Fermi-Surface Script Tutorial

Materials Theory and Design Group

Yongjin Shin

Supervisor: James M. Rondinelli

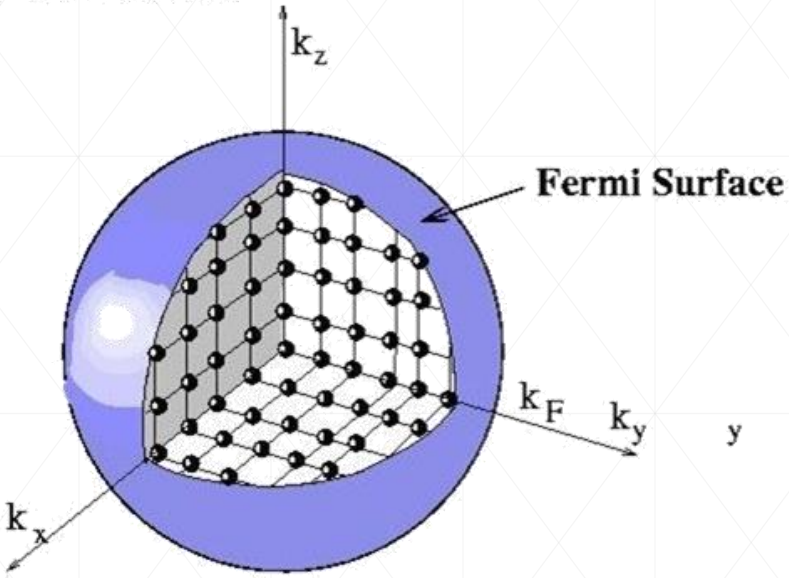
MATERIALS
THEORY AND
DESIGN GROUP

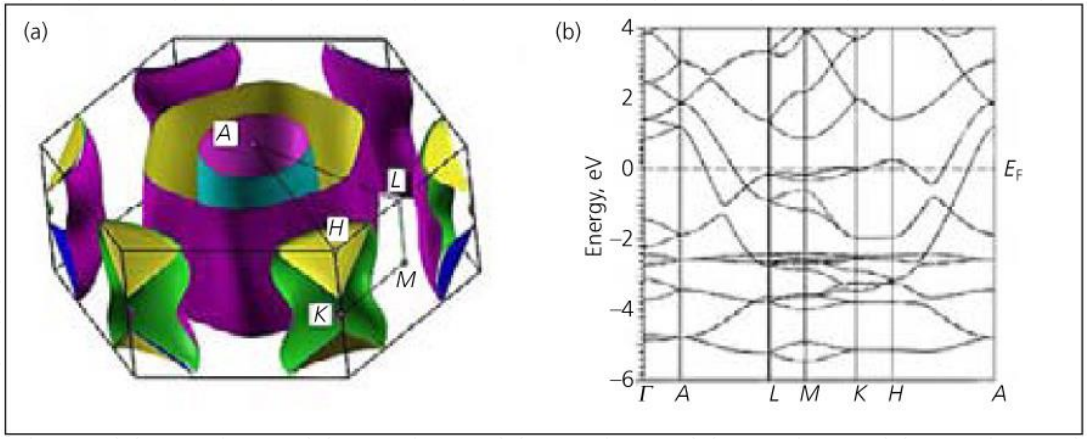
NORTHWESTERN
UNIVERSITY

CONTENTS

- What is fermi surface
- How to draw fermi surface
- Fermi surface with VASP and Xcrysden: Python script

