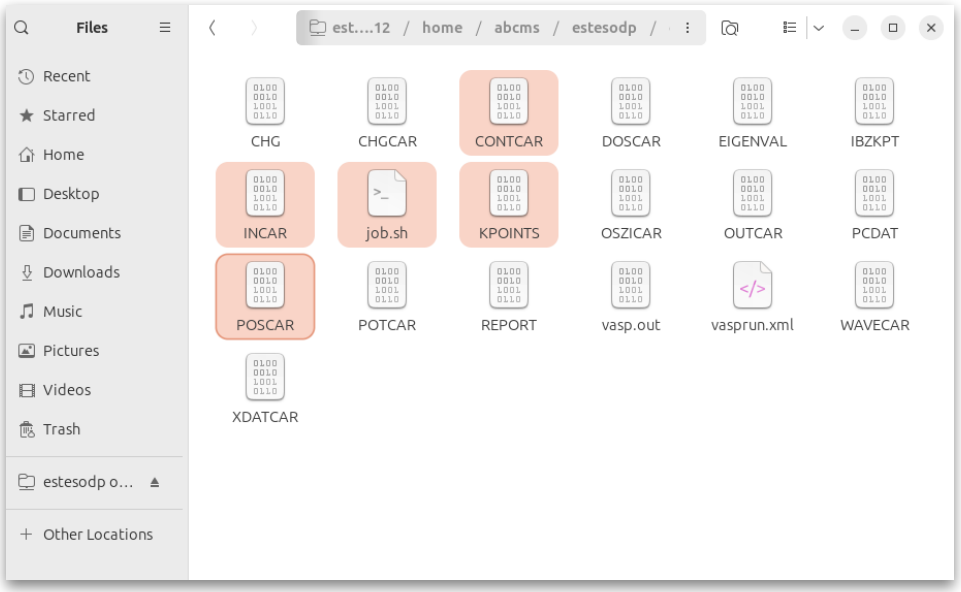
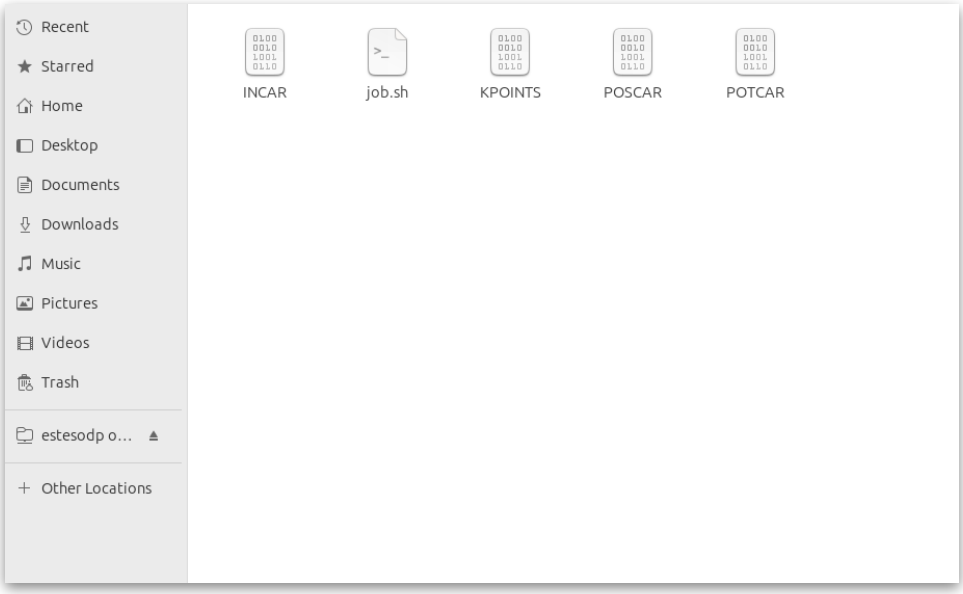
Calculating Band Structure

Band structures are calculated using Non-Self Consistent Field (NSCF) calculations on a special high-symmetry k-points path. For this calculation, charge density and wave functions from a Self Consistent Field (SCF) calculation is taken as input. In this exercise we calculate the band structure of Silicon diamond-FCC and Fe BCC structure.

1. Performing SCF calculation:

- Create a new folder named **scf** in the Silicon diamiond-FCC directory
- Copy the relaxed geometry (CONTCAR) and other input files (INCAR, POTCAR, KPOINTS) along with job script (job.sh) into **scf** folder.





- Rename CONTCAR to **POSCAR** in the **scf** folder using "right click >> rename" option
- Update the INCAR file to write wave functions and charge densities as below:

```
Global Parameters
ISTART =  0            (Read existing wavefunction, if there)
ISPIN  =  1            (Non-Spin polarised DFT)
LREAL  = .FALSE.       (Projection operators: automatic)
LWAVE  = .TRUE.        (Write WAVECAR or not)
LCHARG = .TRUE.        (Write CHGCAR or not)
ADDGRID= .TRUE.        (Increase grid, helps GGA convergence)
LASPH  = .TRUE.        (Give more accurate total energies and band structure calculations)
PREC   = Accurate      (Accurate strictly avoids any aliasing or wrap around errors)
ENCUT  =  450          (Cut-off energy for plane wave basis set, in eV)
LORBIT =  11

Electronic Relaxation
ISMEAR =  0            (Gaussian smearing, metals:1)
SIGMA  =  0.05         (Smearing value in eV, metals:0.2)
NELM   =  90           (Max electronic SCF steps)
NELMIN =  6            (Min electronic SCF steps)
EDIFF  =  1E-06        (SCF energy convergence, in eV)

Ionic Relaxation
NSW    =  00         (Max ionic steps)
IBRION =  -1           (Algorithm: 0-MD, 1-Quasi-New, 2-CG)
ISIF   =  3            (Stress/relaxation: 2-Ions, 3-Shape/Ions/V, 4-Shape/Ions)
EDIFFG = -2E-03        (Ionic convergence, eV/AA)
ISYM =  2              (Symmetry: 0=none, 2=GGA, 3=hybrids)
```

- Optionally, the k-points mesh can also be increased as shown below in the KPOINTS file:

```
Automatic
 0
Monkhorst
21 21 21
0. 0. 0.
```

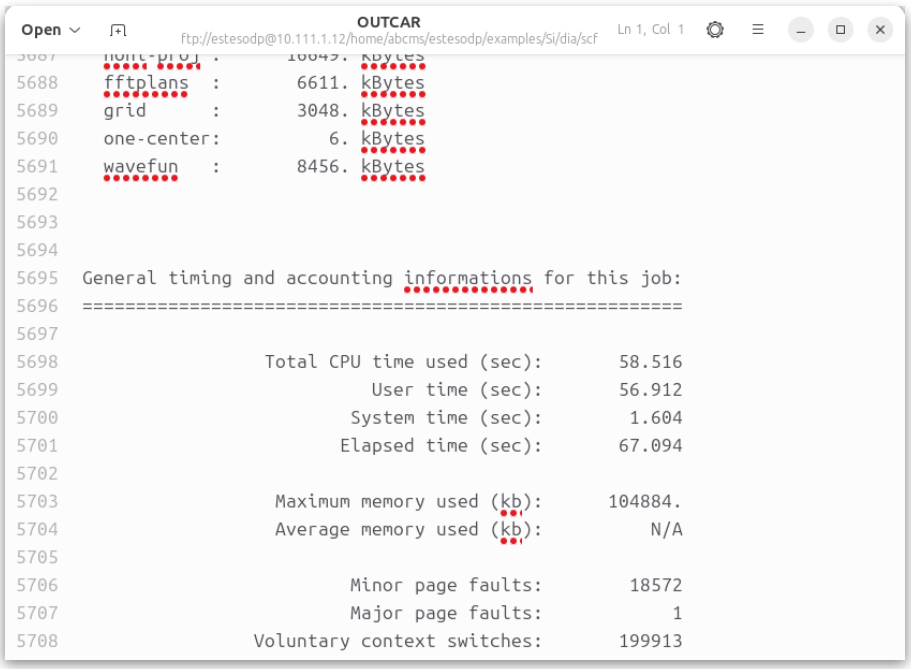
- Submit the job to run using **qsub** command:

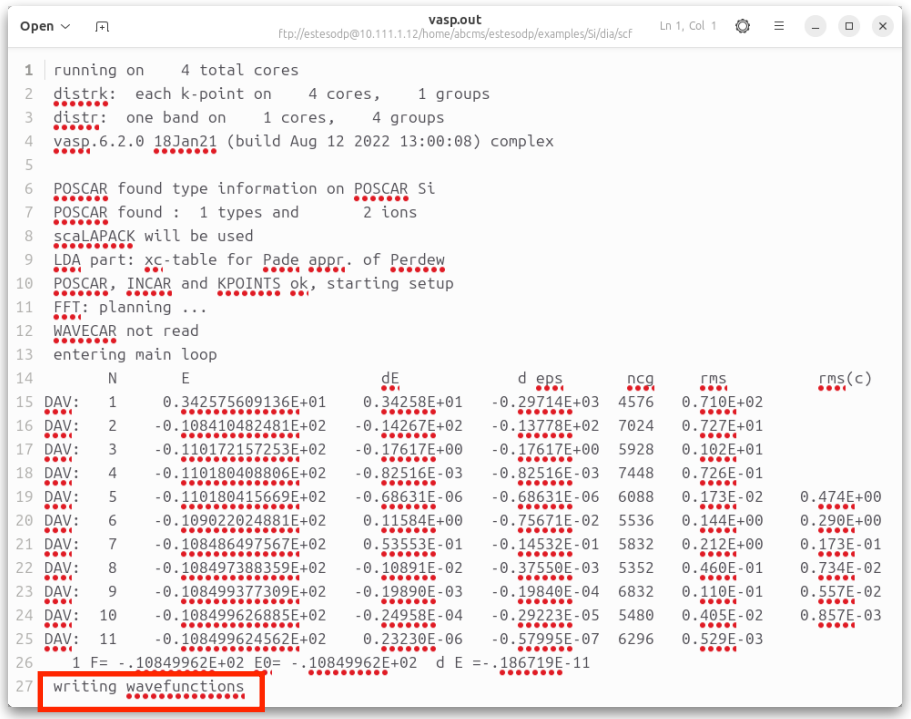
```
qsub job.sh
```

- Verify the running of job using **qstat** command:

```
qstat
```

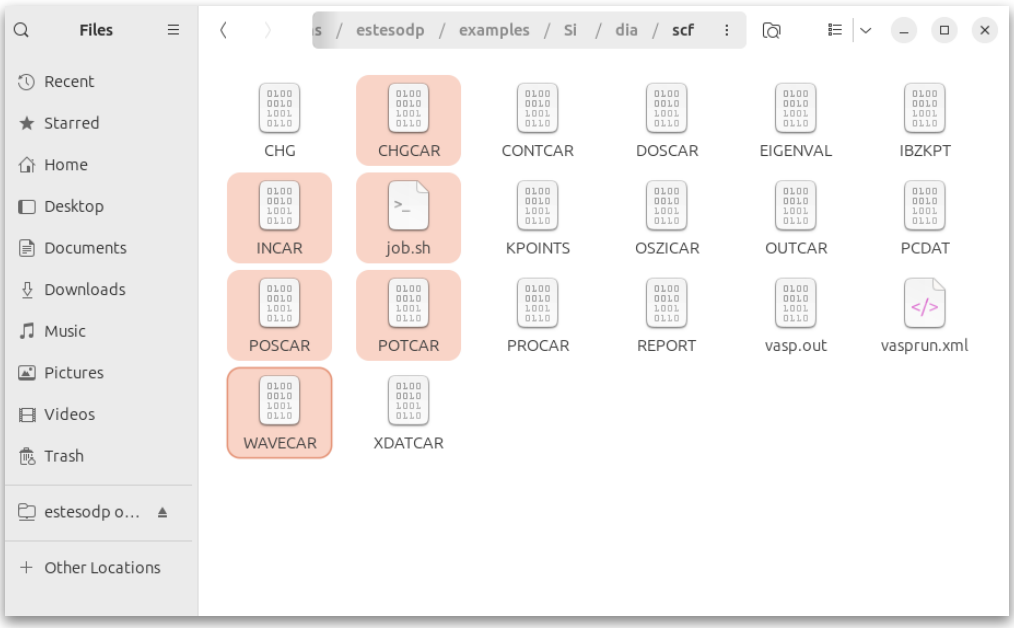
- Once the job is ended, verify the successful completion of the job by opening **vast.out** and **OUTCAR** files

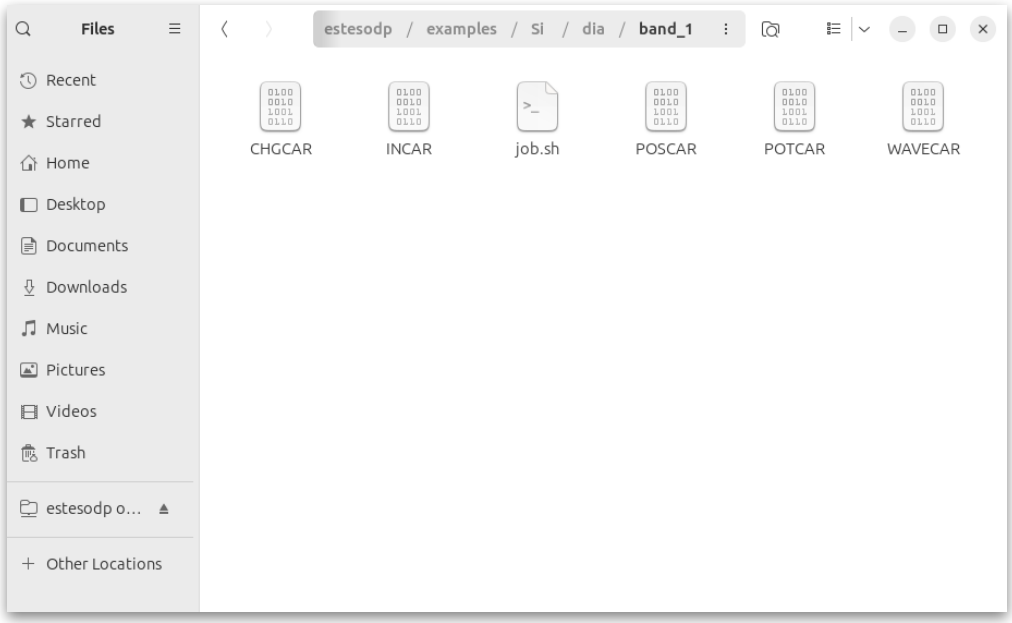




2. Performing band structure calculations:

- Create a folder named **band**
- Copy the following files from **scf** folder to **band** folder





- In the terminal app, move to the band directory using “cd” command:

```
cd ~/<your name>/Si/diamond/band
```

- To generate the high-symmetry k-path for band structure, run “vaspkit” package

```
[estesodp@dendrite band_1]$ vaspkit
```

- Go through the options listed on the screen, we need to select option “03”

```
                (_/
===================== Structural Utilities =====================
01) VASP Input-Files Generator    02) Mechanical Properties
03) K-Path for Band-Structure     04) Structure Editor
05) Catalysis-ElectroChem Kit     06) Symmetry Analysis
07) Materials Databases           08) Advanced Structure Models
===================== Electronic Utilities =====================
11) Density-of-States             21) Band-Structure
23) 3D Band-Structure             25) Hybrid-DFT Band-Structure
26) Fermi-Surface                 28) Band-Structure Unfolding
31) Charge-Density Analysis       42) Potential Analysis
44) Piezoelectric Properties      51) Wave-Function Analysis
62) Magnetic Analysis             65) Spin-Texture
68) Transport Properties
======================== Misc Utilities ========================
71) Optical Properties            72) Molecular-Dynamics Kit
74) User Interface                78) VASP2other Interface
84) ABACUS Interface              91) Semiconductor Kit
92) 2D-Material Kit               95) Phonon Analysis
0)  Quit
------------>>
03
```

- After typing “03” and pressing “Enter” will show another list of options, where we need to select “303”

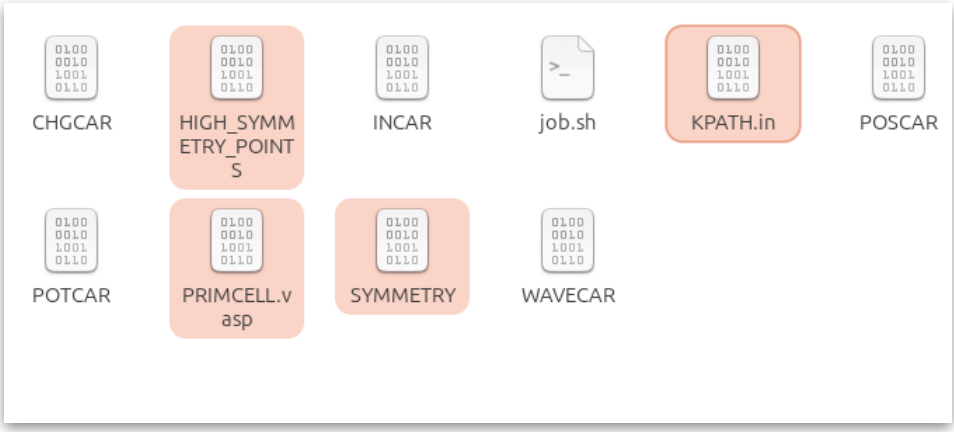
```
03
 ===================== K-Path Options ============================
 301) 1D Structure
 302) 2D Structure
 303) Bulk Structure
 304) K-Path for Wannier90 Code
 305) K-Path for Phonopy Code
 306) K-Path for CP2K Code
 309) Visualize K-Path in First Brillouin Zone

 0) Quit
 9) Back
 ------------>>
303
```

- This will generate the following output:

```
+-------------------------------------------------------------+
+------------------------- Summary ---------------------------+
                          Prototype: A
          Total Atoms in Input Cell:   2
    Lattice Constants in Input Cell:   3.867   3.867   3.867
       Lattice Angles in Input Cell:  60.000  60.000  60.000
      Total Atoms in Primitive Cell:   2
Lattice Constants in Primitive Cell:   3.867   3.867   3.867
   Lattice Angles in Primitive Cell:  60.000  60.000  60.000
                     Crystal System: Cubic
                      Crystal Class: m-3m
                    Bravais Lattice: cF
           Extended Bravais Lattice: cF2
                 Space Group Number: 227
                        Point Group: 32 [ Oh ]
                      International: Fd-3m
                Symmetry Operations:  48
                   Suggested K-Path: (shown in the next line)
[ GAMMA-X-U|K-GAMMA-L-W-X ]
+-------------------------------------------------------------+
-->> (01) Written HIGH_SYMMETRY_POINTS File for Reference.
-->> (02) Written PRIMCELL.vasp file.
-->> (03) Written KPATH.in File for Band-Structure Calculation.
```

```
 -->> (02) Written PRIMCELL.vasp file.
 -->> (03) Written KPATH.in File for Band-Structure Calculation.
 o---------------------------WARNING---------------------------o
 | Do NOT forget to copy PRIMCELL.vasp to POSCAR unless you know |
 |   what you are doing. Otherwise you might get wrong results!  |
 o---------------------------------------------------------------o
 o---------------------------------------------------------------o
 |                        * ACKNOWLEDGMENTS *                    |
 | Other Contributors (in no particular order): Peng-Fei LIU,    |
 | Xue-Fei LIU, Dao-Xiong WU, Zhao-Fu ZHANG, Tian WANG, Qiang LI,|
 | Ya-Chao LIU, Jiang-Shan ZHAO, Qi-Jing ZHENG, Yue QIU and You! |
 | Advisors: Wen-Tong GENG, Yoshiyuki KAWAZOE                    |
 :) Any Suggestions for Improvement are Welcome and Appreciated (:
 |---------------------------------------------------------------|
 |                          * CITATIONS *                        |
 | When using VASPKIT in your research PLEASE cite the paper:    |
 | [1] V. WANG, N. XU, J.-C. LIU, G. TANG, W.-T. GENG, VASPKIT: A|
 | User-Friendly Interface Facilitating High-Throughput Computing|
 | and Analysis Using VASP Code, Computer Physics Communications |
 | 267, 108033, (2021), DOI: 10.1016/j.cpc.2021.108033           |
 o---------------------------------------------------------------o
[estesodp@dendrite band_1]$
```

- It will also generate a set of files as shown below:



- Rename **KPATH.in** file to **KPOINTS**
- Update the **INCAR** file to read the WAVECAR and CHGCAR files in the calculations

```
GGlobal Parameters
ISTART =  1            (Read existing wavefunction, if there)
ICHARG =  11           (Non-self-consistent: GGA/LDA band structures)
ISPIN  =  1            (Non-Spin polarised DFT)
LREAL  = .FALSE.       (Projection operators: automatic)
LWAVE  = .TRUE.        (Write WAVECAR or not)
LCHARG = .TRUE.        (Write CHGCAR or not)
ADDGRID= .TRUE.        (Increase grid, helps GGA convergence)
LASPH  = .TRUE.        (Give more accurate total energies and band structure calculations)
PREC   = Accurate      (Accurate strictly avoids any aliasing or wrap around errors)
ENCUT  =  450          (Cut-off energy for plane wave basis set, in eV)
LORBIT =  11

Electronic Relaxation
ISMEAR =  0            (Gaussian smearing, metals:1)
SIGMA  =  0.05         (Smearing value in eV, metals:0.2)
NELM   =  90           (Max electronic SCF steps)
NELMIN =  6            (Min electronic SCF steps)
EDIFF  =  1E-06        (SCF energy convergence, in eV)

Ionic Relaxation
NSW    =  00          (Max ionic steps)
IBRION =  -1           (Algorithm: 0-MD, 1-Quasi-New, 2-CG)
ISIF   =  3            (Stress/relaxation: 2-Ions, 3-Shape/Ions/V, 4-Shape/Ions)
EDIFFG = -2E-03        (Ionic convergence, eV/AA)
ISYM =  2              (Symmetry: 0=none, 2=GGA, 3=hybrids)
```

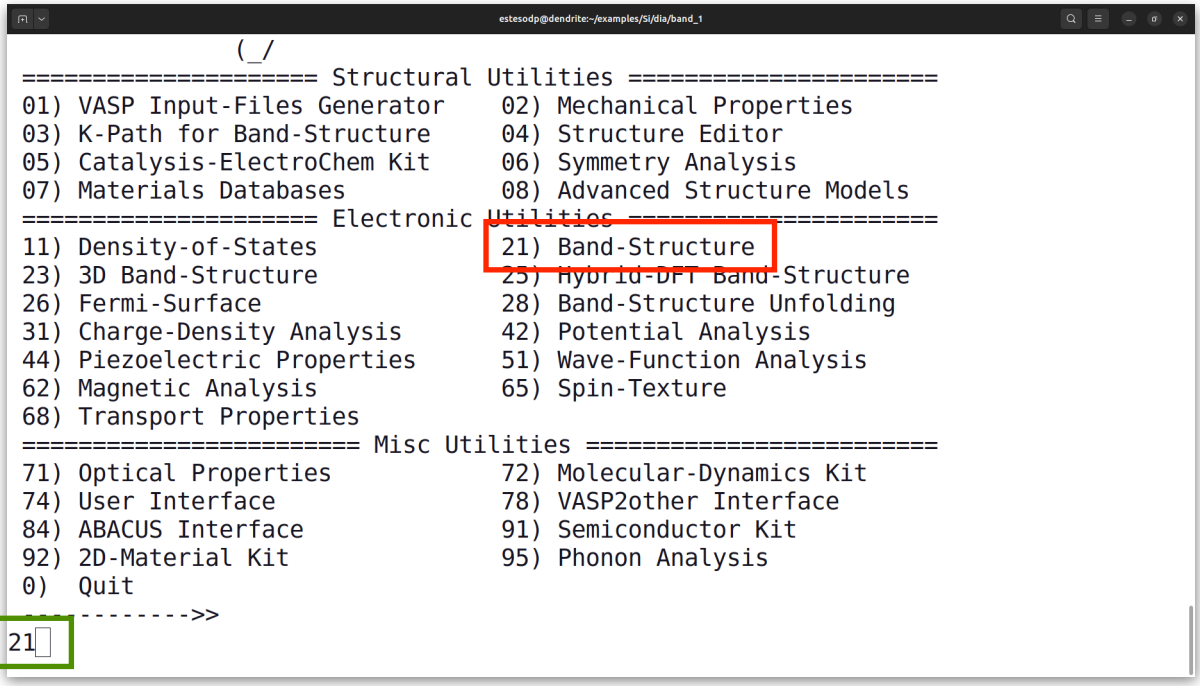
- Submit the job for run using **qsub** command
- Verify the running of job using **qstat** command
- Once the job is ended, verify the successful completion of the job by opening **vast.out** and **OUTCAR** files

3. Extract band structure data from EIGENVAL file using "vaspkit" package:

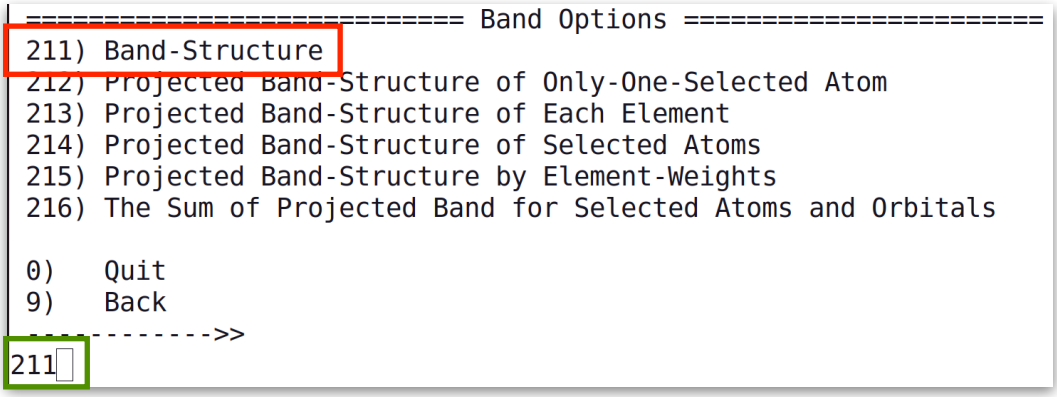
- To extract the band structure data from EIGENVAL file in a readable format, we can use "vaspkit" as shown below:

```
[estesodp@dendrite band_1]$ vaspkit
```

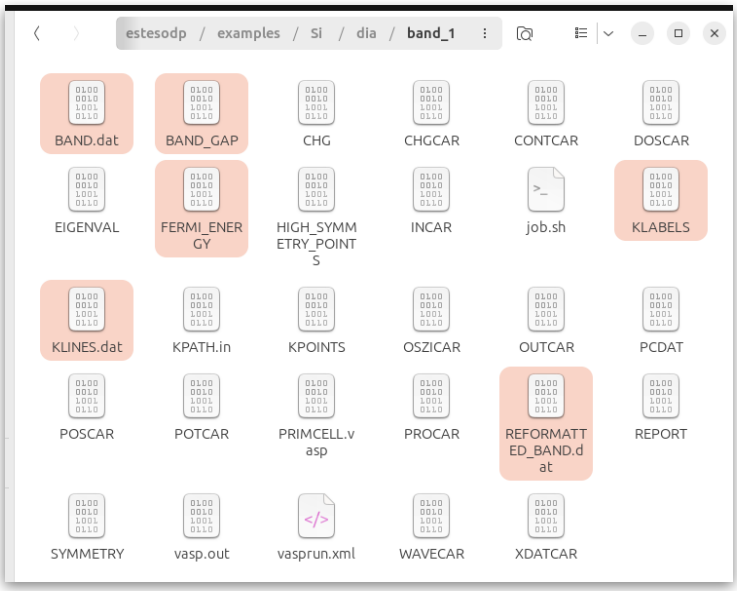
- Select Band-Structure option by typing "21"



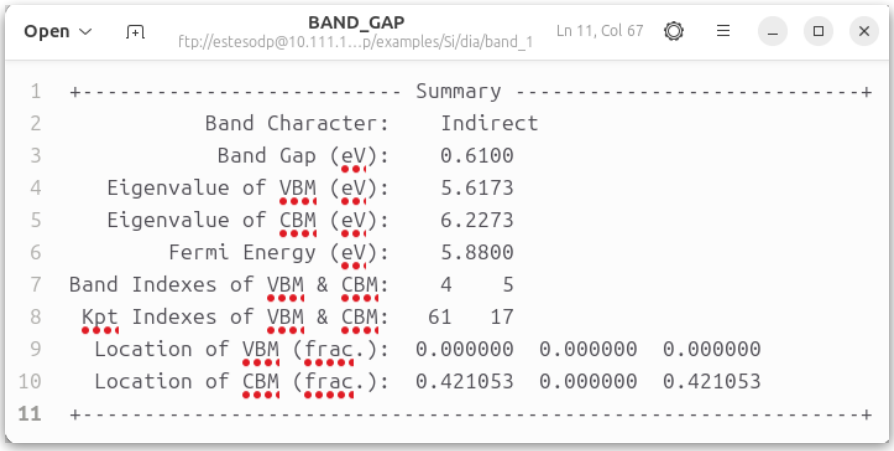
- Select Band-Structure option by typing "211"



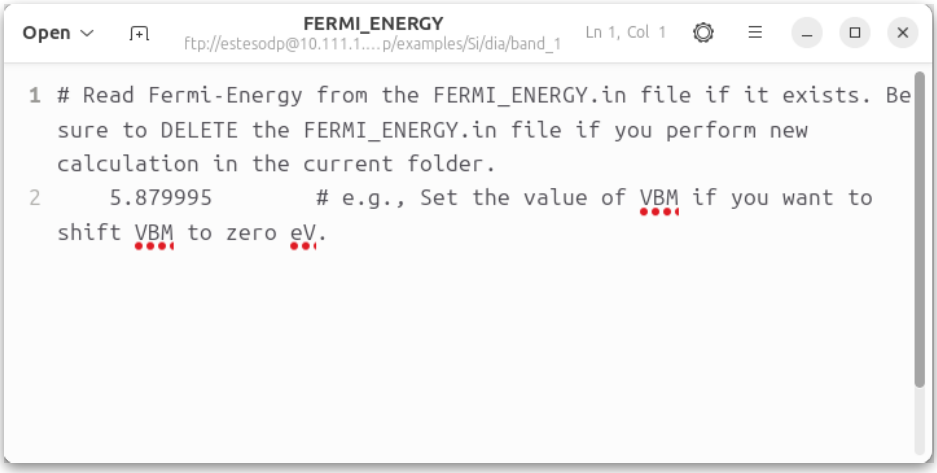
- This will generate the following files:



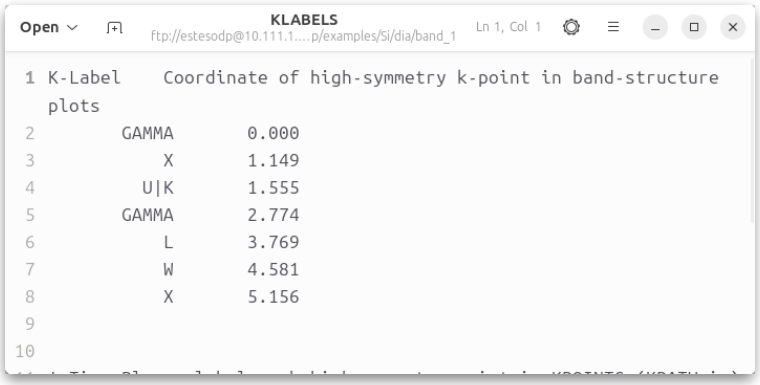
- The BANDGAP file contains the CBm, VBM and band gap details for a insulator system



- Similarly FERMI_ENERGY file contains the value of Fermi energy for the given system



- KLABELS file contains the labels of high symmetry points in the k-path of Brillouin zone

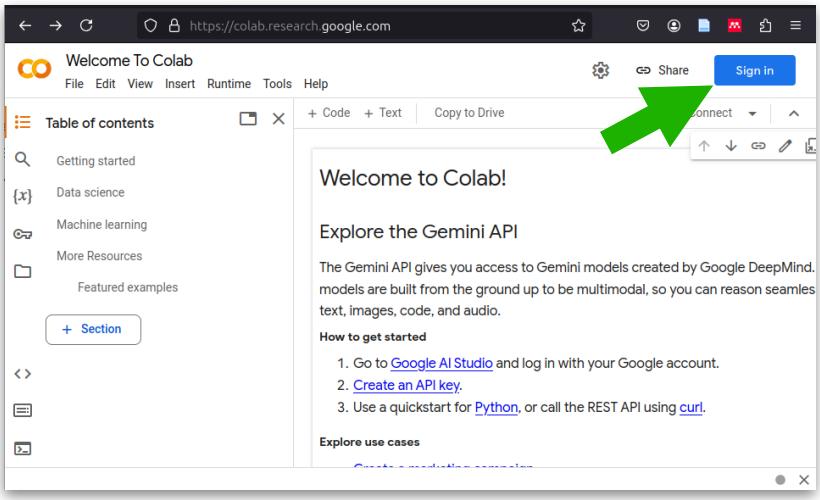


4. Plotting band structure using python in google collab

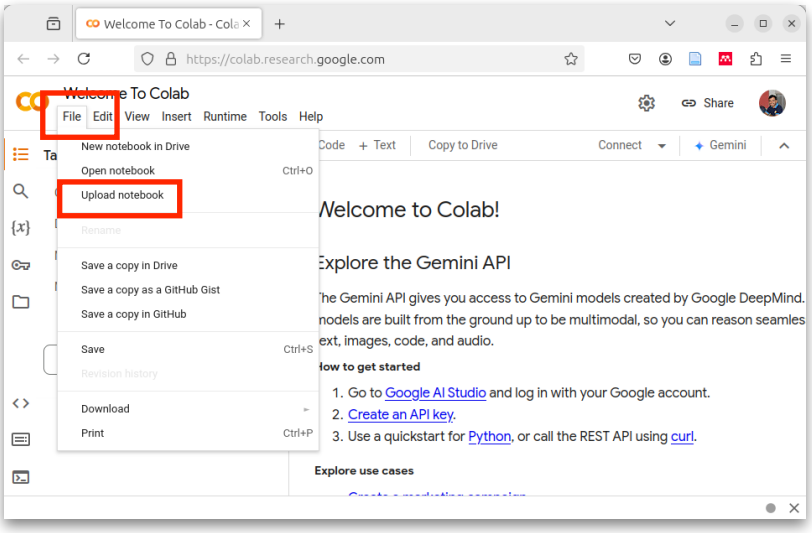
- Open google collab website using the following link:

```
https://colab.research.google.com/
```

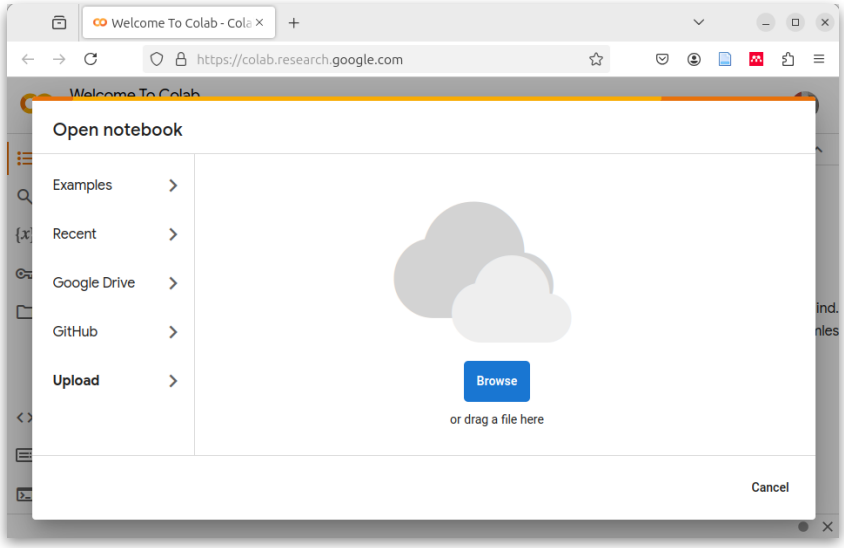
- Sign into your google account



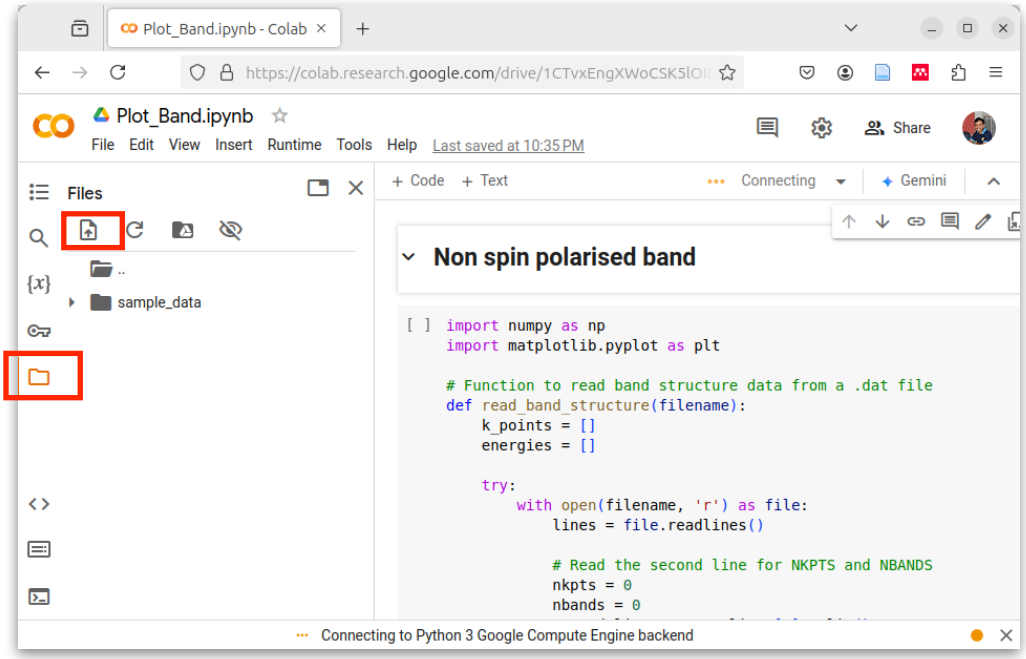
- After logging in, click on **File** and select **upload notebook** option



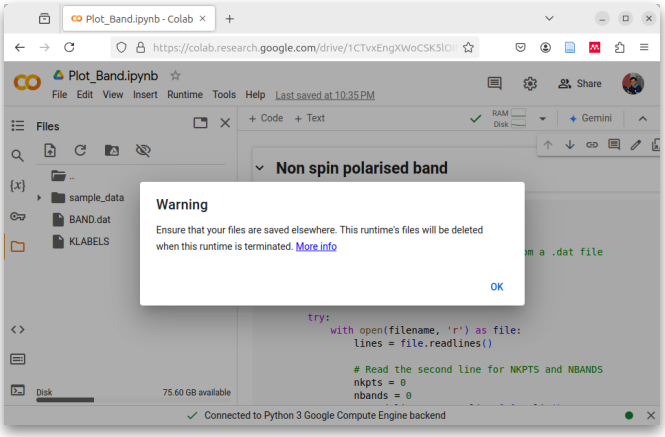
- Select the **Plot_Band.ipynb** file supplied to you



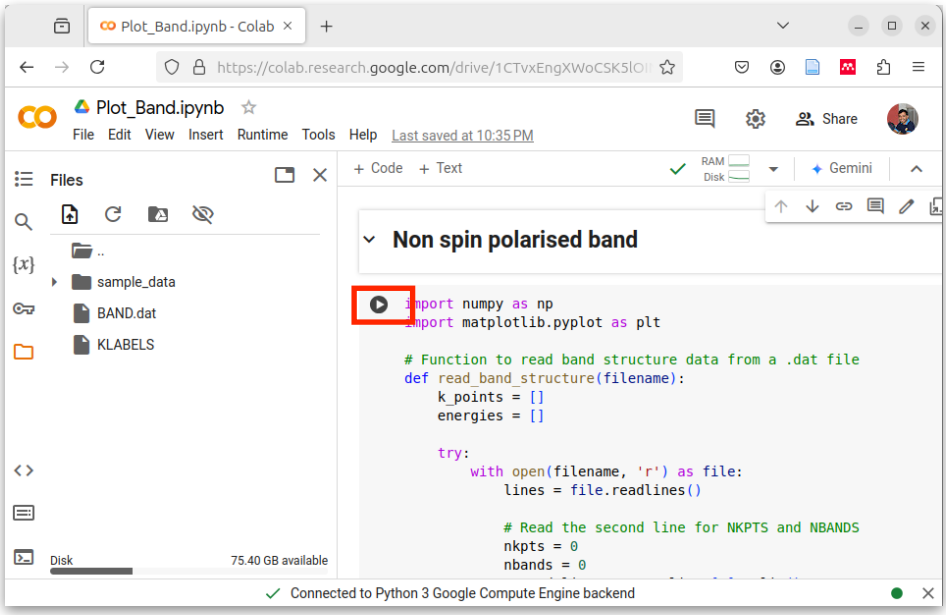
- Once the python notebook is opened, click on the folder icon on the side to open the contents and click on the upload icon to upload the **KLABELS** and **BAND.dat** files



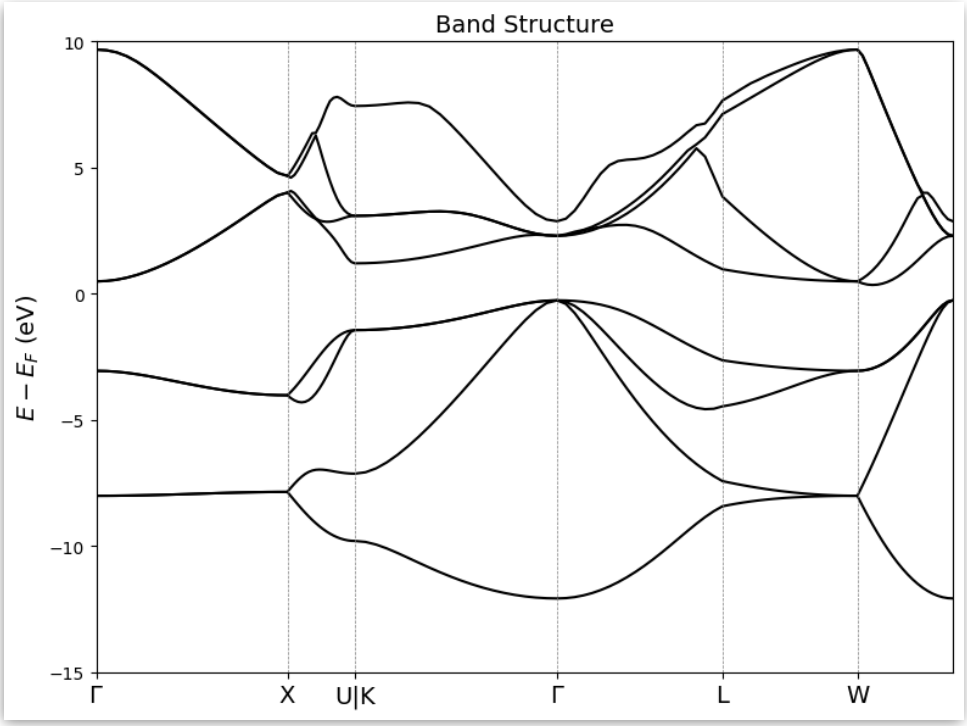
- Ignore the warning after uploading the files



- To plot the simple non spin-polarised band structure, click on the play button on the side of the first code cell



- After successful execution of the code following band structure is generated for Is diamond structure

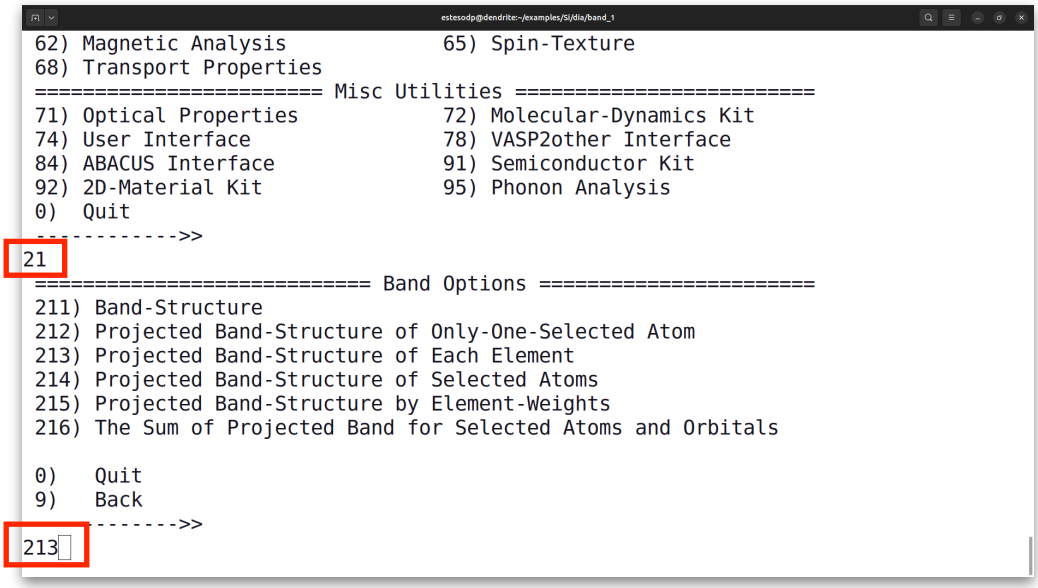


5. Extract fat band structure data from PROCAR file using “vaspkit” package:

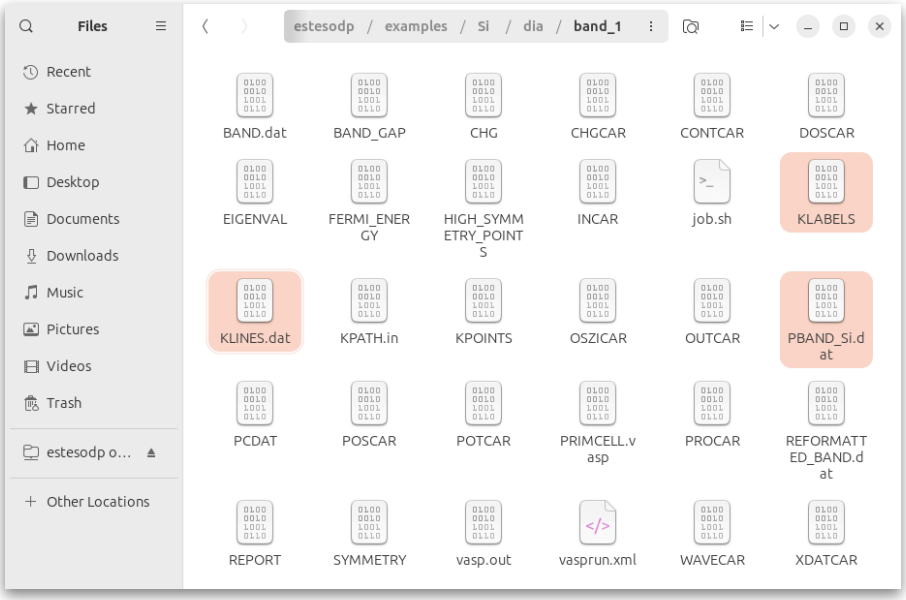
- Run “vaspkit” command in **band** folder in terminal

```
[estesodp@dendrite band_1]$ vaspkit
```

- Type “21” to select Band-Structure option and in the following list, select “213”

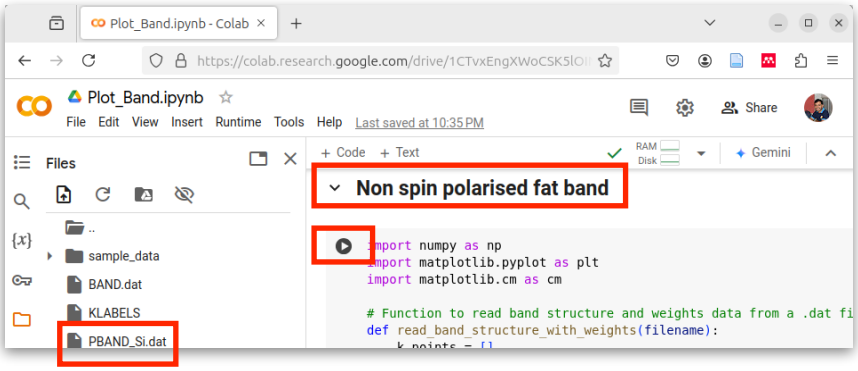


- Following files will be generated

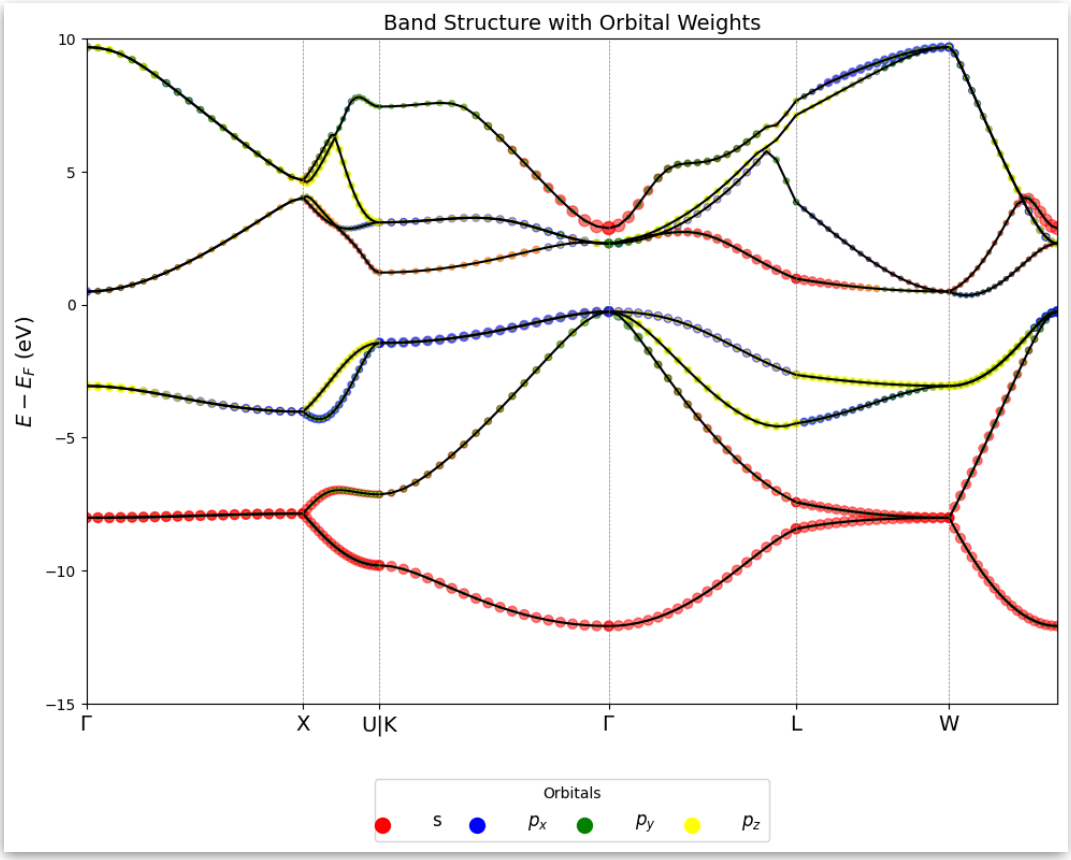


6. Plotting fat band structure using python in google collab

- **PBAND_Si.dat** file contains the orbital contribution details of **Si** atoms on the band structure. Upload this file to the collab notebook and run the code shown below:

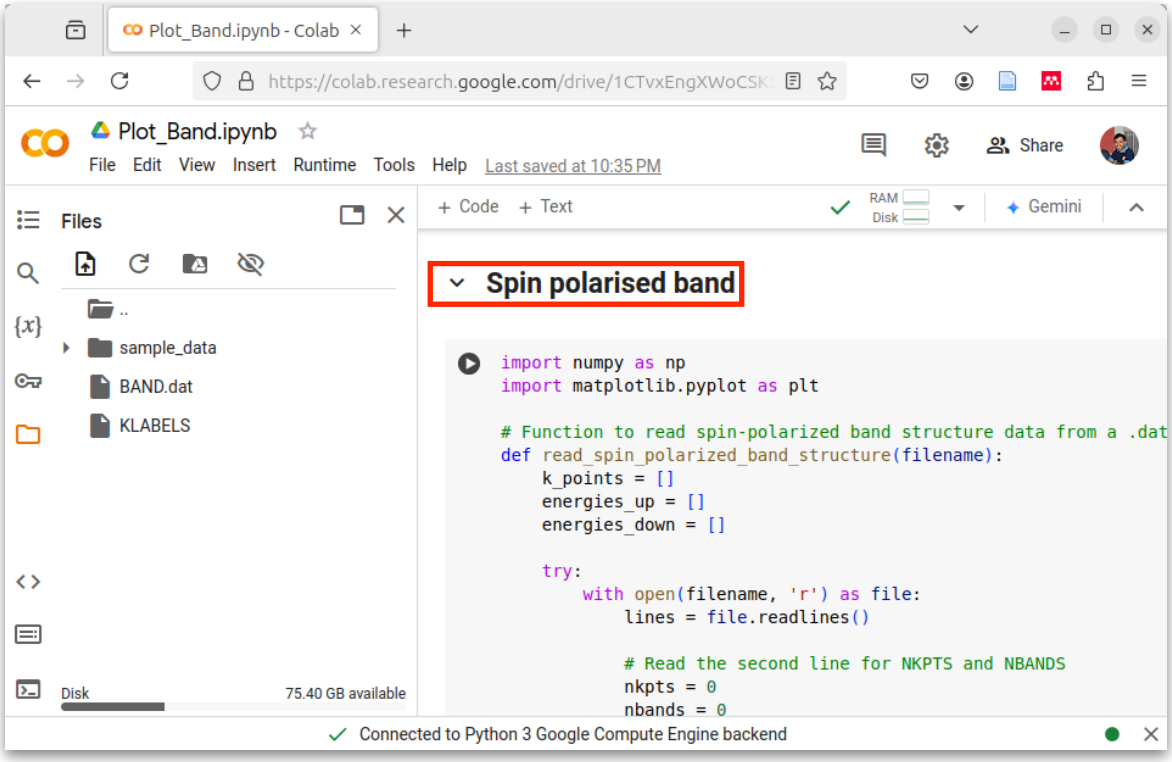


- Below is the fat band generated using the given code:

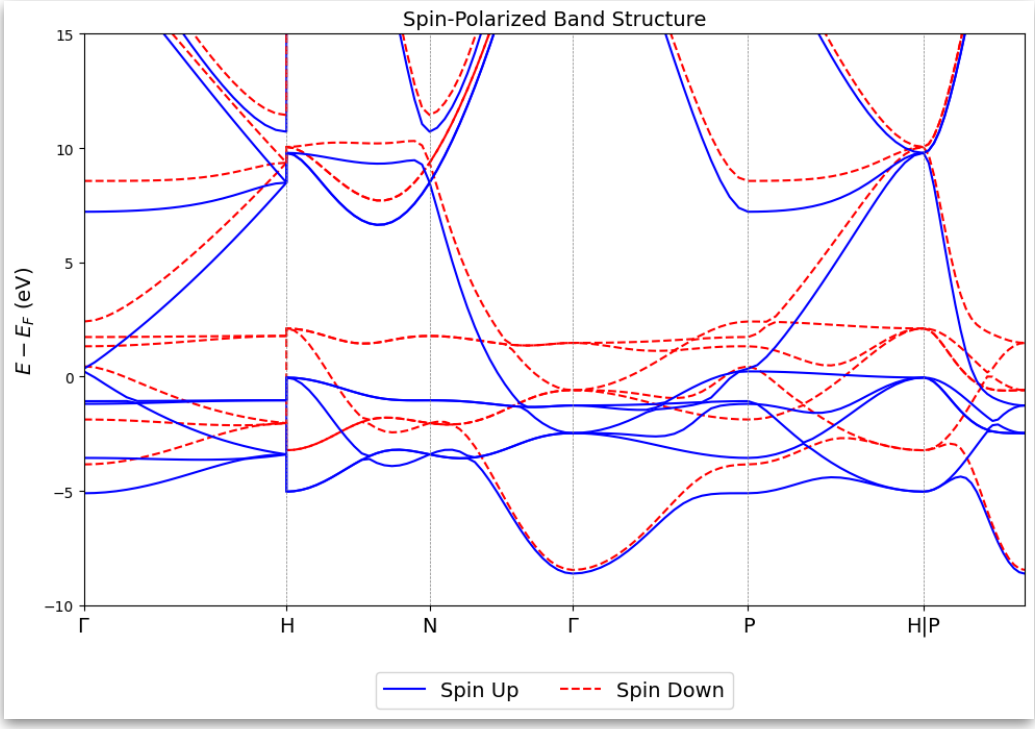


7. Plotting spin polarised band structure:

- Perform steps 1, 2 and 3 for BCC Fe system
- Upload the **KLABELS** and **BAND.dat** files and run the code shown below:



- Below is the spin polarised band generated using the given code:



8. Plotting spin polarised fat band structure:

- Repeat step 5 for BCC Fe system to calculate the orbital contributions in the band structure and upload the **PBAND_Fe_UP.dat** and **PBAND_Fe_DW.dat** files to the collab notebook
- Run the spin polarised fat band code. Below is the spin polarised fat band generated using the given code: