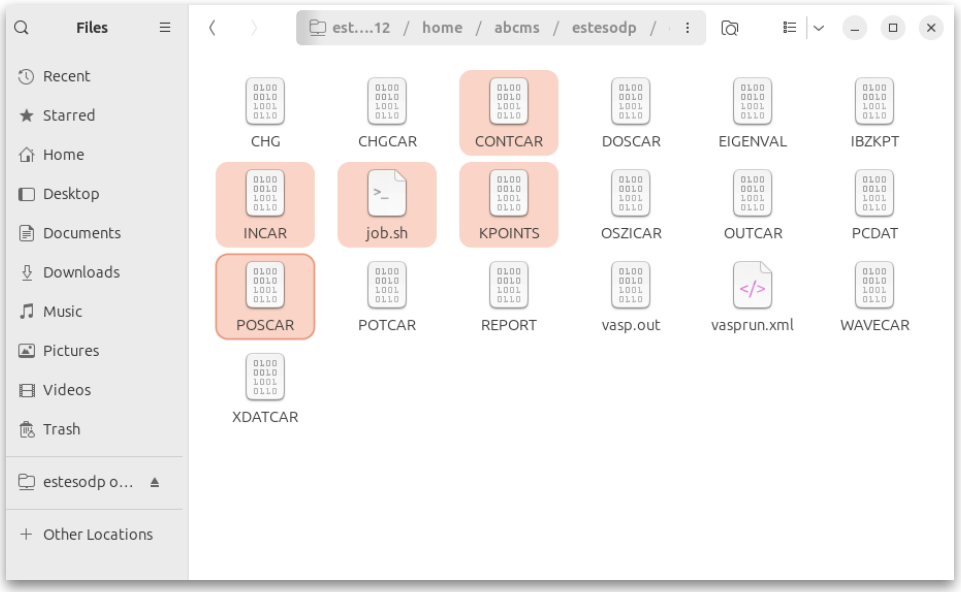
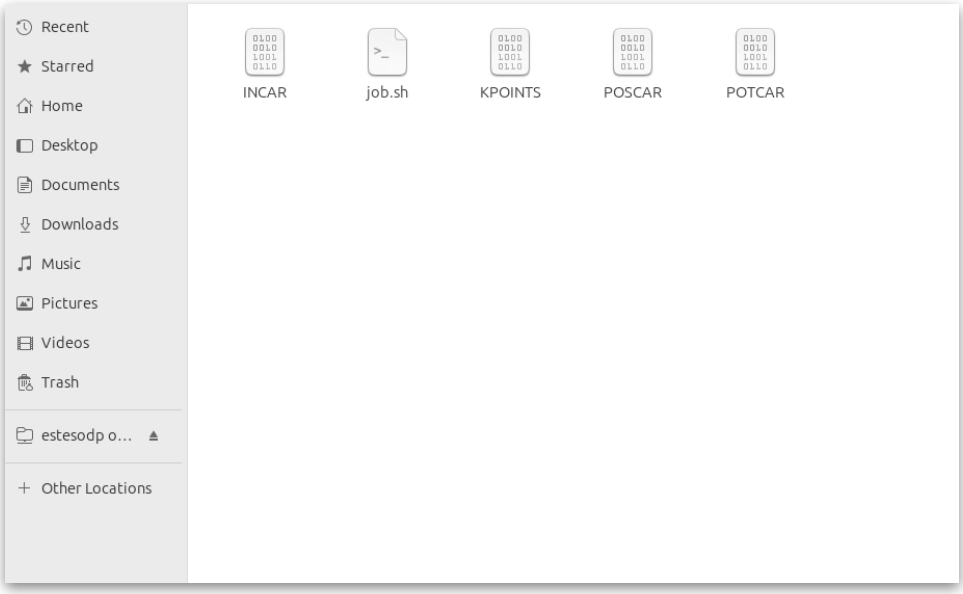
Calculating Density of States

Density of states are calculated using Non-Self Consistent Field (NSCF) calculations on a denser k-mesh. 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 Density of States of Silicon diamond-FCC and Fe-BCC structures.

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

Open OUTCAR ftp://estesodp@10.111.1.12/home/abcms/estesodp/examples/Si/dia/scf Ln 1, Col 1

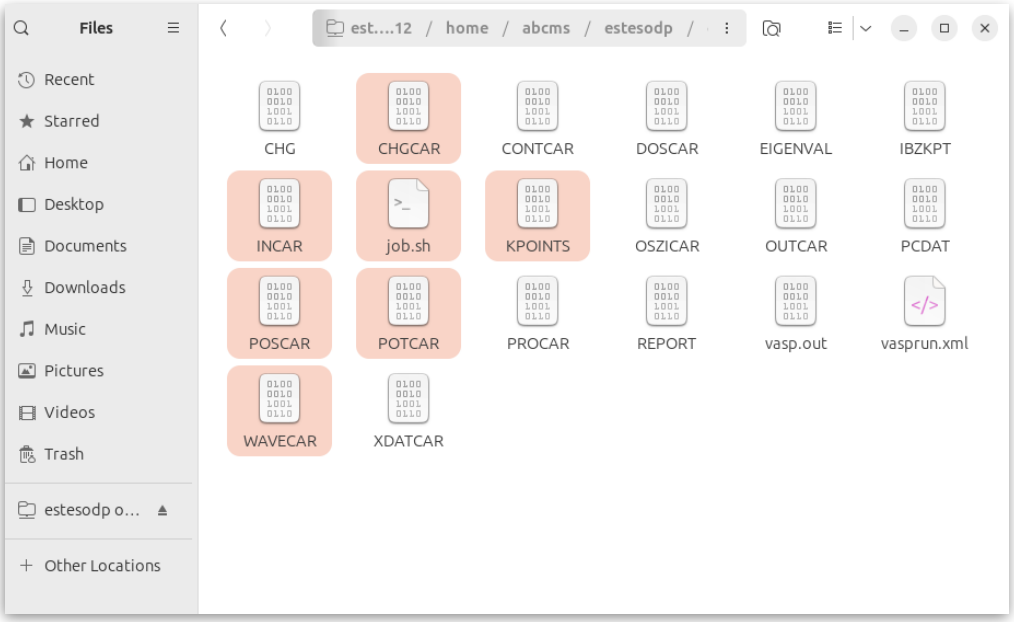
```
5687     nonl-proj  :      16649. kBytes
5688     fftplans   :       6611. kBytes
5689     grid       :       3048. kBytes
5690     one-center:          6. kBytes
5691     wavefun    :       8456. kBytes
5692
5693
5694
5695  General timing and accounting informations for this job:
5696  ========================================================
5697
5698                   Total CPU time used (sec):       58.516
5699                             User time (sec):       56.912
5700                           System time (sec):        1.604
5701                          Elapsed time (sec):       67.094
5702
5703                    Maximum memory used (kb):      104884.
5704                    Average memory used (kb):         N/A
5705
5706                         Minor page faults:        18572
5707                         Major page faults:            1
5708                 Voluntary context switches:       199913
```

