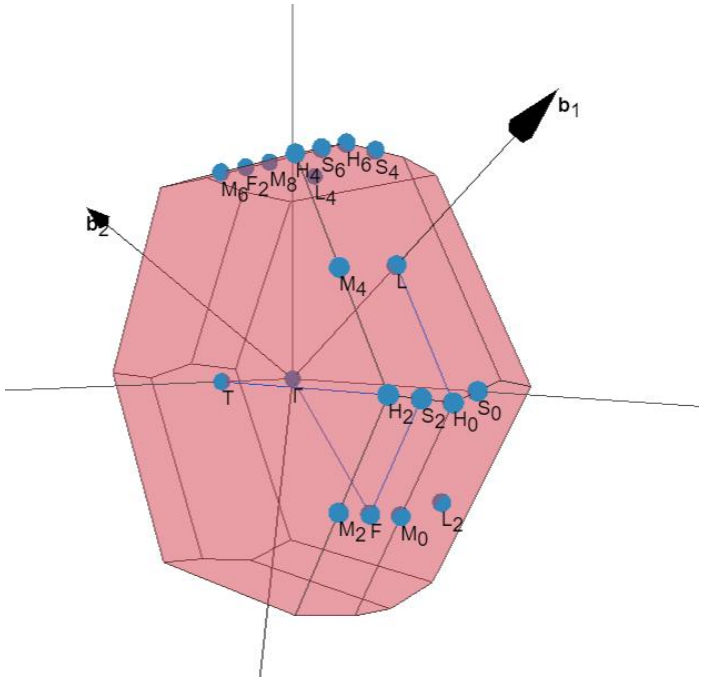
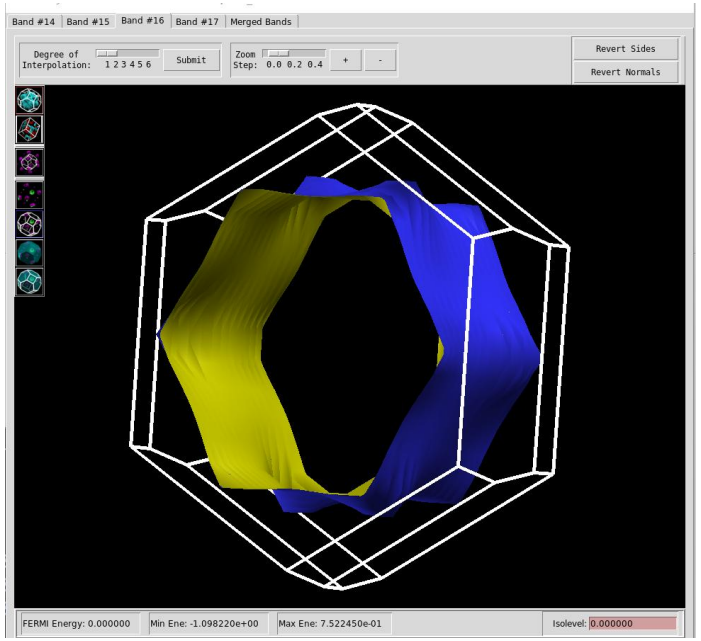


```
The OUTCAR-scf exists, we use it to get the Fermi level,
the RWIGS tag and the number of spins.
Fermi level: 2.1961
ISPIN:  1
  Primitive Cell
 pa_xyz=     5.45900000       0.00000000       0.00000000
 pb_xyz=    -2.72950000       4.72763268       0.00000000
 pc_xyz=     0.00000000       0.00000000       9.67500000
          1   249.693820252038
  Primitive Riciprocal Cell
 pra_xyz=     1.15097734       0.66451708       0.00000000
 prb_xyz=     0.00000000       1.32903416       0.00000000
 prc_xyz=     0.00000000       0.00000000       0.64942484
 writing FS3D.dat!!!
ibktn,nconb,gap:    1   72   73    2.024520    2.197264    0.172744
ibktn,nconb,gap:   38   72   73    2.060718    2.195634    0.134916
ibktn,nconb,gap:   75   72   73    2.152175    2.190804    0.038629
```








```
The OUTCAR-scf exists, we use it to get the Fermi level,
the RWIGS tag and the number of spins.
Fermi level: 8.0479
ISPIN:  1
  Primitive Cell
 pa_xyz=     1.41500000       0.81695063       5.91433333
 pb_xyz=    -1.41500000       0.81695063       5.91433333
 pc_xyz=    -0.00000000      -1.63390126       5.91433333
          1   41.0212887748529
  Primitive Riciprocal Cell
 pra_xyz=     2.22020682       1.28183701       0.35412192
 prb_xyz=    -2.22020682       1.28183701       0.35412192
 prc_xyz=     0.00000000      -2.56367401       0.35412192
 writing FS3D.dat!!!
ibktn,nconb,gap:    7   16   17    8.346311    9.161843    0.815532
ibktn,nconb,gap:    8   16   17    8.800145    9.199257    0.399112
~
```