Fermi Surface



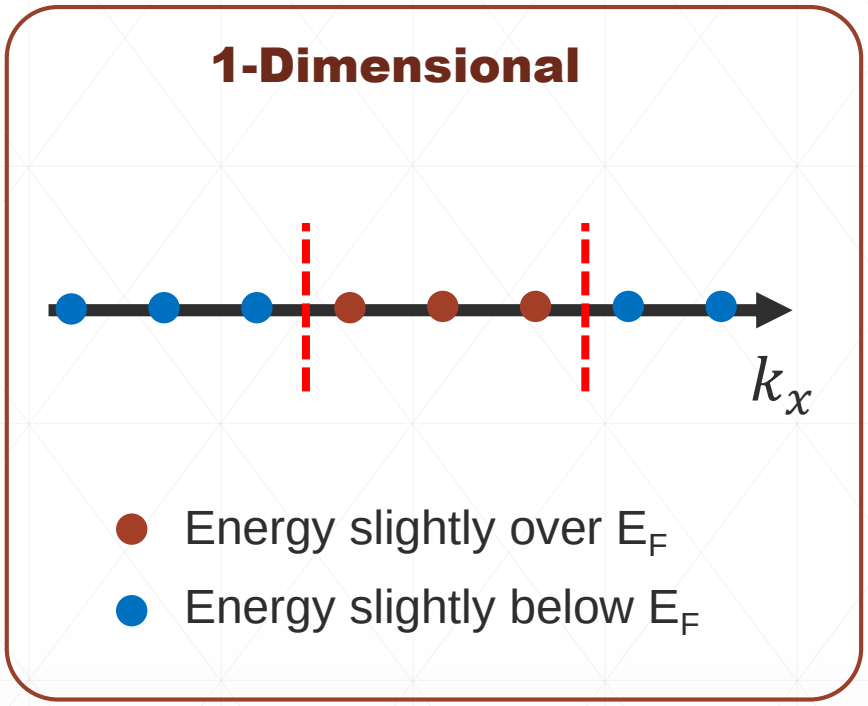


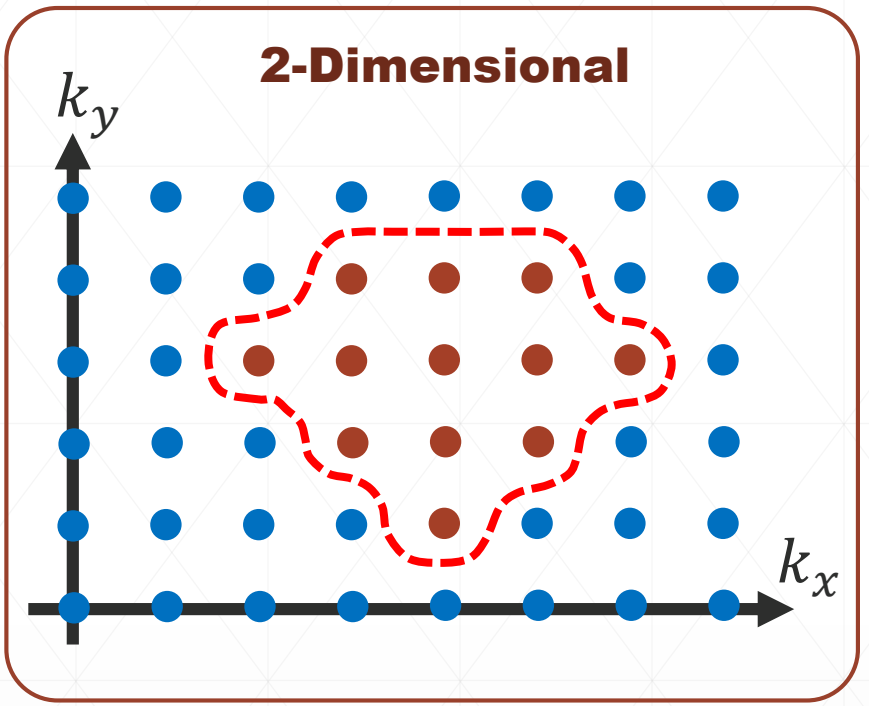
A. Ivanovskii, Platinum Metals Rev., 2013, 57, (2), 87

Fermi Surface

- Abstract boundary in reciprocal space
- Useful for predicting the thermal, electrical, magnetic, and optical properties
- Derived from periodicity and symmetry of the crystalline lattice
- Direct consequence of Pauli exclusion principle, and occupation of electronic bands
- Visually more intuitive than providing band structure in some cases (e.g., 2DEG)