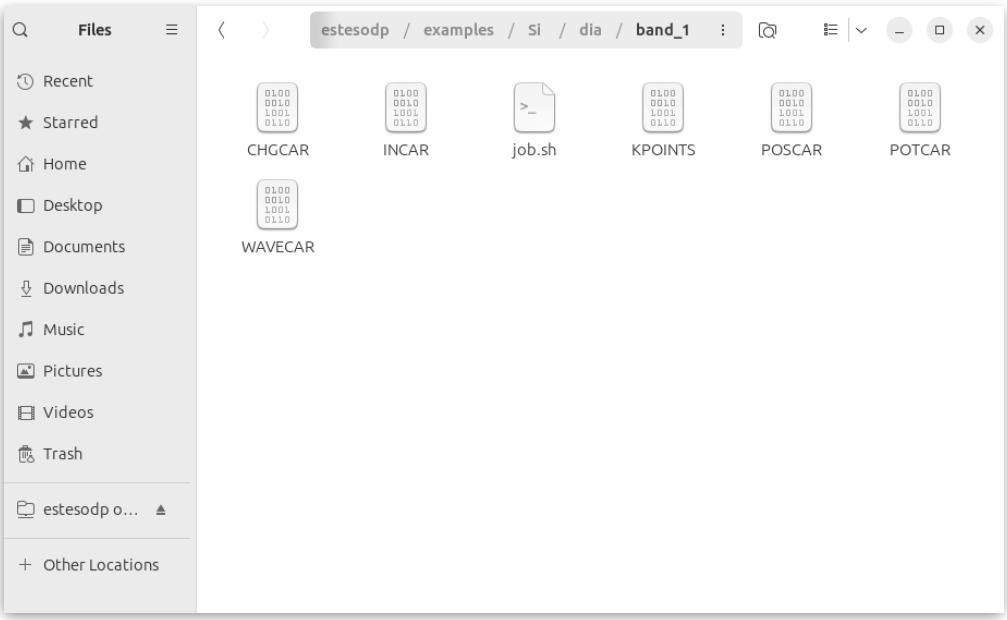
Open vasp.out ftp://estesodp@10.111.1.12/home/abcms/estesodp/examples/Si/dia/scf Ln 1, Col 1

```
 1  running on    4 total cores
 2  distrk:  each k-point on    4 cores,    1 groups
 3  distr:  one band on    1 cores,    4 groups
 4  vasp.6.2.0 18Jan21 (build Aug 12 2022 13:00:08) complex
 5
 6  POSCAR found type information on POSCAR Si
 7  POSCAR found :  1 types and       2 ions
 8  scaLAPACK will be used
 9  LDA part: xc-table for Pade appr. of Perdew
10  POSCAR, INCAR and KPOINTS ok, starting setup
11  FFT: planning ...
12  WAVECAR not read
13  entering main loop
14        N       E                     dE             d eps       ncg     rms          rms(c)
15 DAV:   1     0.342575609136E+01    0.34258E+01   -0.29714E+03  4576   0.710E+02
16 DAV:   2    -0.108410482481E+02   -0.14267E+02   -0.13778E+02  7024   0.727E+01
17 DAV:   3    -0.110172157253E+02   -0.17617E+00   -0.17617E+00  5928   0.102E+01
18 DAV:   4    -0.110180408806E+02   -0.82516E-03   -0.82516E-03  7448   0.726E-01
19 DAV:   5    -0.110180415669E+02   -0.68631E-06   -0.68631E-06  6088   0.173E-02    0.474E+00
20 DAV:   6    -0.109022024881E+02    0.11584E+00   -0.75671E-02  5536   0.144E+00    0.290E+00
21 DAV:   7    -0.108486497567E+02    0.53553E-01   -0.14532E-01  5832   0.212E+00    0.173E-01
22 DAV:   8    -0.108497388359E+02   -0.10891E-02   -0.37550E-03  5352   0.460E-01    0.734E-02
23 DAV:   9    -0.108499377309E+02   -0.19890E-03   -0.19840E-04  6832   0.110E-01    0.557E-02
24 DAV:  10    -0.108499626885E+02   -0.24958E-04   -0.29223E-05  5480   0.405E-02    0.857E-03
25 DAV:  11    -0.108499624562E+02    0.23230E-06   -0.57995E-07  6296   0.529E-03
26    1 F= -.10849962E+02 E0= -.10849962E+02  d E =-.186719E-11
27  writing wavefunctions
```

