

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,

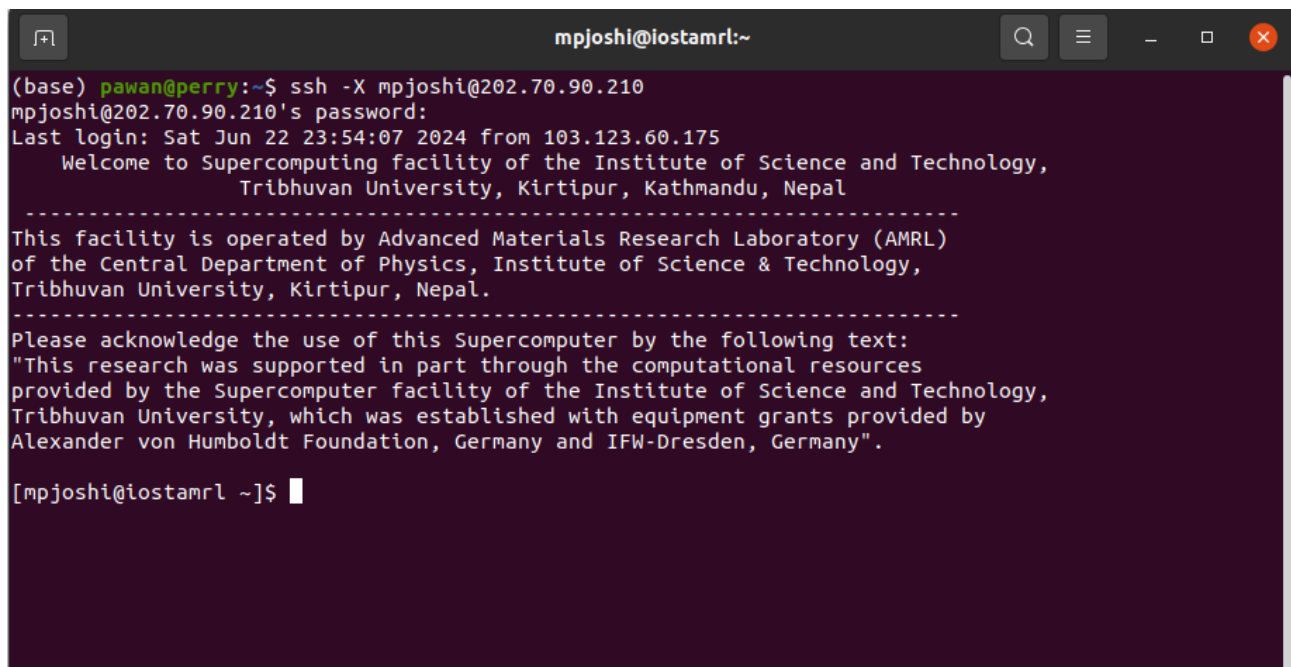
\$ passwd <>

! type old password

! type new password

! retype new password

! After log in, you will see interface like:



```
(base) pawan@perry:~$ ssh -X mpjoshi@202.70.90.210
mpjoshi@202.70.90.210's password:
Last login: Sat Jun 22 23:54:07 2024 from 103.123.60.175
Welcome to Supercomputing facility of the Institute of Science and Technology,
Tribhuvan University, Kirtipur, Kathmandu, Nepal
-----
This facility is operated by Advanced Materials Research Laboratory (AMRL)
of the Central Department of Physics, Institute of Science & Technology,
Tribhuvan University, Kirtipur, Nepal.
-----
Please acknowledge the use of this Supercomputer by the following text:
"This research was supported in part through the computational resources
provided by the Supercomputer facility of the Institute of Science and Technology,
Tribhuvan University, which was established with equipment grants provided by
Alexander von Humboldt Foundation, Germany and IFW-Dresden, Germany".

[mpjoshi@iostamrl ~]$
```

! 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.
```

```
mpjoshi@iostamr:~/storage0/fplo/Al/Al
MAIN MENU
[ ] (Q)uit/save (+) Symmetry (//) Search (H)elp

GENERAL DATA
(S)pin sorts : 1 (I)nitia] polarization : [X]
(K)-mesh subdivision : 12 12 12 (O)ccupied bands : -1
(N)umber of iterat. : 30 (A)ccuracy of density : 1.e-6
(T)otal energy calc. : [X] A(C)curacy of Etot : 1.e-8
Conver(G)ence condit : Energy (-) Options : ...

(R)elativistic : scalar relativistic
(V)xc-version : Perdew Wang 92 (LSDA)
(F)inite nucleus : Point charge
xc-field str(E)ngth : 1.0 (Y) spin moment : 1.0
(W) fixed spin mom. : [ ]

RELATIVISTIC SETTINGS
Q(U)antization-axis : 0 0 1

OTHERS
(>) verbosity level : more information
use (D)ata directories : [X]

STATUS: OK (18.00-52:M-CPA)
```

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)nitia] polarization : [X] ie. make it true for scf convergence but not necessarily.

(I)nitia] 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/Al/Al/
 \$ type your password <>

```

pawan@perry: ~
(base) pawan@perry:~/Downloads$ pwd
/home/pawan/Downloads
(base) pawan@perry:~/Downloads$ cd
(base) pawan@perry:~$ scp -r /home/pawan/Downloads/fplo.slurm mpjoshi@202.70.90.210:/home/mpjoshi/storage0/fplo/Al/Al
mpjoshi@202.70.90.210's password:
fplo.slurm                               100% 591    75.3KB/s   00:00
(base) pawan@perry:~$
  
```

! 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

\$ queue

! look for your ID like this

11646	fplo	Al	mpjoshi	R	0:03	1 cnode2
tamrl AlJ\$						

! 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:

```
e(X)it BANDPLOT (/) 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) : S~G : 0 0 0
(2) : X : 0 1 0
(3) : W : 1/2 1 0
(4) : K : 3/4 3/4 0
(5) : S~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).

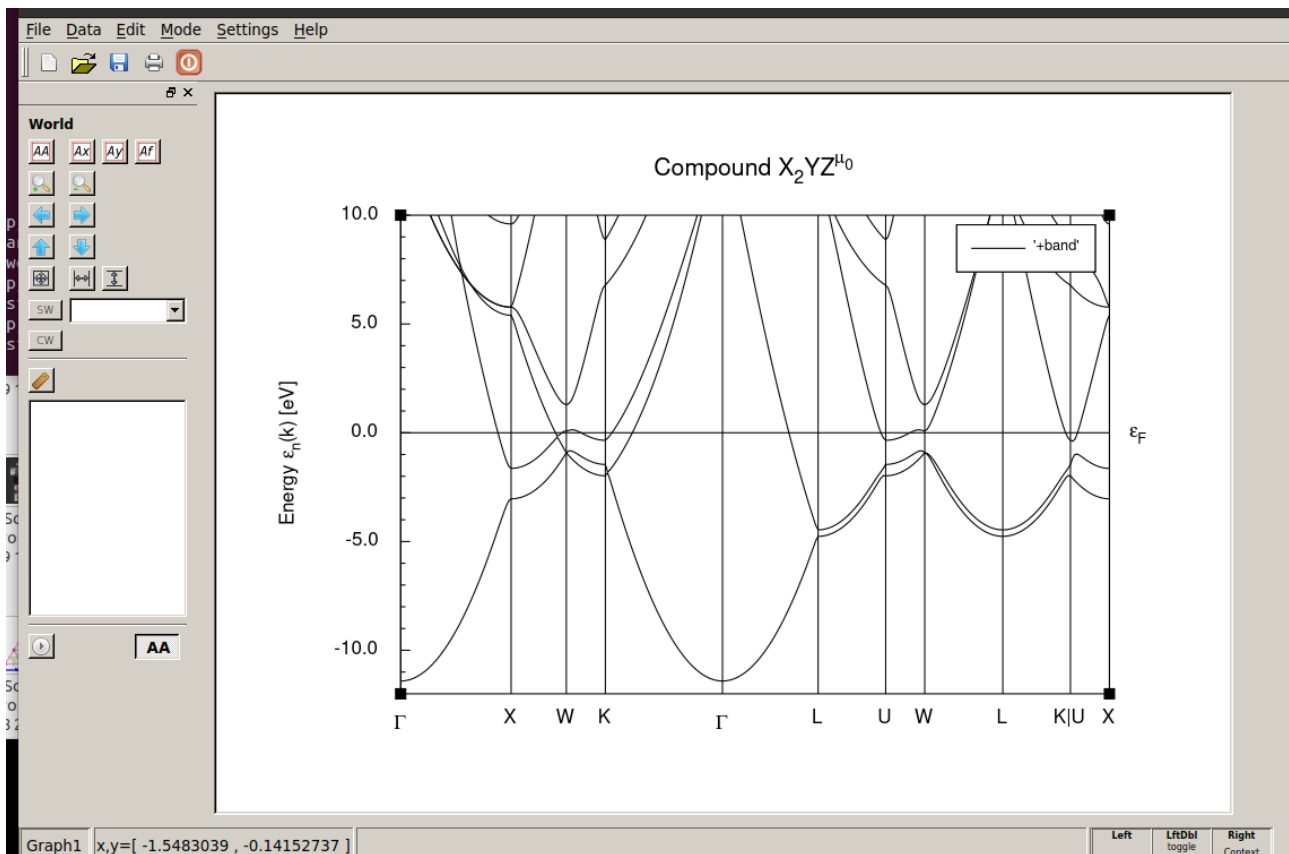
\$ sbatch fplo.slurm <>

\$ queue

! 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 direcorey

\$ 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

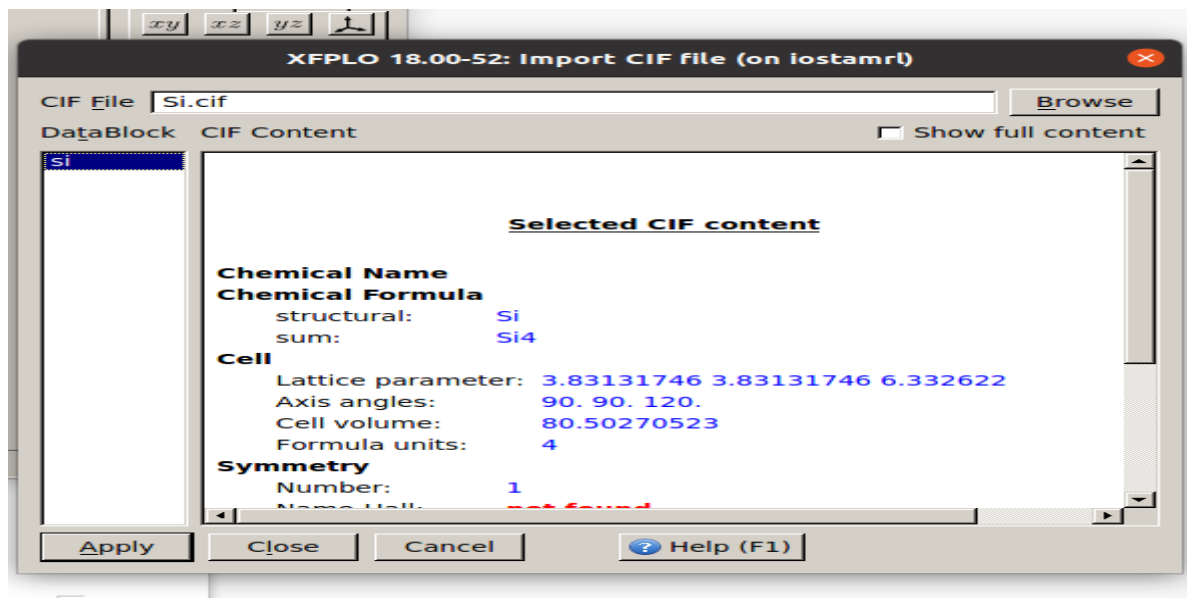
! copy here your Cif file which, you have downloaded from above website. To copy, follow as :

\$ scp -r /home/pawan/Downloads/Si.cif mpjoshi@202.70.90.210:/home/mpjoshi/storage0/fplo_calculations/Si/

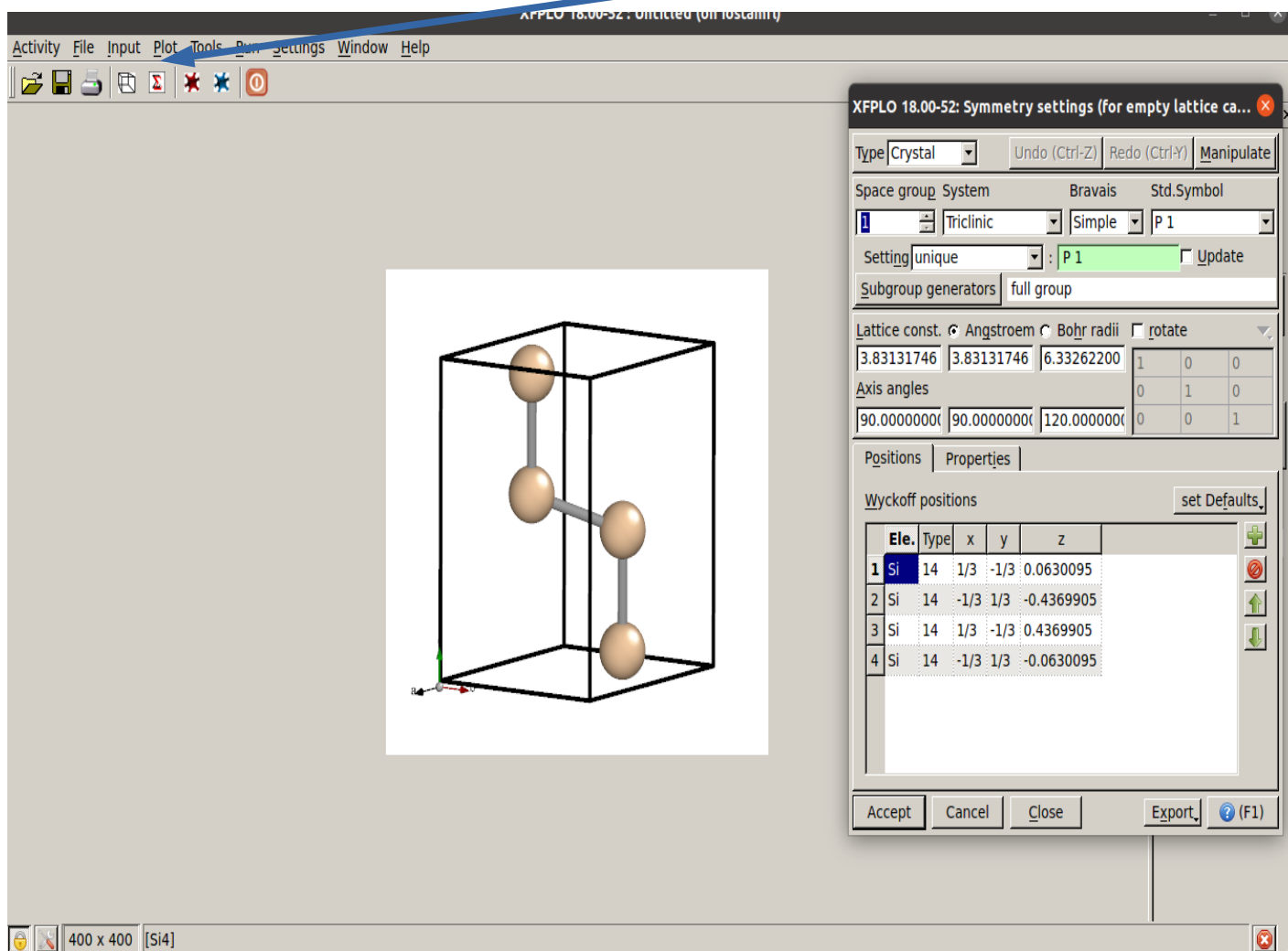
! Then do:

\$ xfplo Si.cif <>

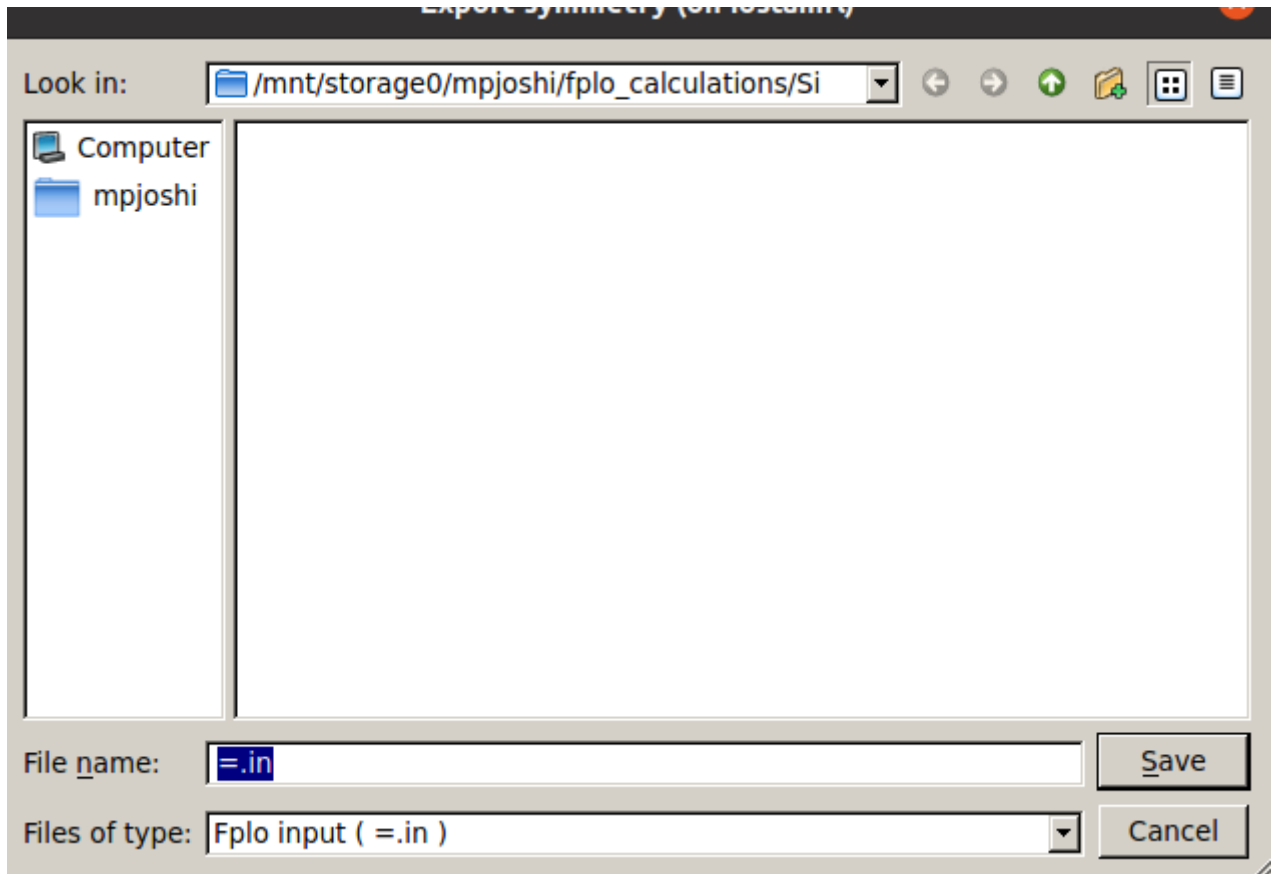
! click on apply at bottom and see the modifications.



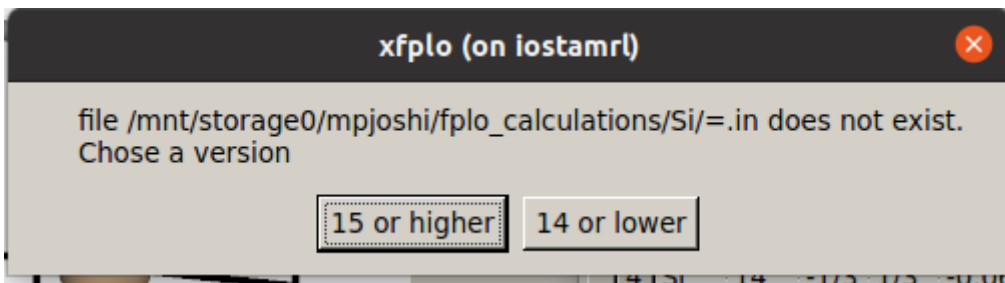
! Click on export ie summation like icon here below.



! 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.

```
mpjoshi@iostamr1:~/storage0/fplo_calculations/Rb2Ni3S4
[ ] e(X)it (+) Update (//) Search (H)elp

(C)ompound      : Al example
s(T)tructure type : Crystal
(S)pacegroup/Layergr. : F m -3 m (225)
S(E)tting      : F m -3 m (unique)
(U)nit of length : Bohr radii
(L)attice constants : 7.55 7.55 7.55
(A)xis angles    : 90. 90. 90.

change gl(0)bal axes : [ ]
new X-ax(I)s        : 1 0 0
new (Z)-axis        : 0 0 1

Subgroup (G)enerators :

(N)umber of atoms    : 1

Wyckoff positions

(1) -th atom sort    : Al      0. 0. 0.

STATUS: OK (18.00-52:M-CPA)
```

! edit every steps one by one here like below:

```
mpjoshi@iostamr1:~/storage0/fplo_calculations/Rb2Ni3S4
[ ] e(X)it (+) Update (//) Search (H)elp

(C)ompound      : Rb2Ni3S4
s(T)tructure type : Crystal
(S)pacegroup/Layergr. : F m m m (69)
S(E)tting      : F m m m (unique)
(U)nit of length : Angstroem
(L)attice constants : 5.862 9.937 13.758
(A)xis angles    : 90. 90. 90.

change gl(0)bal axes : [ ]
new X-ax(I)s        : 1 0 0
new (Z)-axis        : 0 0 1

Subgroup (G)enerators :

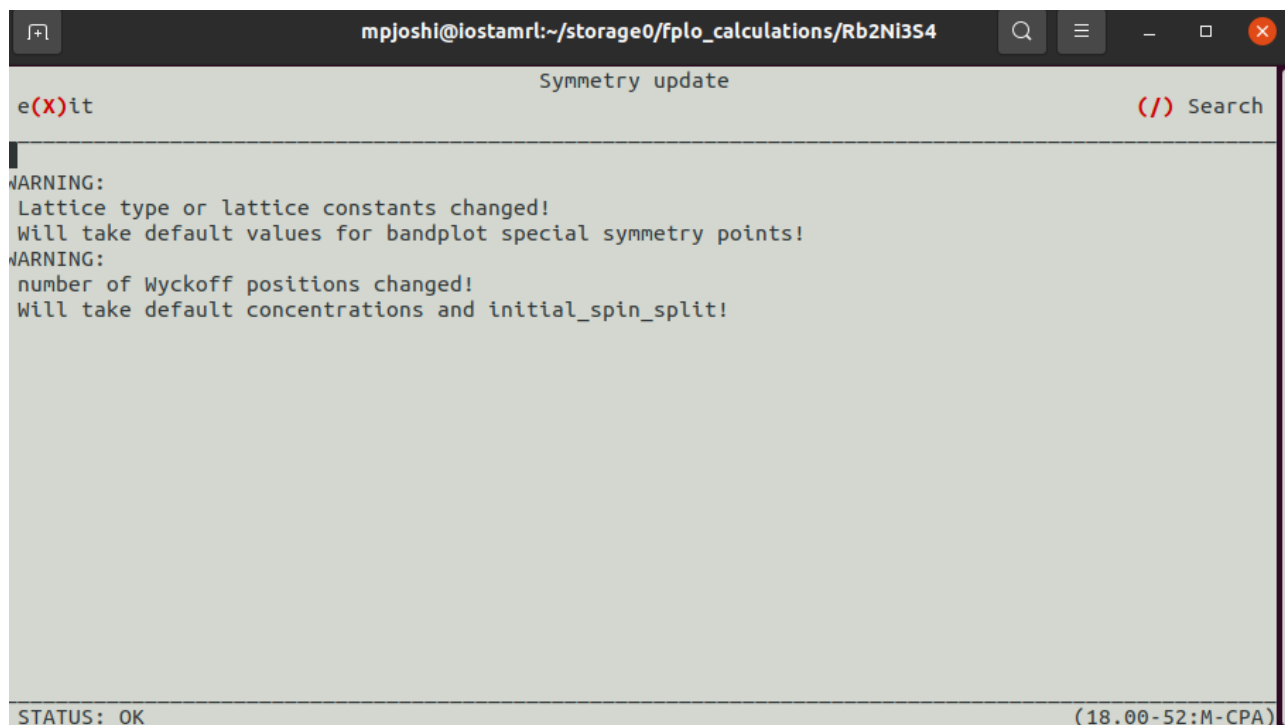
(N)umber of atoms    : 4

Wyckoff positions

(1) -th atom sort    : Rb      0.0 0.0 0.3425
(2) -th atom sort    : Ni      -1/4 -1/4 0.0
(3) -th atom sort    : Ni      0. 0. 0.
(4) -th atom sort    : S       0.0 0.1677 0.1061

STATUS: OK (18.00-52:M-CPA)
```


! 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 :



```
mpjoshi@iostamrl:~/storage0/fplo_calculations/Rb2Ni3S4
Symmetry update
e(x)it (//) Search

WARNING:
Lattice type or lattice constants changed!
Will take default values for bandplot special symmetry points!
WARNING:
number of Wyckoff positions changed!
Will take default concentrations and initial_spin_split!

STATUS: OK (18.00-52:M-CPA)
```

! click x
! Now, proceed as usual....

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