# Calculating Electronic properties in FPLO

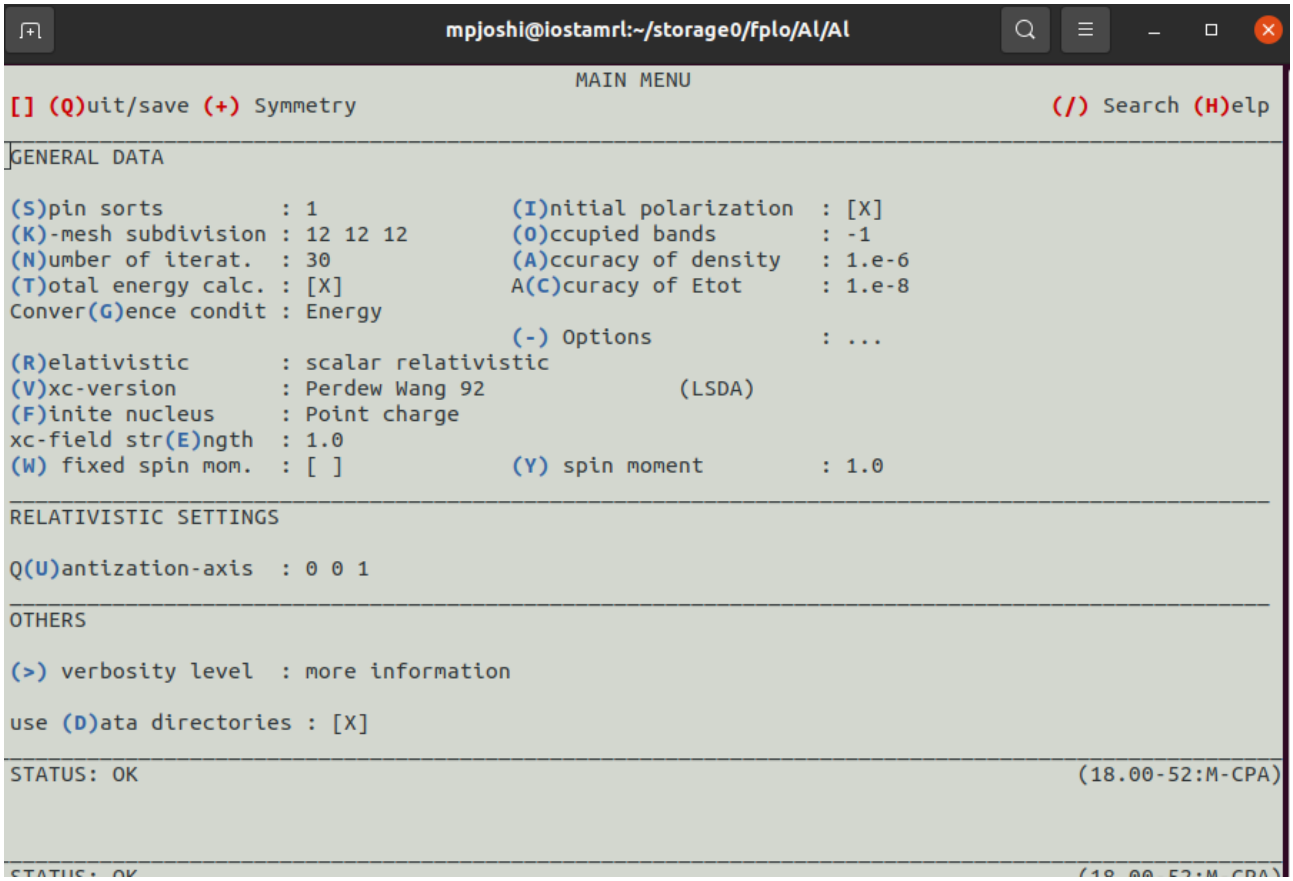
Note: lines ! are suggestions, with $ are commands to be run on terminal, and <> tells just hit enter key

## 1. Default case (Aluminium).

! Open your terminal and login to your ssh (supercomputer). In my case:
$ ssh -X mpjoshi@202.70.90.210 <>
$ inter your password
! If you are logging in first time, grant permission your local pc to ssh and change password. For this,
$ passwd <>
! type old password
! type new password
! retype new password
! After log in, you will see interface like:


! Now, lets begin your calculation.
$ ls <>
$ cd storage0/
$ ls <>
$ mkdir fplo_calculations <>
$ ls <>
$ cd fplo_calculations/ <>  ! For auto direction, just hit Tab key.
$ ls <>
$ mkdir Al <>
$ cd Al/
$ ls <>

$ module load fplo/18.52 <>
$ module load gnu/8.3.0 <>
$ fedit18.00-52-x86_64 <>
$ x
! Edit the file as below.



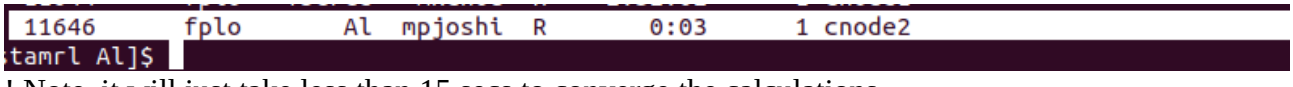

This file is called input file for FPLO calculation names as =.in, which is similar like scf.in in QE and case.struct in Wien2k.
! Here, lets describe some necessary terminologies:
! To change these parameter, just enter blue lettered letter in your keyboard and <>.

(S)pin sorts : 1 for namagnetic case
(S)pin sorts : 2 for magnetic case
(K)-mesh subdivision : 12 12 12 ! Note: initially just take smaller value of K-mesh like 4 4 4 and just analyze the results and increase its value because in some case smaller value K-mesh is enough. This checking is called K-points convergence.
(N)umber of iterat. : 30 ! 30-80 are enough in most of case but maximum value you can take is 999.
(T)otal energy calc. : [X] i.e. ON or True. ! Its calculate Total energy, make it always ON
(T)otal energy calc. : [ ] I.e OF or False.
Conver(G)ence condit : Energy ! 3 or 4 options are most used. To quit from here type x.
(R)elativistic : scalar relativistic ! you can choose full-relativistic or other
V)xc-version : Perdew Wang 92 ! Exchange potential, generally GGA but you can choose other too.
(I)nitial polarization : [X] ie. make it true for scf convergence but not necessarily.
(I)nitial polarization : [ ] ie No polarization.
(A)ccuracy of density : 1.e-6 ! just follow same idea as K-mesh

A(C)curacy of Etot : 1.e-8 ! just follow same idea as K-mesh
use (D)ata directories : [X] make it on as it will create separate file DOS data.
! Do not change other values

! just type '+' key to see your input crystal structure file. To quit from here, type x.
! Now to save your input file, type q and you will see at bottom like:
CHOOSE: Save now the file '=.in'? (Esc: abort) (y/n):
! type y
! Now, you your input file is ready
! To view crystal structure
$ xfplo =.in <>
! quit after viewing crystal structure just by clicking on red power of button like key or just clicking on cross icon at top right corner.
! Now to submit your job, you need fplo.slurm file, which is provided by ssh server. So, copy this file to your current directory ie. Al. For this, there are two options:
> one copying from your local pc to ssh
> second is from ssh to ssh
! Copying from local pc to ssh;
! scp -r path_of_your_fplo.slurm_downloaded directory/fplo.slurm your ssh ID:path of your current directory i.e Al in ssh
! In my case, fplo.slurm file is located in Download directory. So,
$ scp -r /home/pawan/Downloads/fplo.slurm mpjoshi@202.70.90.210:/home/mpjoshi/storage0/fplo_calculations/Al/
$ type your password <>


! Now, edit this file for proper job submission. For this:
$ vi fplo.slurm
$ i ! to go in insert mode
! Edit this as #SBATCH -J Al # Job name
! #SBATCH -o job.%j.out # Name of stdout output file (%j expands to jobId)
! Do not change if don't know its purpose.
!click Esc key to quit insert mode. Then,
$ shift ; wq <>
$ sbatch fplo.slurm
$ squeue
! look for your ID like this




! Note, it will just take less than 15 secs to converge the calculations.
! Now analyze your scf file.
$ vi job.11646.out <> ! to open file using vi.
$ shift g ! to go to bottom of file
$ ? words (like Gap) ! to search for pattern or information in this case, it will search Band Gap.

$  shift ; q <>   ! to quit scf file   !  To save changes and quit.

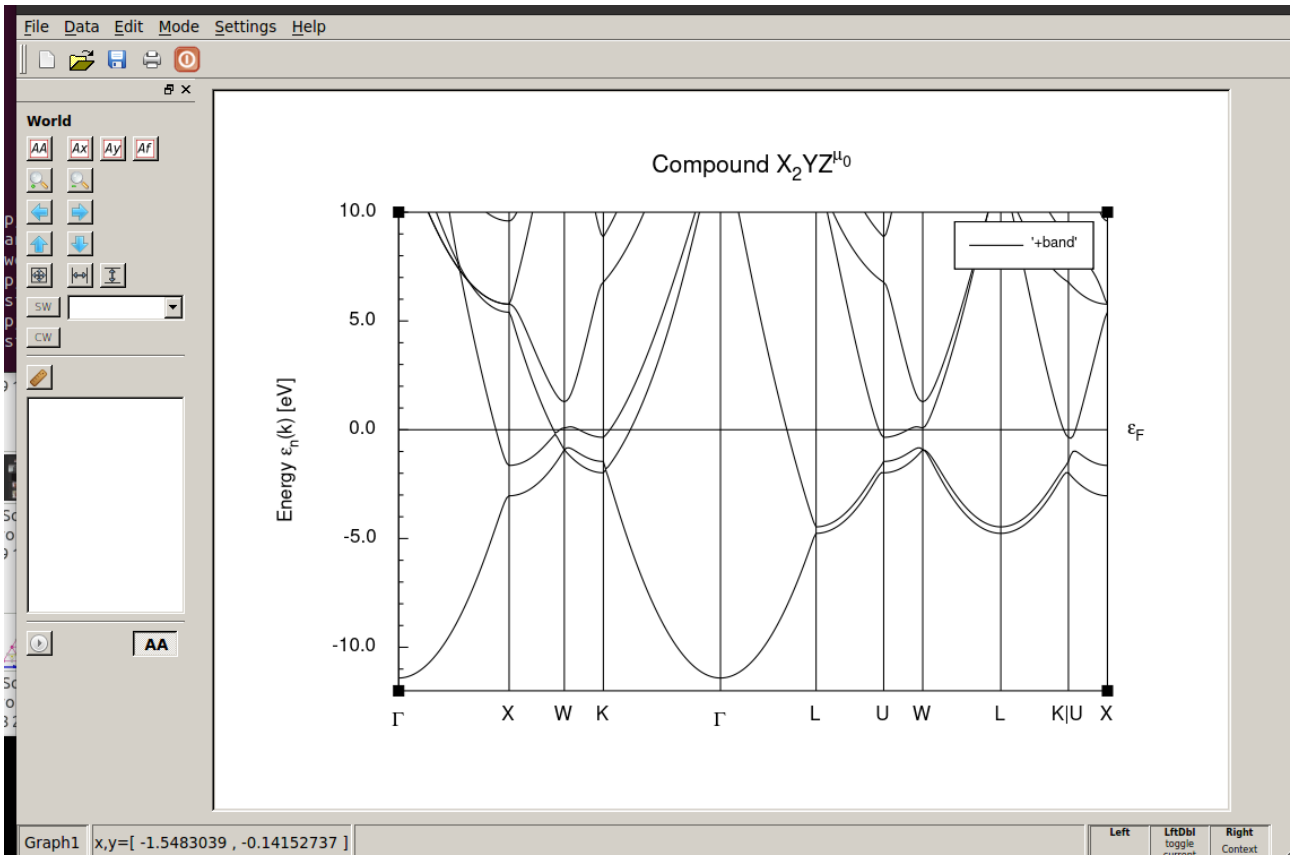
! Now, lets calculate Band structure.
$ fedit18.00-52-x86_64 <>
! Now make following changes
        (N)umber of iterat.  : 1
        (I)nitial polarization  : [ ]
$ hit space key
$ type b
! make changes as:

```
                                        BANDPLOT
e(X)it                                                                  (/) Search (H)elp
_____________________________________________________________________________________________

(B)andstructure plot        : [X]
(R)ead sym-points           : [X]
(S)teps between sym-points  : 50
_____________________________________________________________________________________________
DOS/AKBL/BANDS

Number of e(-)pts (non-CPA) : 1000              (P)lot IDOS      : [ ]
                                                plot n(E)t DOS   : [ ]

(L)ower energy bound [eV] relative to E_f : -20.0
(U)pper energy bound [eV] relative to E_f : 20.0

Restr(I)ct bands to window  : [ ]

Local (D)OS sites    :

Output +(C)oeff file : [ ]

_____________________________________________________________________________________________
BAND WEIGHTS/FAT BANDS

Weights def (F)ile          :

(W)eights                   : [ ]
(T)ransform quant. axis     : [ ]
X-(A)xis                    : 1.0 0.0 0.0
(Z)-axis                    : 0.0 0.0 1.0


(N)umber of sym-points      : 13
_____________________________________________________________________________________________
No.    Label                k-point
_____________________________________________________________________________________________

(1)   : $~G                 : 0 0 0
(2)   : X                   : 0 1 0
(3)   : W                   : 1/2 1 0
(4)   : K                   : 3/4 3/4 0
(5)   : $~G                 : 0 0 0
(6)   : L                   : 1/2 1/2 1/2
(7)   : U                   : 1/4 1 1/4
(8)   : W                   : 1/2 1 0
(9)   : L                   : 1/2 1/2 1/2
[...]_______________________________________________________________________________________
STATUS: OK                                                          (18.00-52:M-CPA)
```

$ x ! to quit
$ q y ! to save changes and quit file.
! open and edit fplo.slurm file (follow steps above to open and save using vi) to make change as :
 #SBATCH -o job.%j.outband   # Name of stdout output file (%j expands to jobId).

$ sbatch fplo.slurm <>
$ squeue

! wait for convergence.
$ ls <>
$ xfbp +band <>



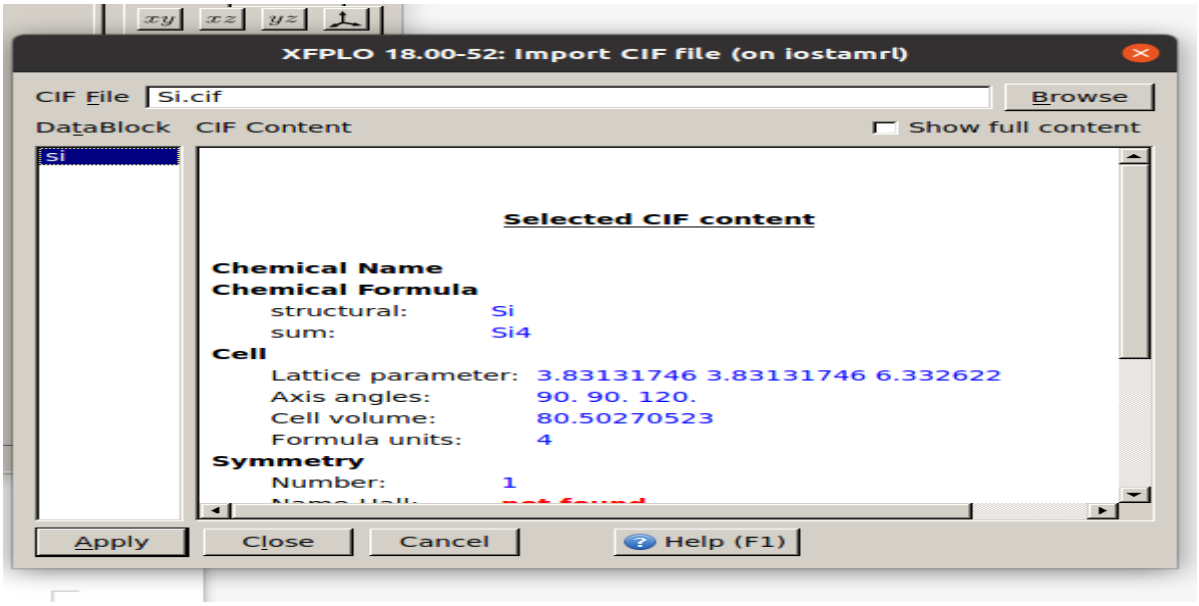

! you will see band structure of Al like this

Look and analyze.
! Quit after viewing.
! To get dos and pdos, go to + dos direcory
$ cd +dos <>
$ xfbp +dos.total <> ! To plot toal dos and so on…
! Play with it more and analyze output.
! For more documentation go to *DOC* directory

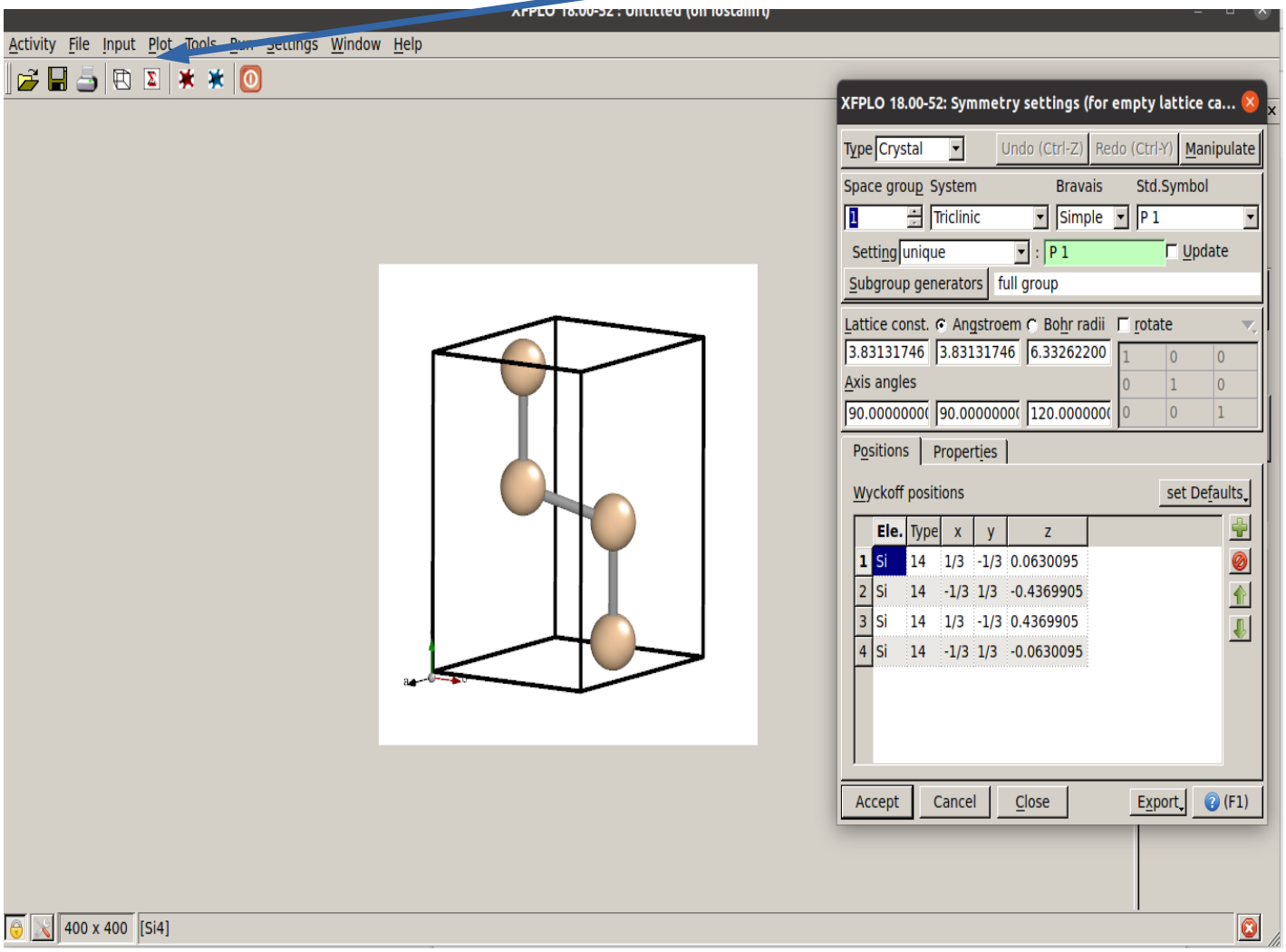
# 2. From cif file (Any compounds having cif).

! Download CIF file of your system from materials project (website link : https://next-gen.materialsproject.org/ )or crystallographic open data base(website link: http://www.crystallography.net/cod/ )
! log in to your ssh
! navigate to fplo_calculations
! make new directory say Si ie.
$ mkdir Si <>
$ cd Si/ <>
$ pwd <>

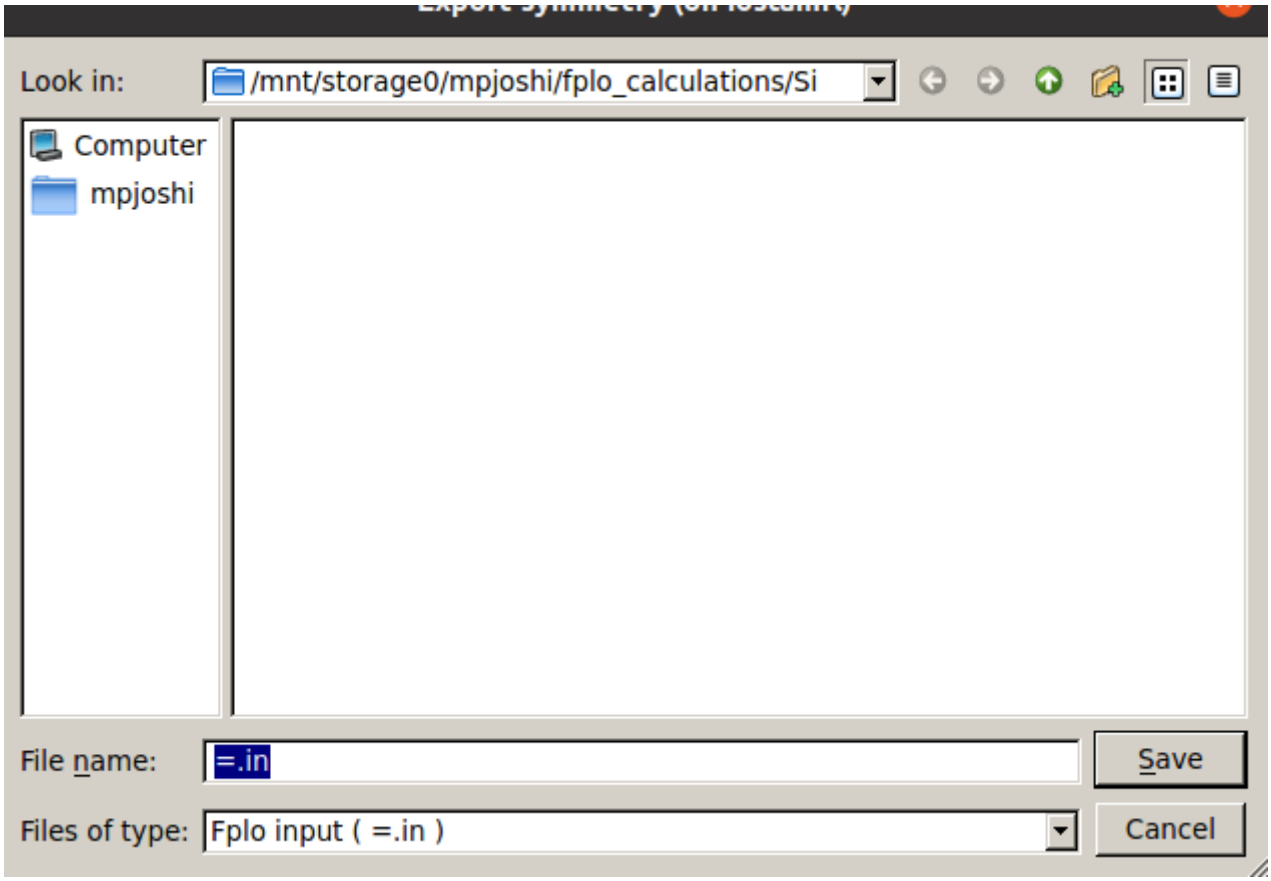
! You will see path of your new current directory
! copy here your Cif file which, you have downloaded from above website. To copy, follow as :
$ scp -r /home/pawan/Downloads/Si.cif mpjoshi@202.70.90.210:/home/mpjoshi/storage0/fplo_calculations/Si/
! Then do:
$ xfplo Si.cif <>
! click on apply at bottom and see the modifications.



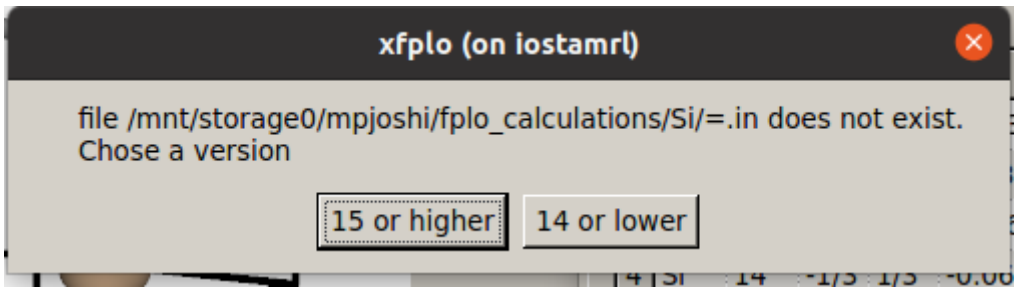

! Click on export ie summation like icon here below.



! Save as =.in




! choose 15 or higher

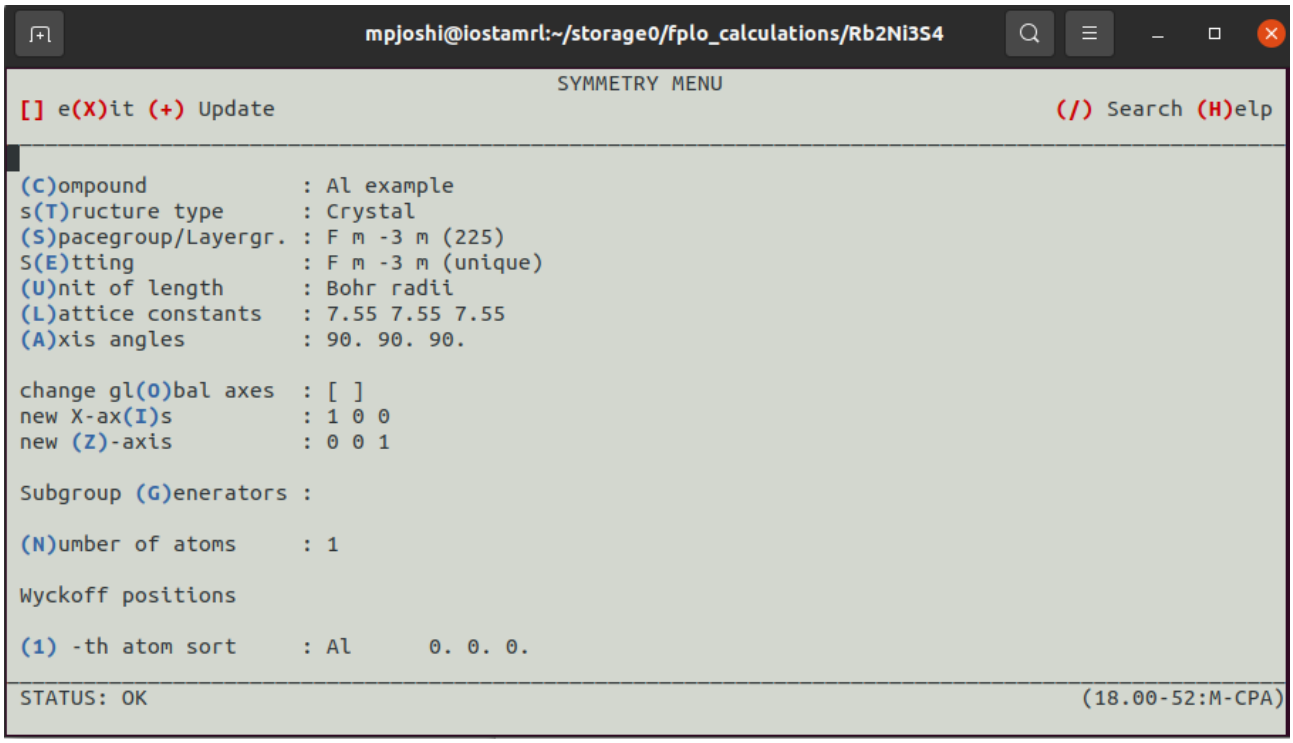



! Then close it and repeat every steps from :
$ fedit18.00-52-x86_64 <>
! follow exactly as same as above

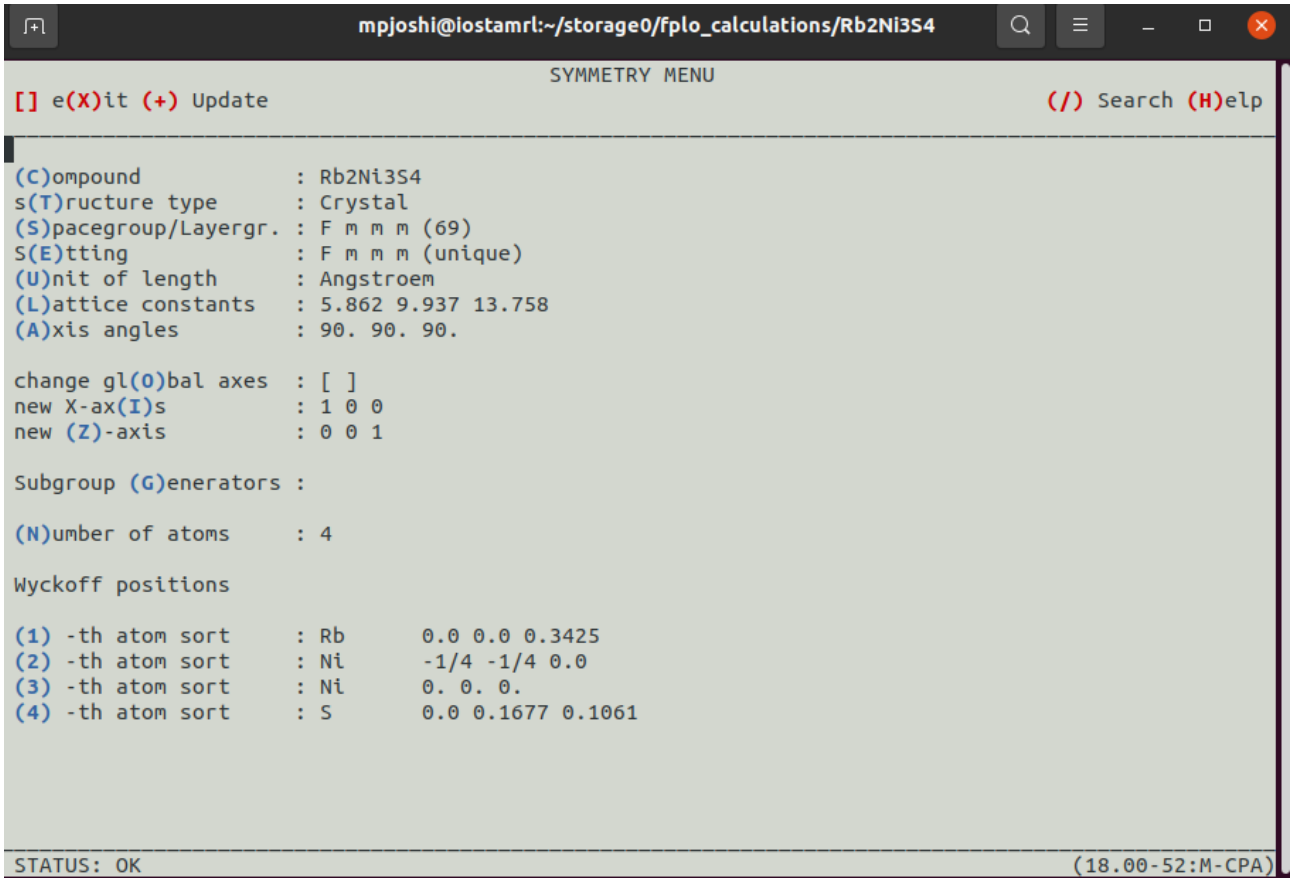
# 3. From paper (Any paper giving information about crystal system).

! Navigate to directory fplo_calculations
! Make a new directory ie.
$ mkdir Rb2Ni3S4
$ cd Rb2Ni3S4/
$ fedit18.00-52-x86_64 <>

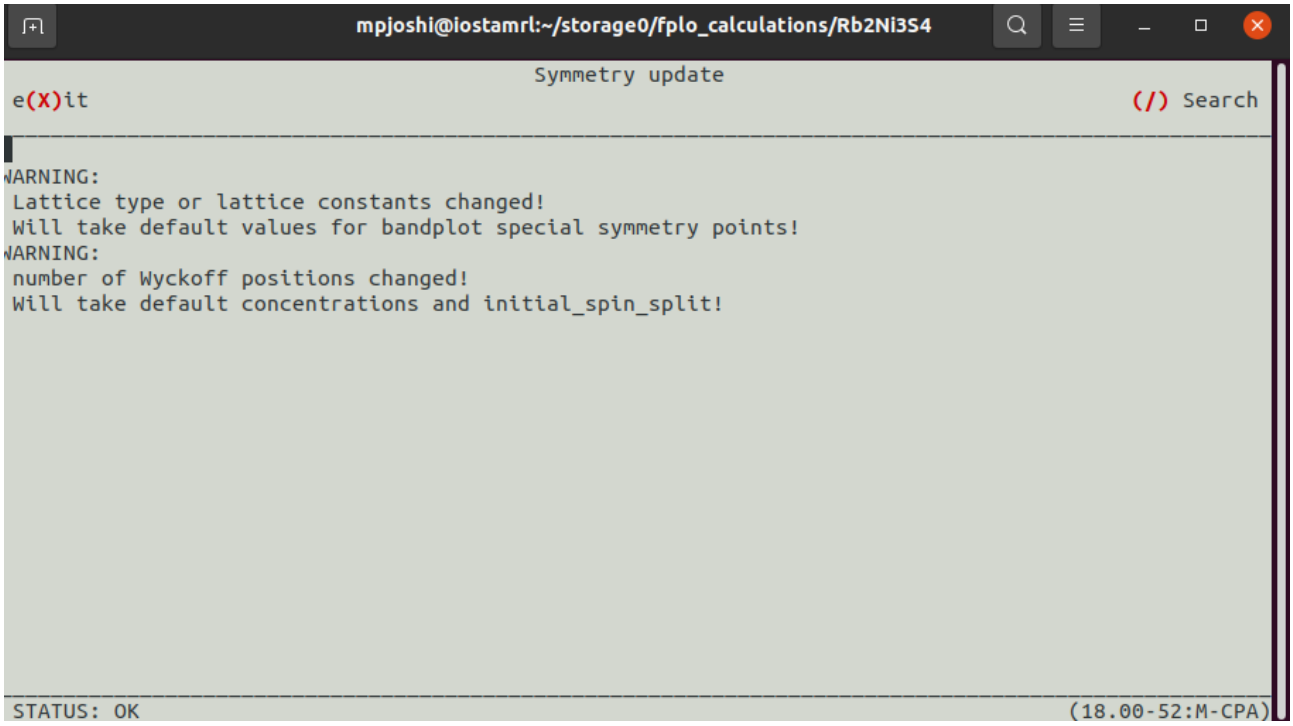
$ x
$ +
! You will see the following interface like this, which is default case of Al.




! edit every steps one by one here like below:



! These all information are from paper by  Mr. Gang Prasad Acharya and Dr,.madhav Prasad Ghimire.  **DOI** 10.1088/1361-651X/ad54e1
! After this, update the structure by clicking '+' button
! You should have like :




! click x
! Now,  proceed as usual….

**For magnetic calculations(Ferro + antiferro) and optical properties,  will be updated soon….. Check the Githublink.**