2. Performing density of states calculations:

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





- Update **KPOINTS** file to increase the mesh to 31x31x31
- 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)
```

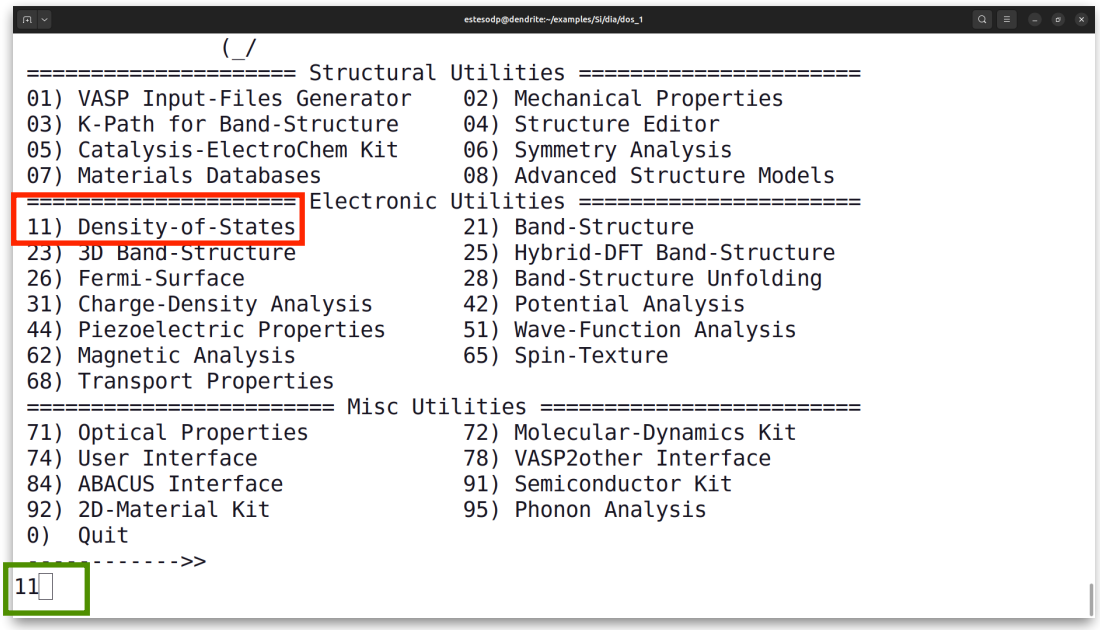
- Submit the job for run using **qsub** command
- Verify the running of job using **qstat** command
- Once the job is ended, verify the successful completion of the job by opening **vast.out** and **OUTCAR** files

3. Extract density of states data from DOSCAR file using "vaspkit" package:

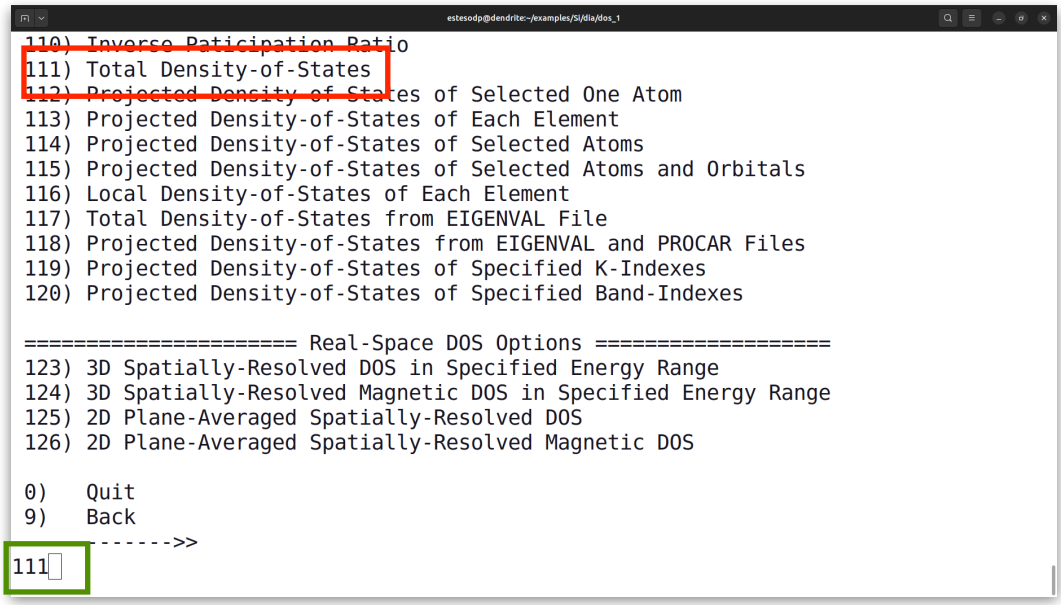
- To extract the density of states data from DOSCAR file in a readable format, we can use "vaspkit" as shown below:

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