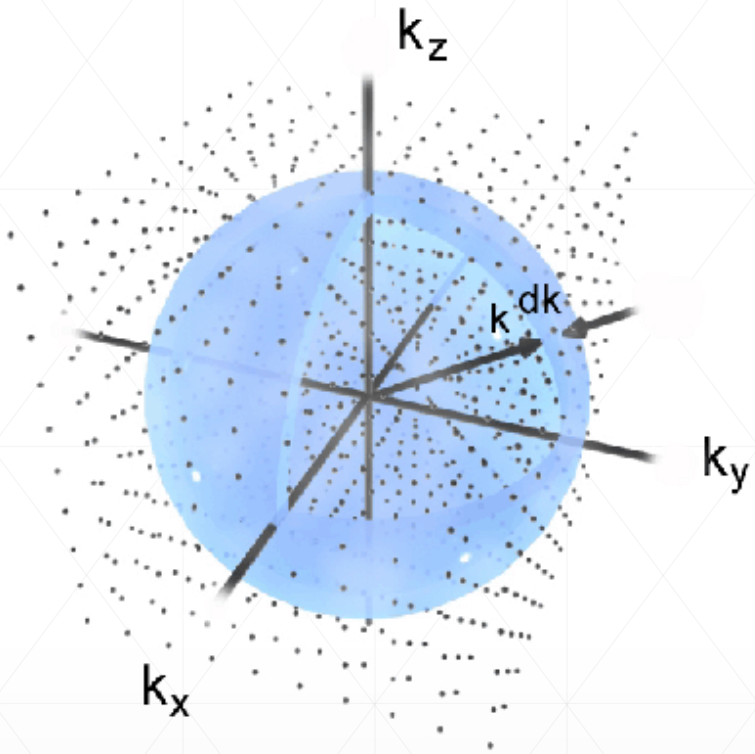
Drawing Fermi Surface in 1-D and 2-D Cases



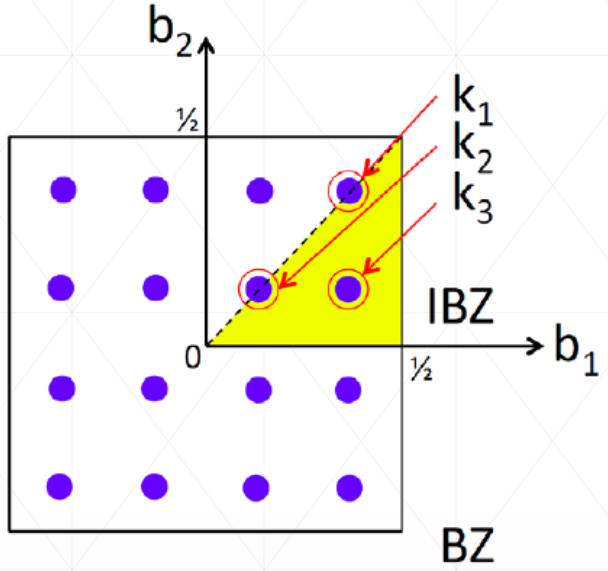


- Fermi surface is drawn where eigen energy of electronic band is equal to E_F
- Multiple boundary can be given depending on electronic bands
- Total fermi surface is collection of the boundaries of all bands

Drawing Fermi Surface in 3-D with VASP



When ISYM ≠ -1



- To draw fermi surface using VASP, 3-dimensional mesh grid should be prepared
- INCAR is very similar to band structure calculation, except for ISYM -tag
- ISYM = -1 # This is to turn off symmetry, and has easier data for do post-process
- Otherwise only Irreducible Brillouin Zone will be calculated on VASP

J. Rondinelli, MSE 458 Course Material, Northwestern Univ. 2015

Step 1: Prepare k-mesh grid

Python script ‘ Fermi_kpoints.py ’

- How to use:
  $ python Fermi_kpoints.py KX KY KZ

  KX, KY, KZ (Optional): number of points along each reciprocal axis
  If not given, default value of 9 is assigned, which is quite high for usual structures.
- Output filename: ‘KPOINTS’

Output example

```
k-points for fermi-surface. RP-phase 9x9x9
1000
Reciprocal
0.0000 0.0000 0.0000 1
0.0000 0.0000 0.1111 1
0.0000 0.0000 0.2222 1
0.0000 0.0000 0.3333 1
0.0000 0.0000 0.4444 1
0.0000 0.0000 0.5556 1
0.0000 0.0000 0.6667 1
0.0000 0.0000 0.7778 1
0.0000 0.0000 0.8889 1
0.0000 0.0000 1.0000 1
0.0000 0.1111 0.0000 1
0.0000 0.1111 0.1111 1
```

- Line 1: Comment
- Line 2: Total number of k-points
- Line 3: Reciprocal
- Line 4-end: reciprocal coordinate of each k-point and its **weight**.

Step 2 & 3: VASP Calculation and Post-processing

Step 2: VASP Calculation

- After self-consistent calculation, use CHGCAR for non self-consistent calculation
- INCAR: ISYM = -1, ICHARG = 11, ISMEAR = 0
- Required files for fermi surface: OUTCAR and EIGENVAL
- OUTCAR: information on reciprocal lattice and fermi energy (E_F)
  EIGENVAL: eigen energy values of electronic bands

Step 3: Create .bxsf file (Script ‘ Fermi_surface.py ’)

- How to use:
  $ python Fermi_surface.py [OUTCAR_file] [EIGENVAL_file] [output.bxsf]

  [OUTCAR_file] (optional): OUTCAR filename from calculation
  default: ‘OUTCAR’

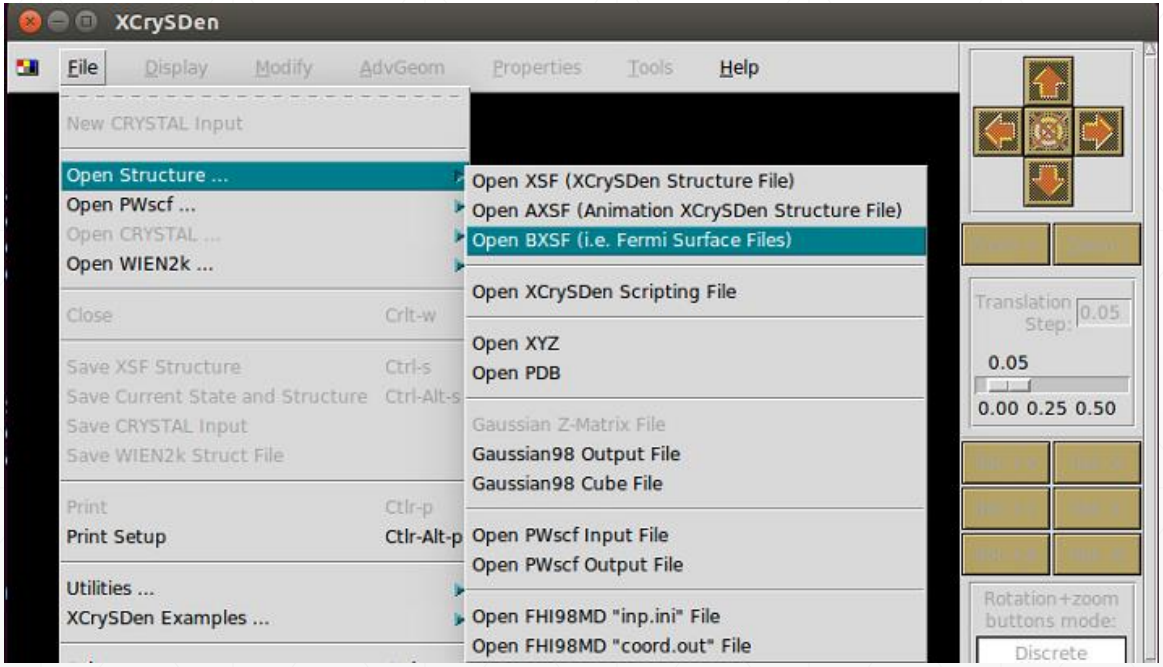
  [EIGENVAL_file] (optional): EIGENVAL filename from calculation
  default: ‘EIGENVAL’
- Output filename: [output.bxsf] (optional)
  default: ‘Xcrysden.bxsf’
- Example: $ python Fermi_surface.py OUTCAR_fermi EIGENVAL_fermi Xcrysden.bxsf

Step 4: Run Xcrysden

Xcrysden

- How to install: http://www.xcrysden.org/Download.html
- Input file: .bxsf file
  Information is given here, http://www.xcrysden.org/doc/XSF.html#__toc__14
- Generated bxsf file is ready to use

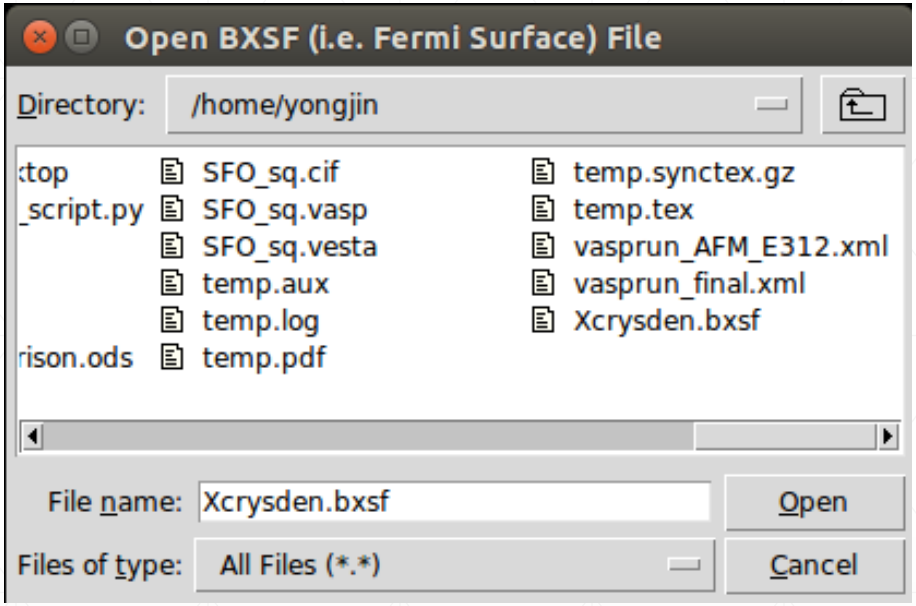
Step by step instruction

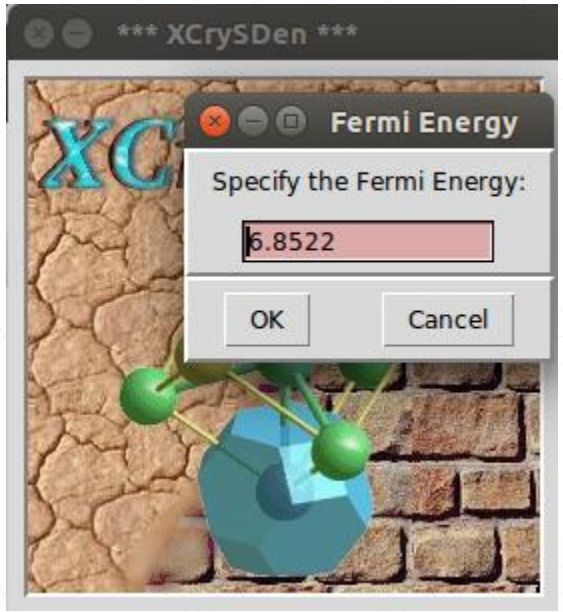


- File
  - Open Structure…
  - Open BXSF

Step 4: Run Xcrysden

Open file

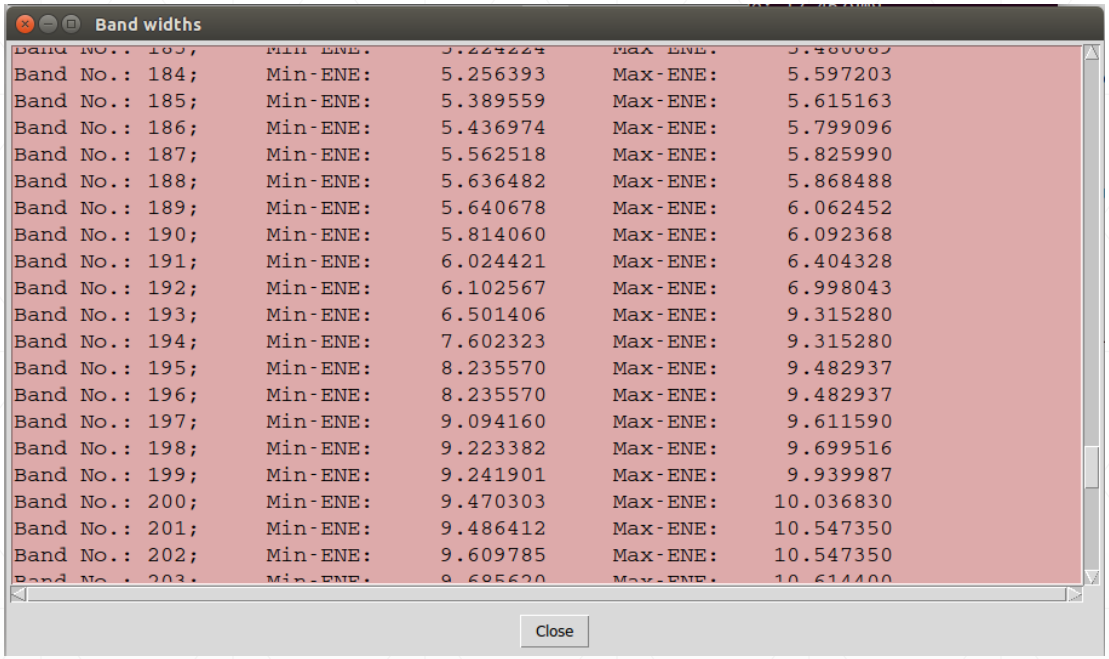


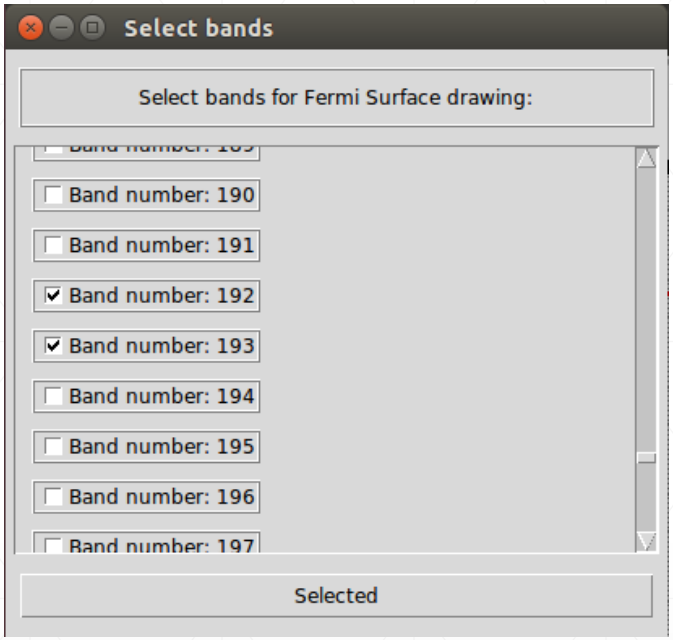


- Fermi energy is automatically filled in.
- Remember the value

Step 4: Run Xcrysden

Select Bands

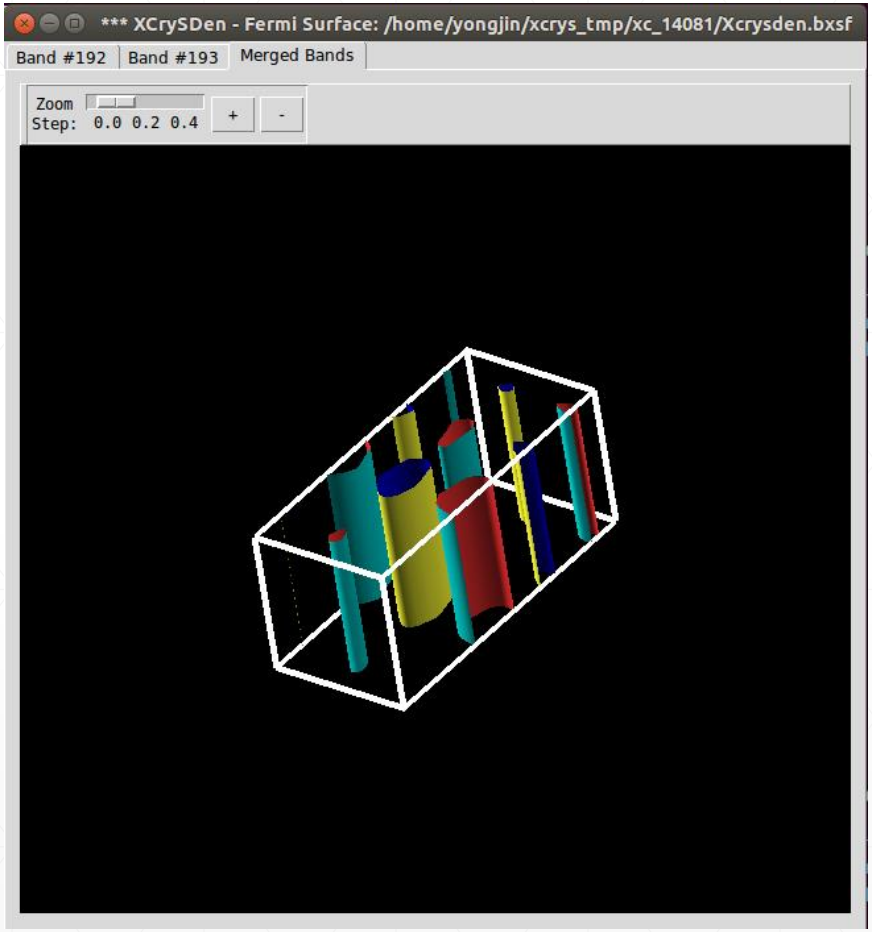




- Find bands goes over E_F, and check on the other window
- You can check based on Min-ENE and Max-ENE of each band
- Bands are listed with increasing order
- Spin polarized system (ISPIN = 2), another set of bands is given below for the other spin.

Step 4: Run Xcrysden

Result



- Ta-da !
- Fermi surface from each bands are given in individual tabs