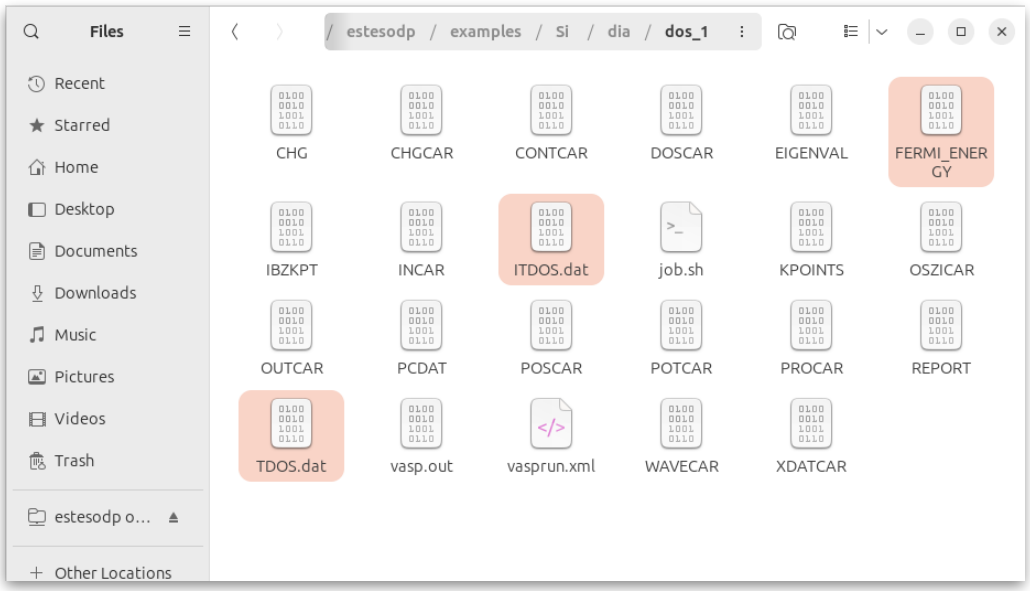
- Select Density-of-States option by typing "11"



- Select Total Density-of-States option by typing “111”



- This will generate the following files:



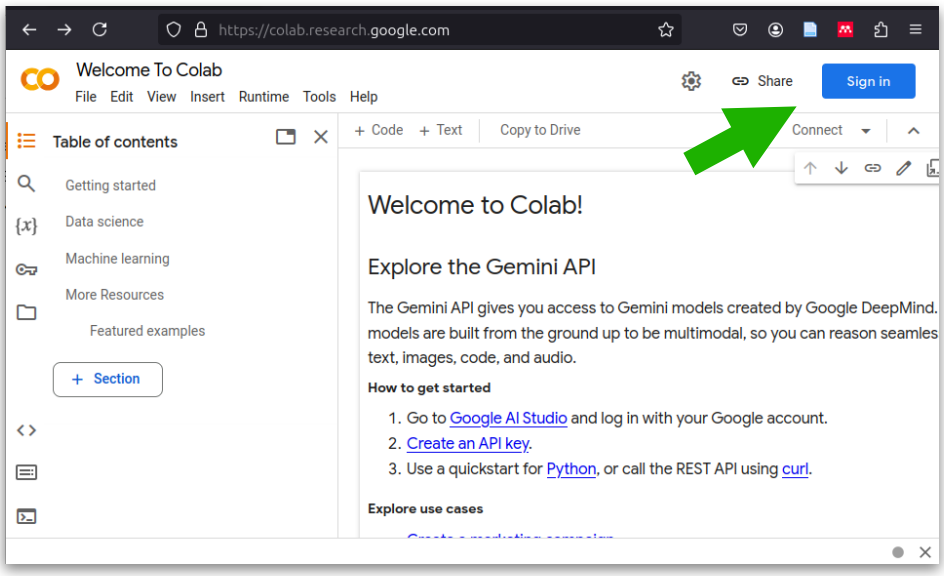
- The **TDOS.dat** file contains the total DOS and Integrated DOS of the system
- Similarly **FERMI_ENERGY** file contains the value of Fermi energy for the given system

4. Plotting band structure using python in google collab

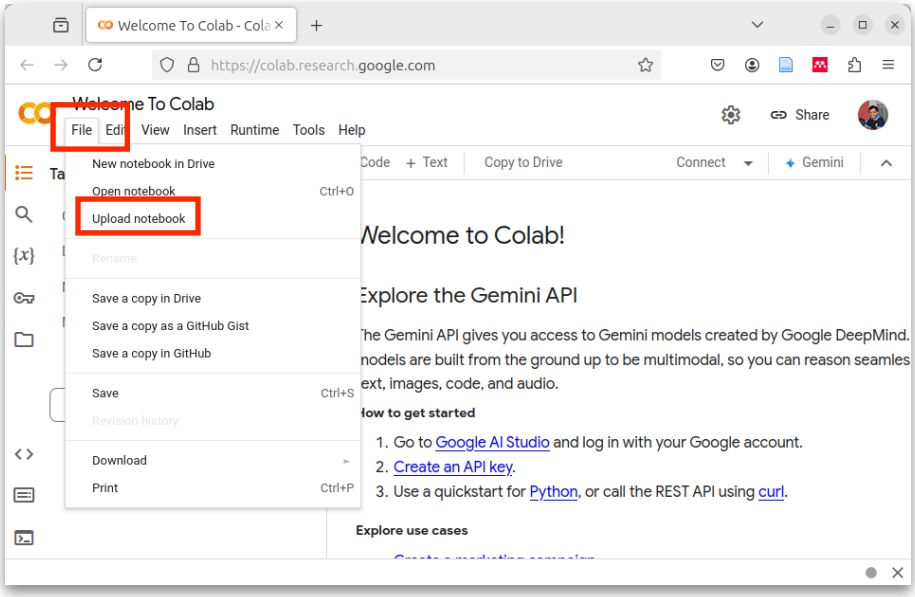
- Open google collab website using the following link:

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

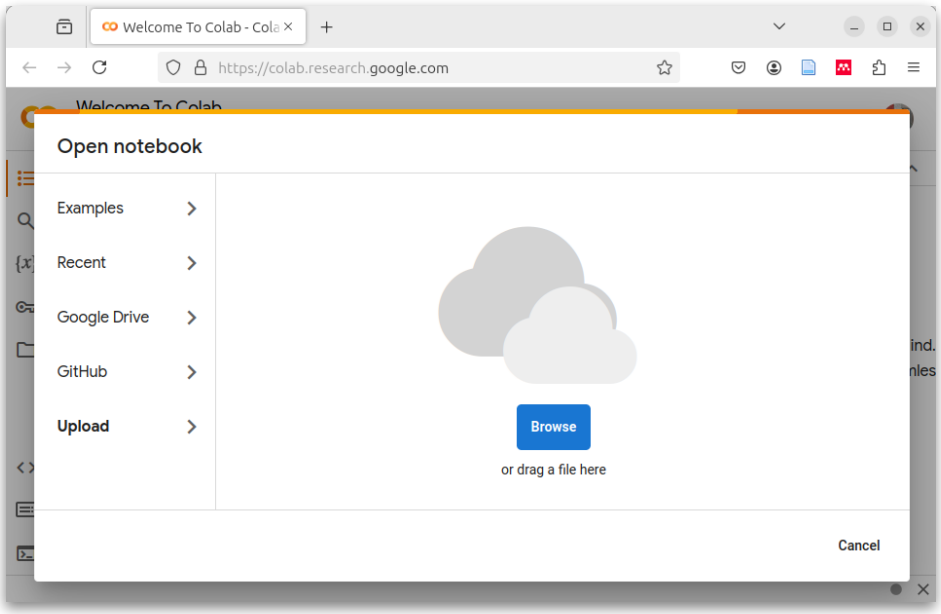
- Sign into your google account



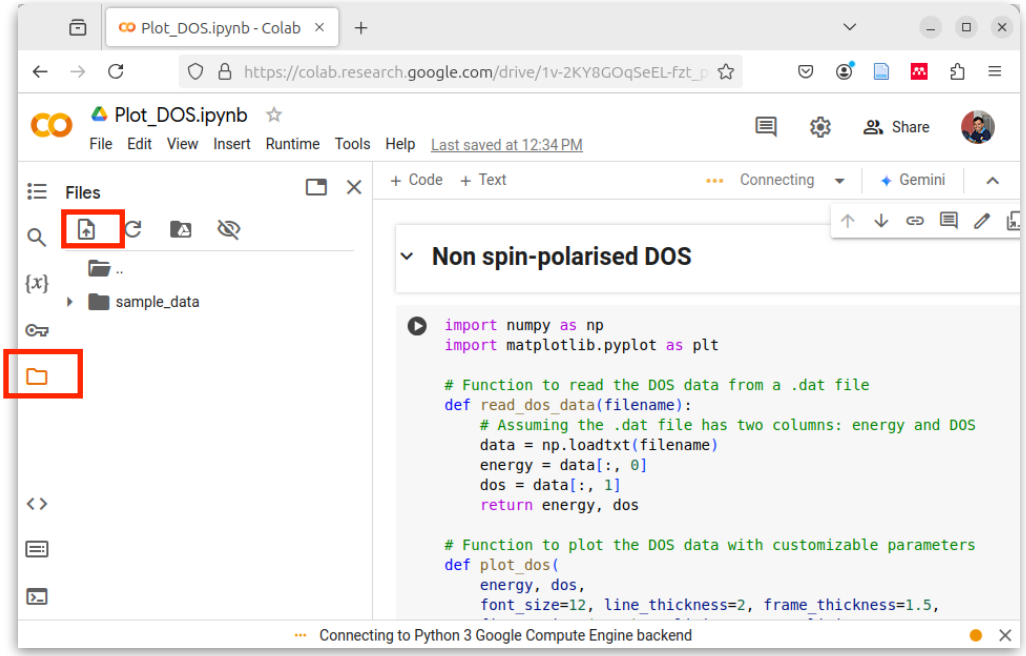
- After logging in, click on **File** and select **upload notebook** option



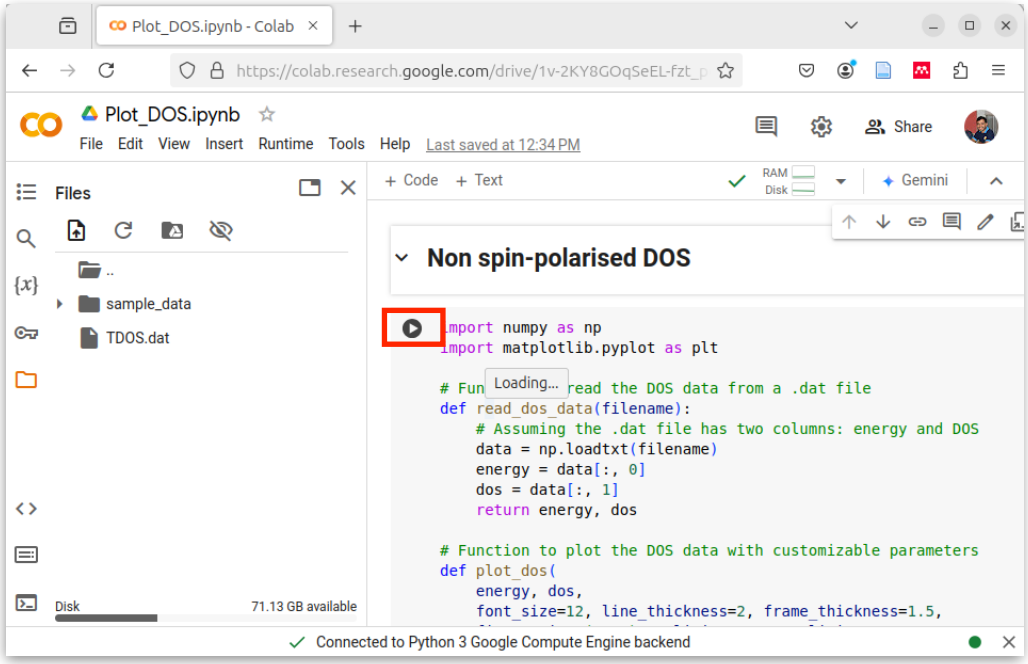
- Select the **Plot_DOS.ipynb** file supplied to you



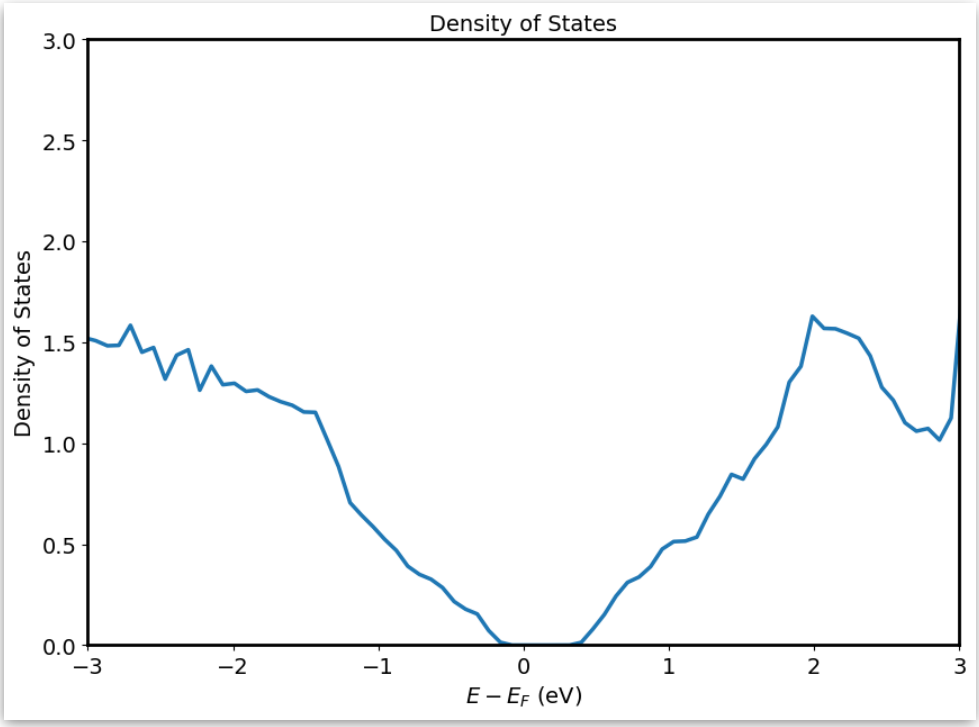
- Once the python notebook is opened, click on the folder icon on the side to open the contents and click on the upload icon to upload the **TDOS.dat** file



- Ignore the warning after uploading the file
- To plot the simple non spin-polarised DOS, click on the play button on the side of the first code cell



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



5. Extract Partial DOS data from DOSCAR file using "vaspkit" package:

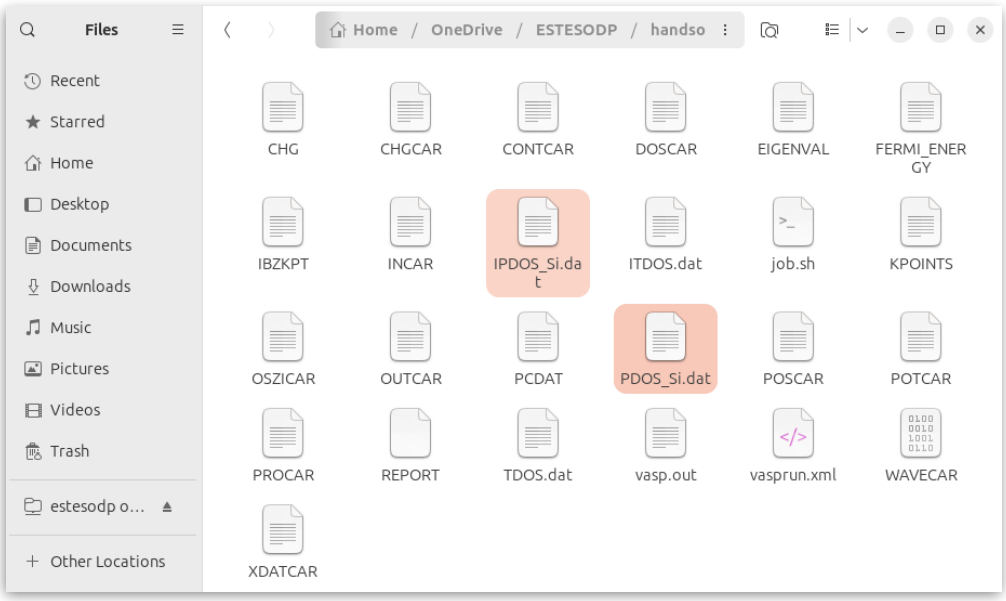
- Run "vaspkit" command in **band** folder in terminal

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

- Type "11" to select Density-of-States option and in the following list, select "113" for orbital contributions of each element in the structure

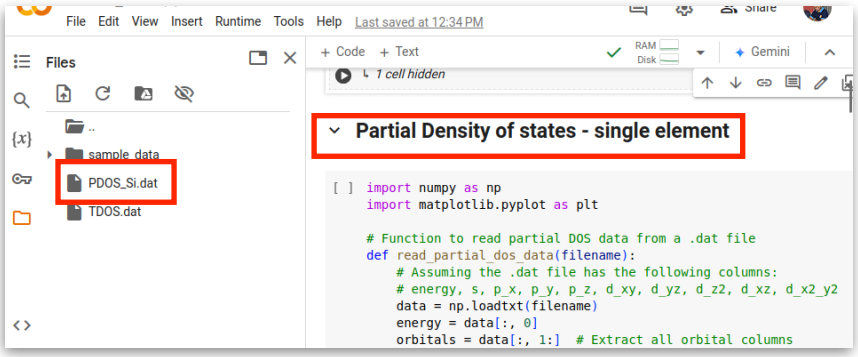
```
110) Inverse Paticipation Ratio
111) Total Density-of-States
112) Projected Density-of-States of Selected One Atom
113) Projected Density-of-States of Each Element
114) Projected Density-of-States of Selected Atoms
115) Projected Density-of-States of Selected Atoms and Orbitals
116) Local Density-of-States of Each Element
117) Total Density-of-States from EIGENVAL File
118) Projected Density-of-States from EIGENVAL and PROCAR Files
119) Projected Density-of-States of Specified K-Indexes
120) Projected Density-of-States of Specified Band-Indexes

====================== Real-Space DOS Options ==================
123) 3D Spatially-Resolved DOS in Specified Energy Range
124) 3D Spatially-Resolved Magnetic DOS in Specified Energy Range
125) 2D Plane-Averaged Spatially-Resolved DOS
126) 2D Plane-Averaged Spatially-Resolved Magnetic DOS

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

- Following files will be generated

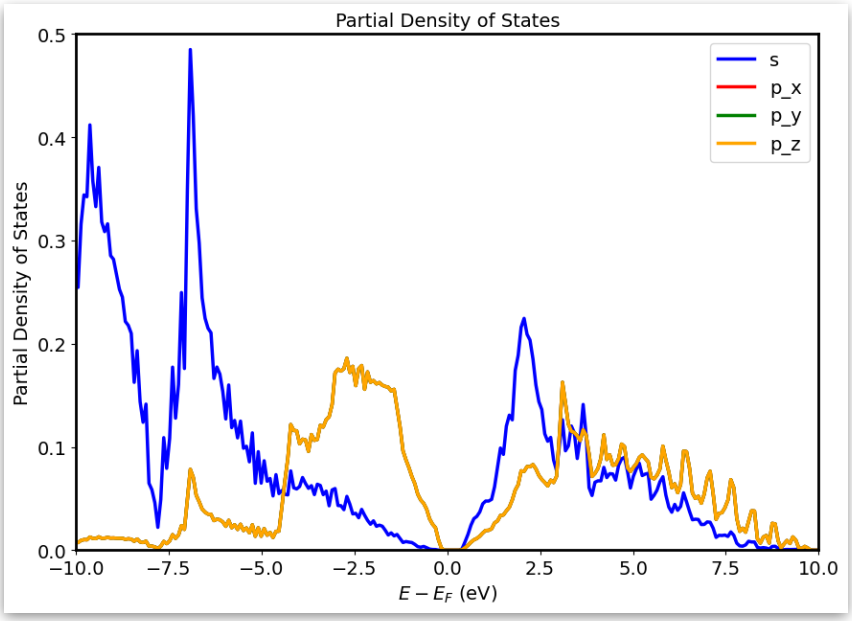


6. Plotting Partial DOS using python in google collab

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

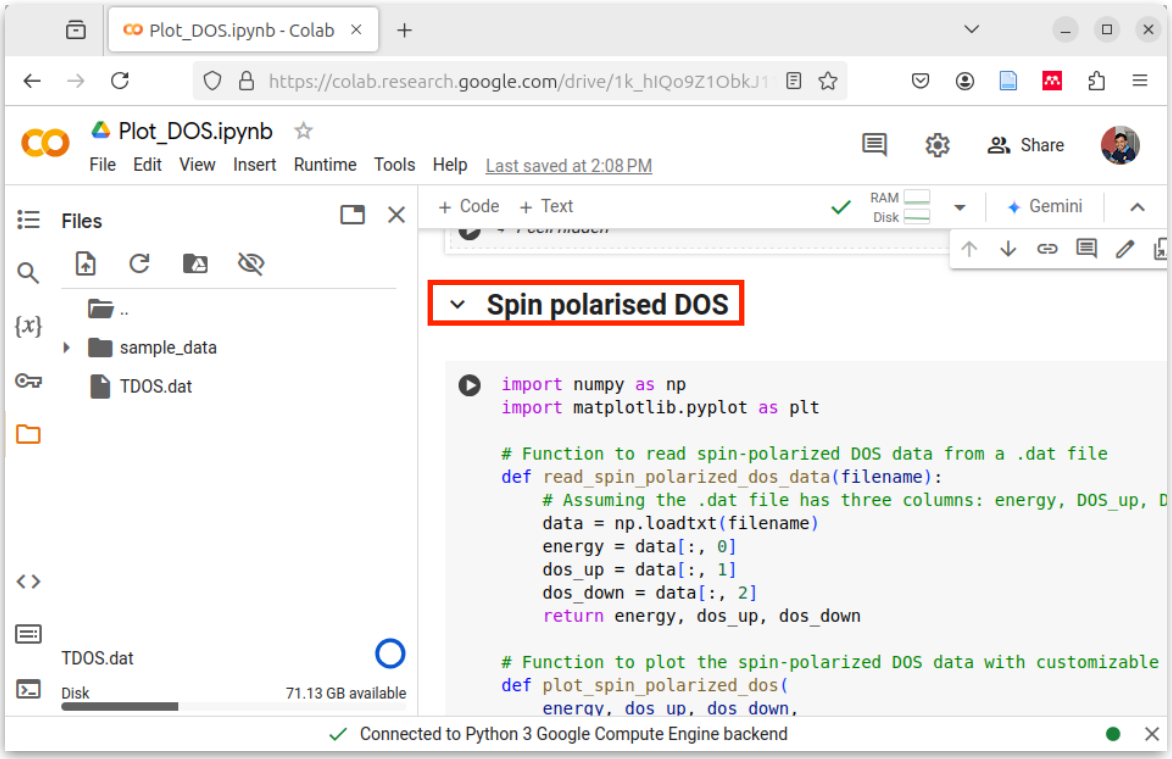


- Below is the PDOS generated using the given code:

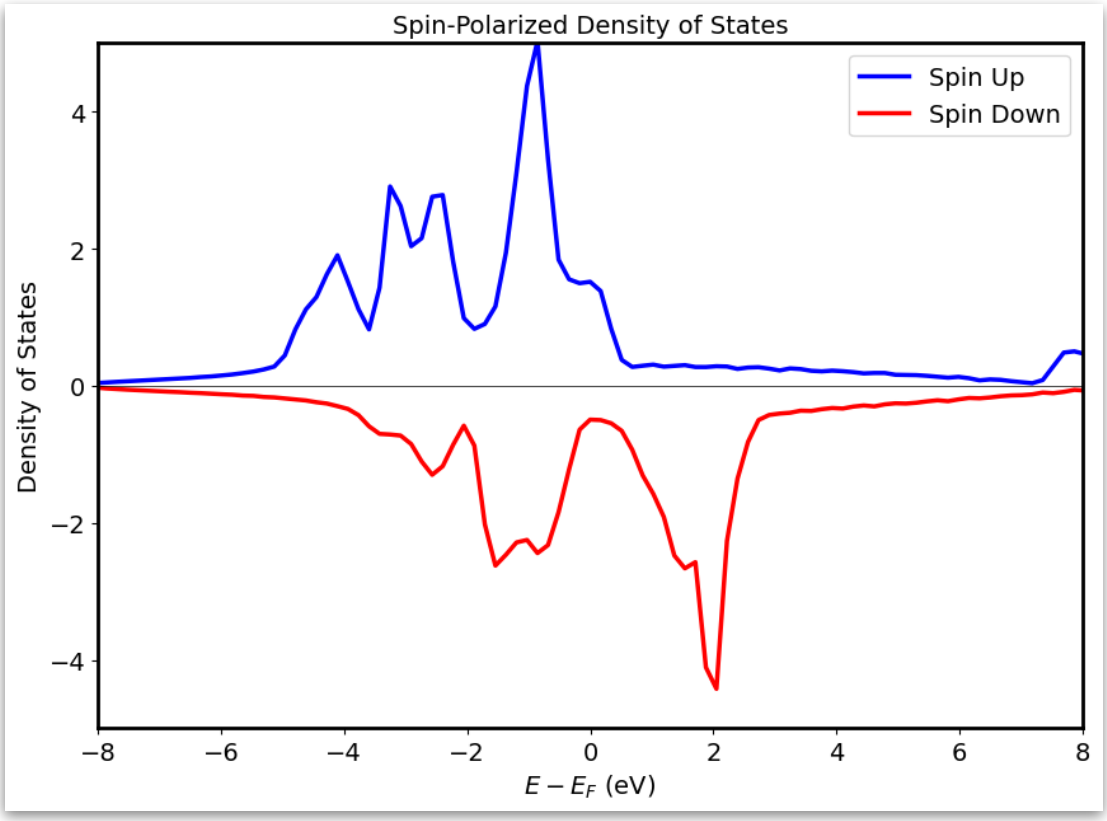


7. Plotting spin polarised DOS:

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

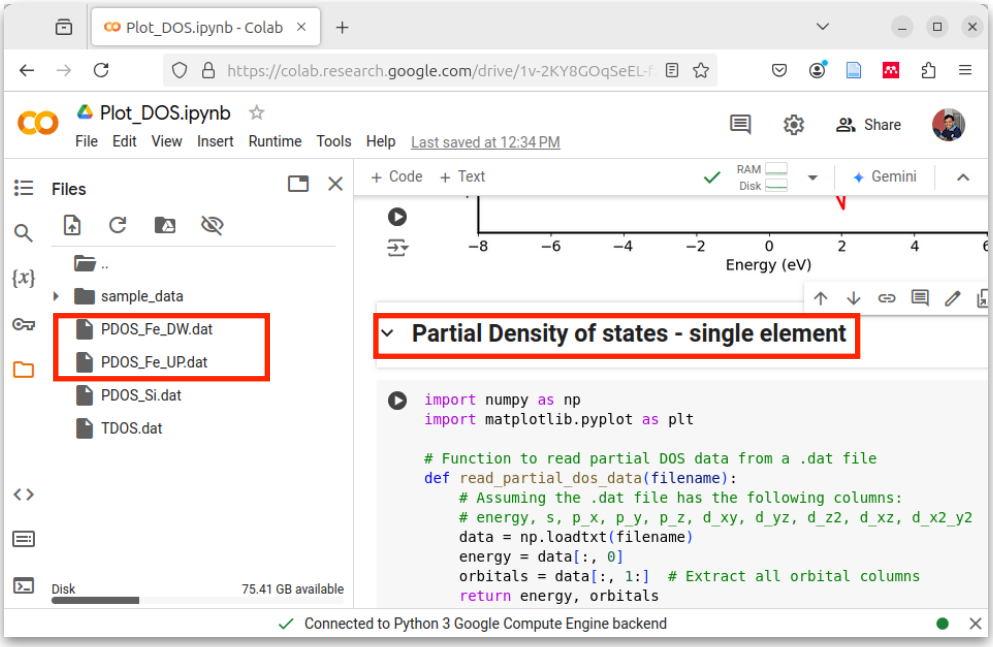


- Below is the spin polarised band generated using the given code:



8. Plotting spin polarised partial density of states:

- Repeat step 5 for BCC Fe system to calculate the orbital contributions in the band structure and upload the **PDOS_Fe_UP.dat** and **PDOS_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: