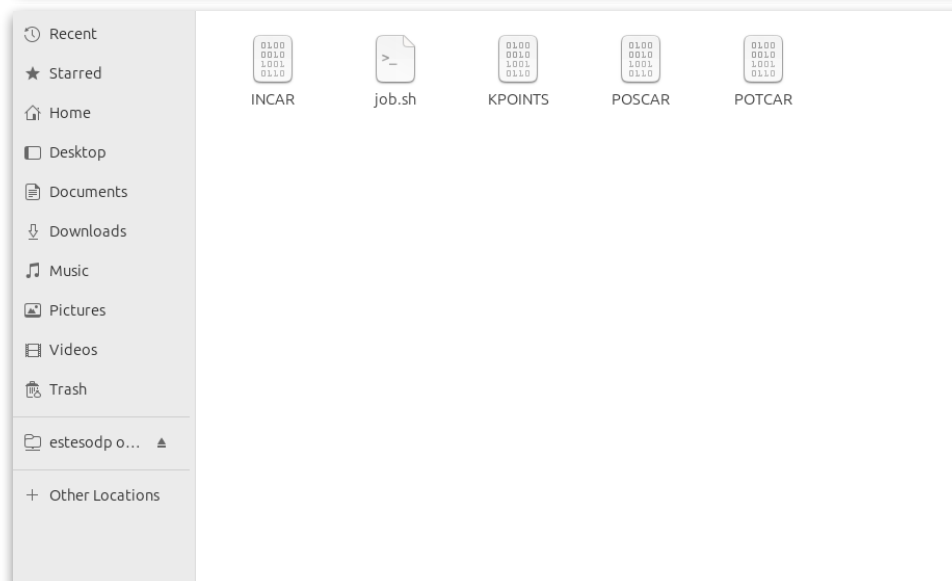
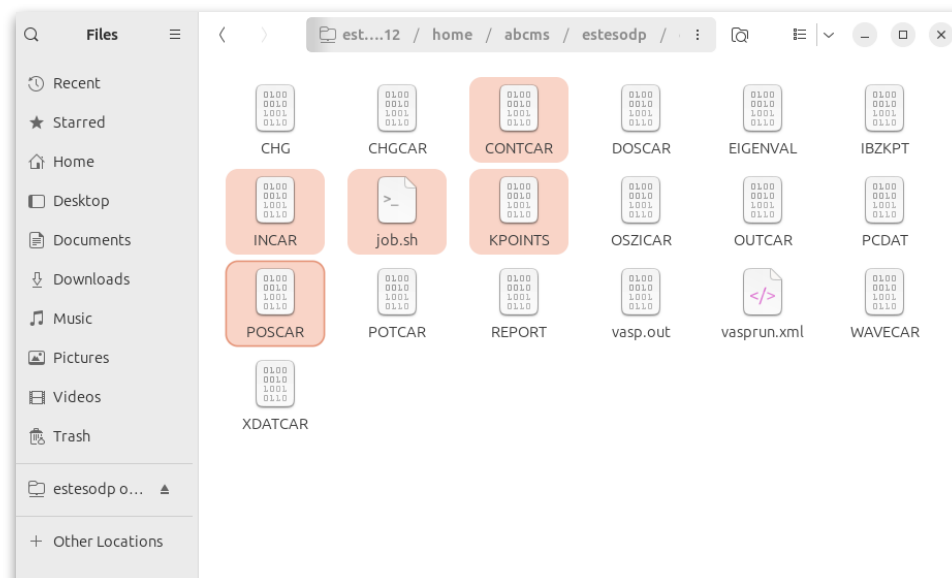


Calculating Band Structure

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 diamond-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

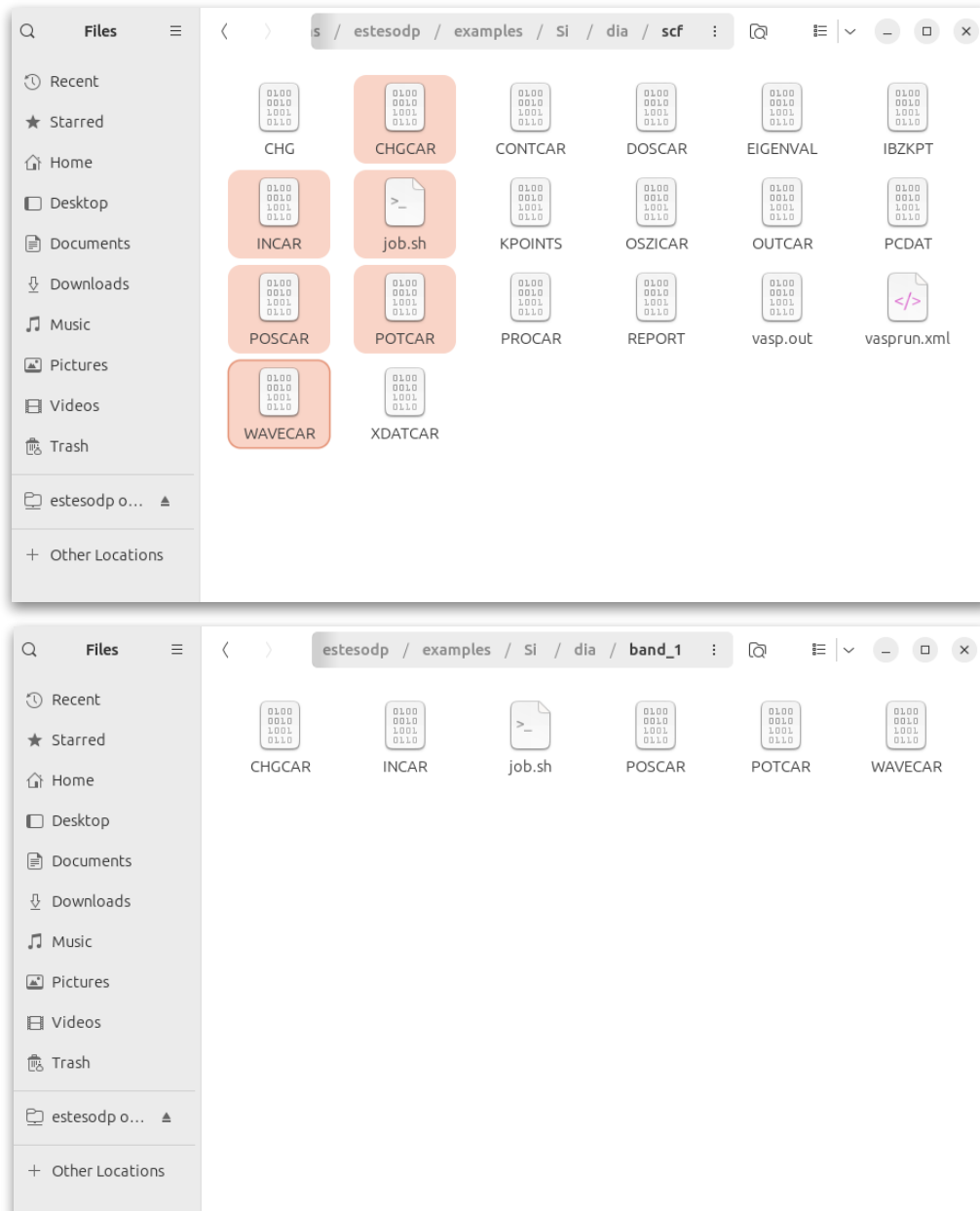
```

OUTCAR
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

vasp.out
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
15 N E dE d eps ncq rms rms(c)
16 DAV: 1 0.342575609136E+01 0.34258E+01 -0.29714E+03 4576 0.710E+02
17 DAV: 2 -0.108410482481E+02 -0.14267E+02 -0.13778E+02 7024 0.727E+01
18 DAV: 3 -0.110172157253E+02 -0.17617E+00 -0.17617E+00 5928 0.102E+01
19 DAV: 4 -0.110180408806E+02 -0.82516E-03 -0.82516E-03 7448 0.726E-01
20 DAV: 5 -0.110180415669E+02 -0.68631E-06 -0.68631E-06 6088 0.173E-02 0.474E+00
21 DAV: 6 -0.109022024881E+02 0.11584E+00 -0.75671E-02 5536 0.144E+00 0.290E+00
22 DAV: 7 -0.108486497567E+02 0.53553E-01 -0.14532E-01 5832 0.212E+00 0.173E-01
23 DAV: 8 -0.108497388359E+02 -0.10891E-02 -0.37550E-03 5352 0.460E-01 0.734E-02
24 DAV: 9 -0.108499377309E+02 -0.19890E-03 -0.19840E-04 6832 0.110E-01 0.557E-02
25 DAV: 10 -0.108499626885E+02 -0.24958E-04 -0.29223E-05 5480 0.405E-02 0.857E-03
26 DAV: 11 -0.108499624562E+02 0.23230E-06 -0.57995E-07 6296 0.529E-03
27 1 F= -.10849962E+02 E0= -.10849962E+02 d E =-.186719E-11
28 writing wavefunctions
  
```

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 [ 0h ]
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.

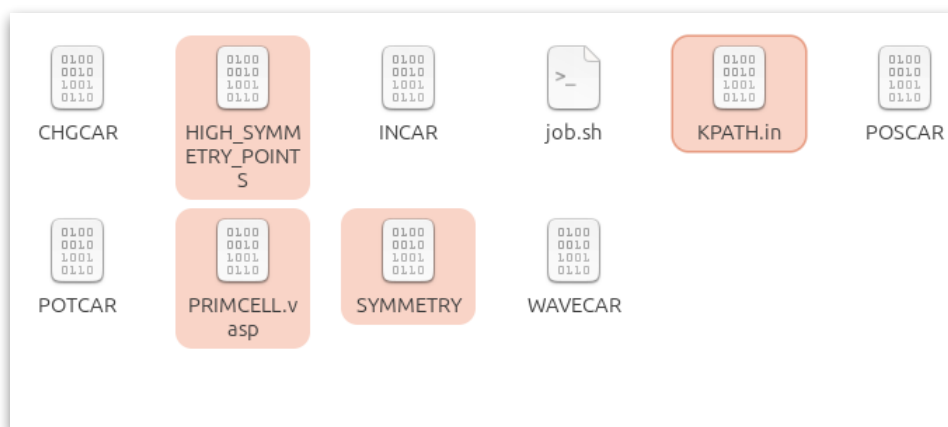
```

```

-->> (02) Written PRIMCELL.vasp file.
-->> (03) Written KPATH.in File for Band-Structure Calculation.
0-----WARNING-----0
| Do NOT forget to copy PRIMCELL.vasp to POSCAR unless you know |
| what you are doing. Otherwise you might get wrong results! |
0-----0
0-----* ACKNOWLEDGMENTS *-----0
| 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 (: |
0-----0
0-----* CITATIONS *-----0
| 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 |
0-----0
[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/Å)
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”

```

(_/
===== 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
----->>
21

```

- Select Band-Structure option by typing “211”

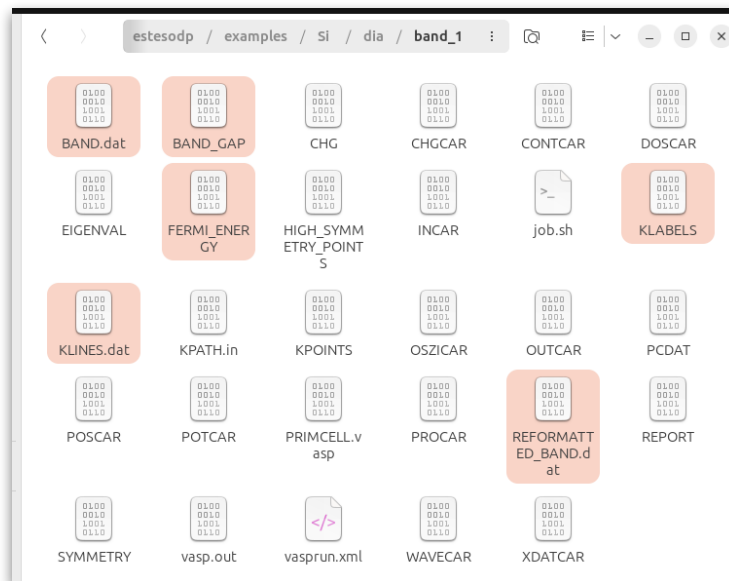
```

===== Band Options =====
211) Band-Structure
212) Projected Band-Structure of Only-One-Selected Atom
213) Projected Band-Structure of Each Element
214) Projected Band-Structure of Selected Atoms
215) Projected Band-Structure by Element-Weights
216) The Sum of Projected Band for Selected Atoms and Orbitals

0) Quit
9) Back
----->>
211

```

- This will generate the following files:



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

```

Open  ftp://estesodp@10.111.1...p/examples/Si/dia/band_1  Ln 11, Col 67
1  +----- Summary -----+
2      Band Character:      Indirect
3      Band Gap (eV):       0.6100
4      Eigenvalue of VBM (eV):  5.6173
5      Eigenvalue of CBM (eV):  6.2273
6      Fermi Energy (eV):     5.8800
7      Band Indexes of VBM & CBM:  4   5
8      Kpt Indexes of VBM & CBM:  61  17
9      Location of VBM (frac.):  0.000000  0.000000  0.000000
10     Location of CBM (frac.):  0.421053  0.000000  0.421053
11  +-----+

```

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

```

Open  ftp://estesodp@10.111.1...p/examples/Si/dia/band_1  Ln 1, Col 1
1  # Read Fermi-Energy from the FERMI_ENERGY.in file if it exists. Be
   sure to DELETE the FERMI_ENERGY.in file if you perform new
   calculation in the current folder.
2      5.879995      # e.g., Set the value of VBM if you want to
   shift VBM to zero eV.

```


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

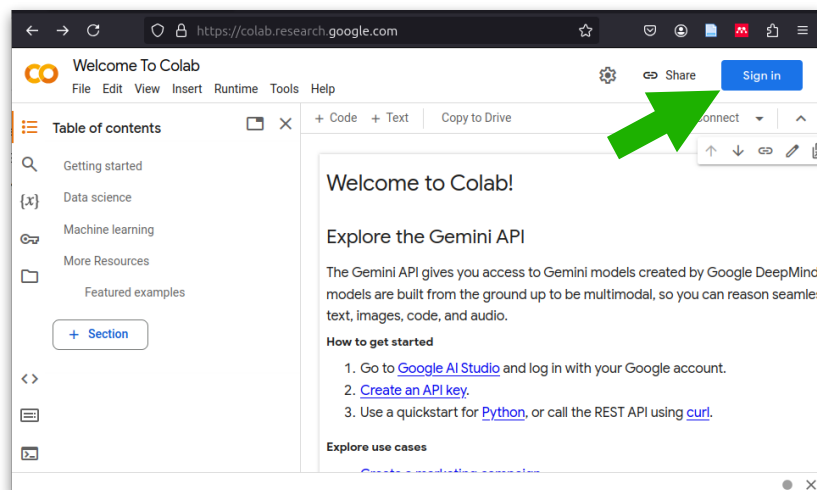
K-Label	Coordinate of high-symmetry k-point in band-structure plots
GAMMA	0.000
X	1.149
U K	1.555
GAMMA	2.774
L	3.769
W	4.581
X	5.156

4. Plotting band structure using python in google collab

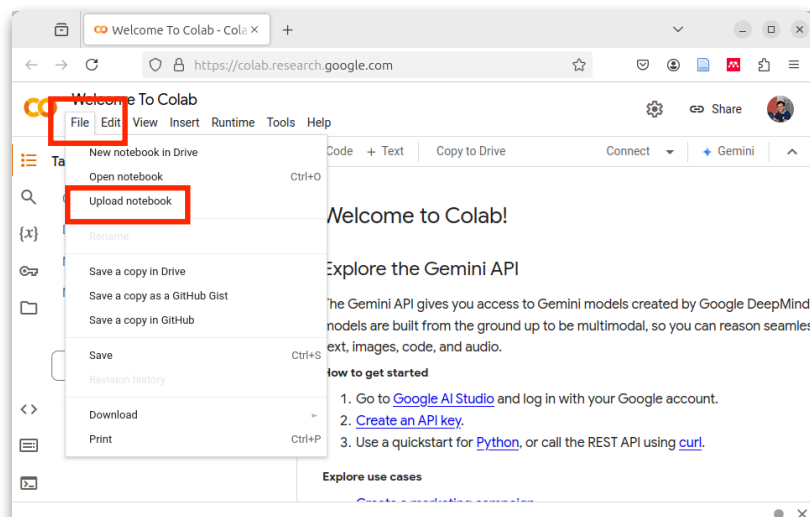
- Open google collab website using the following link:

<https://colab.research.google.com/>

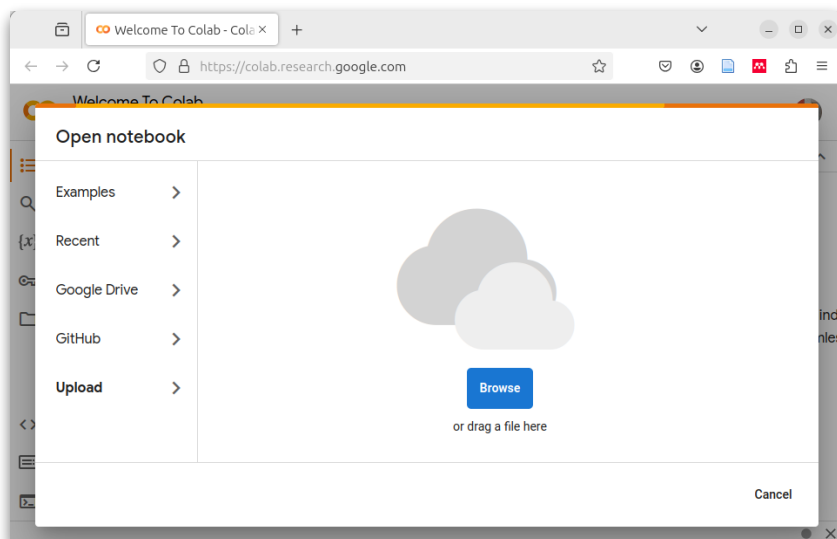
- Sign into your google account



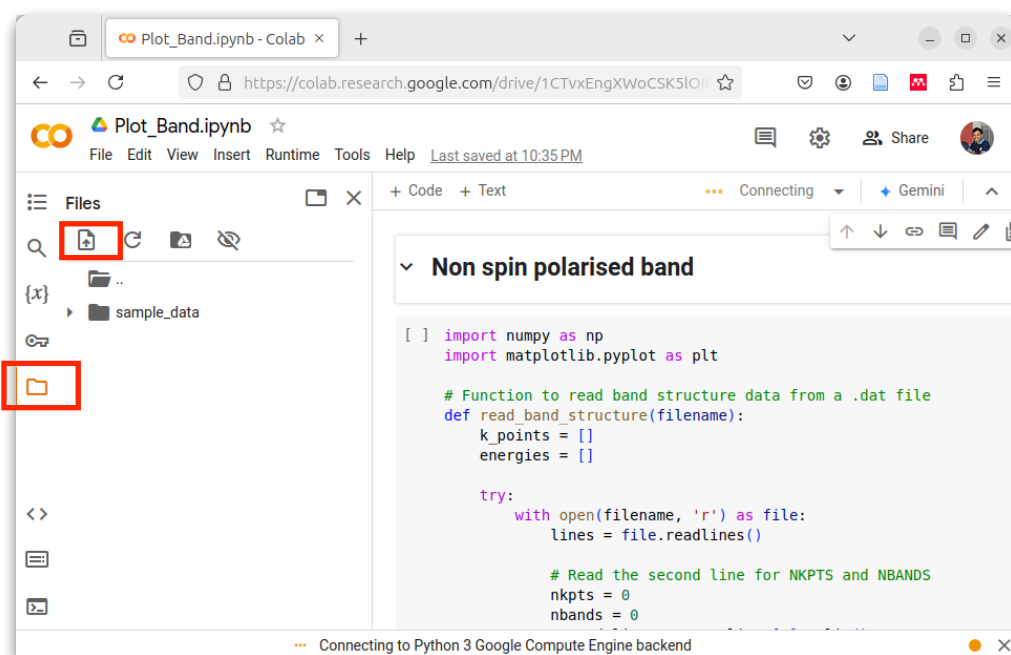
- After logging in, click on **File** and select **upload notebook** option



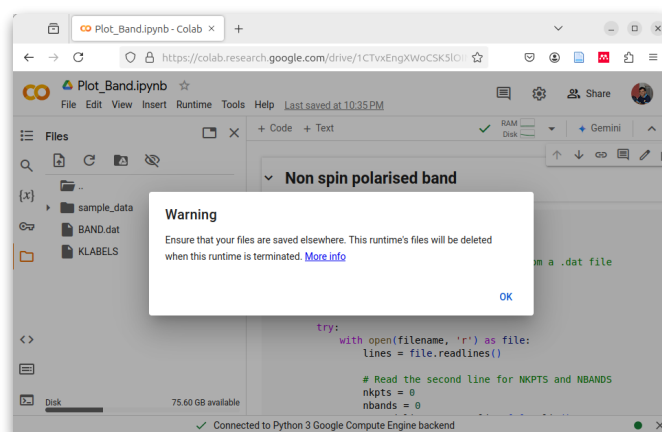
- Select the **Plot_Band.ipynb** file supplied to you



- 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

```

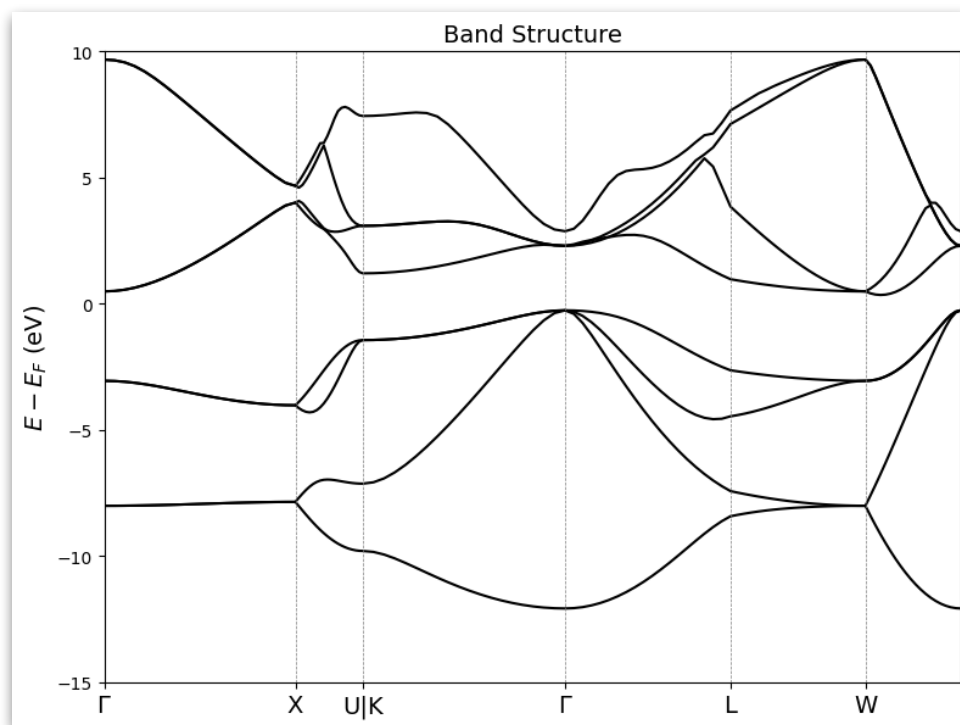
import numpy as np
import matplotlib.pyplot as plt

# Function to read band structure data from a .dat file
def read_band_structure(filename):
    k_points = []
    energies = []

    try:
        with open(filename, 'r') as file:
            lines = file.readlines()

        # Read the second line for NKPTS and NBANDS
        nkpts = 0
        nbands = 0
    
```

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

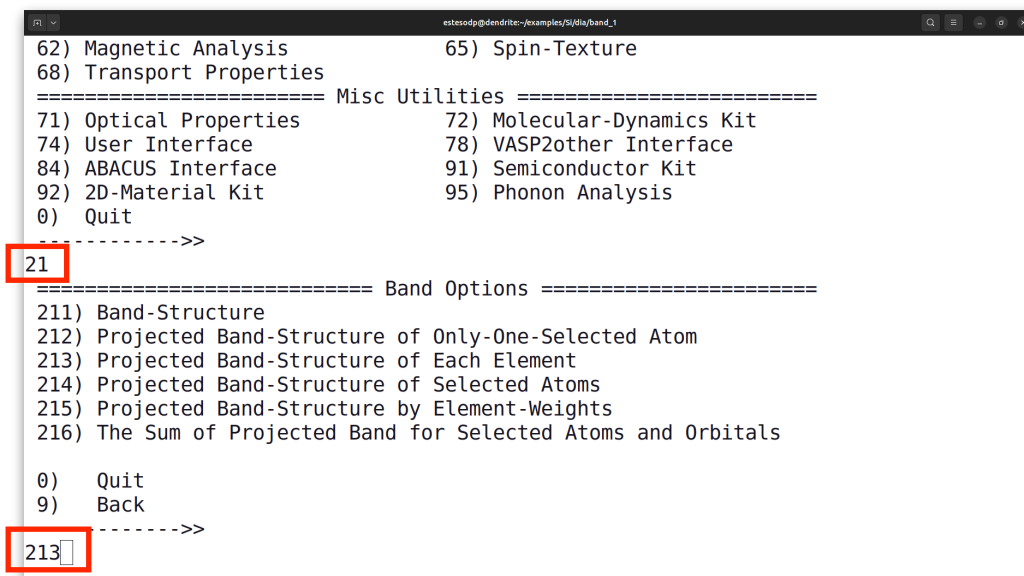


5. Extract fat band structure data from PROCAR file using “vaspkit” package:

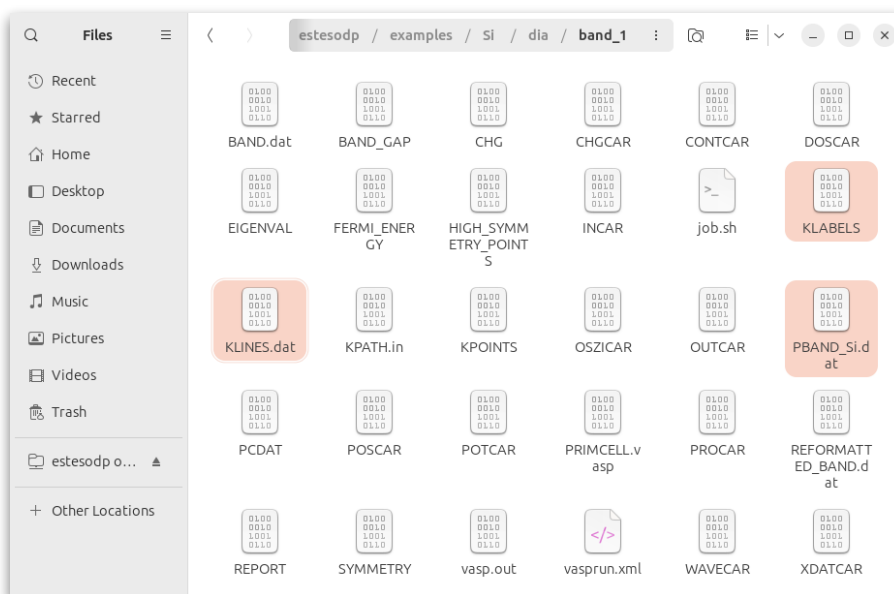
- Run “vaspkit” command in **band** folder in terminal

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

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

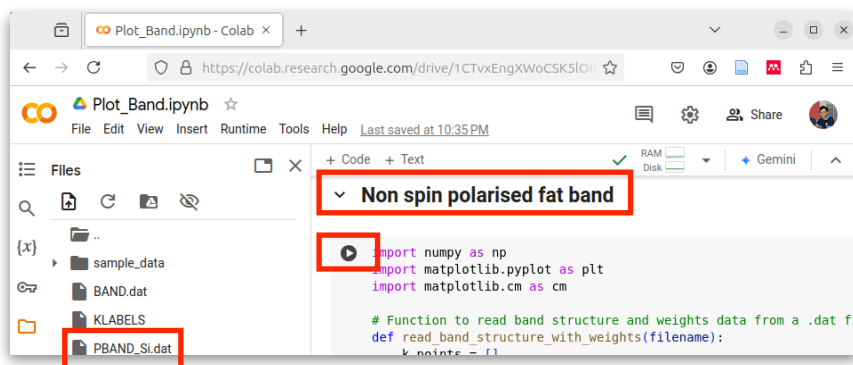


- Following files will be generated

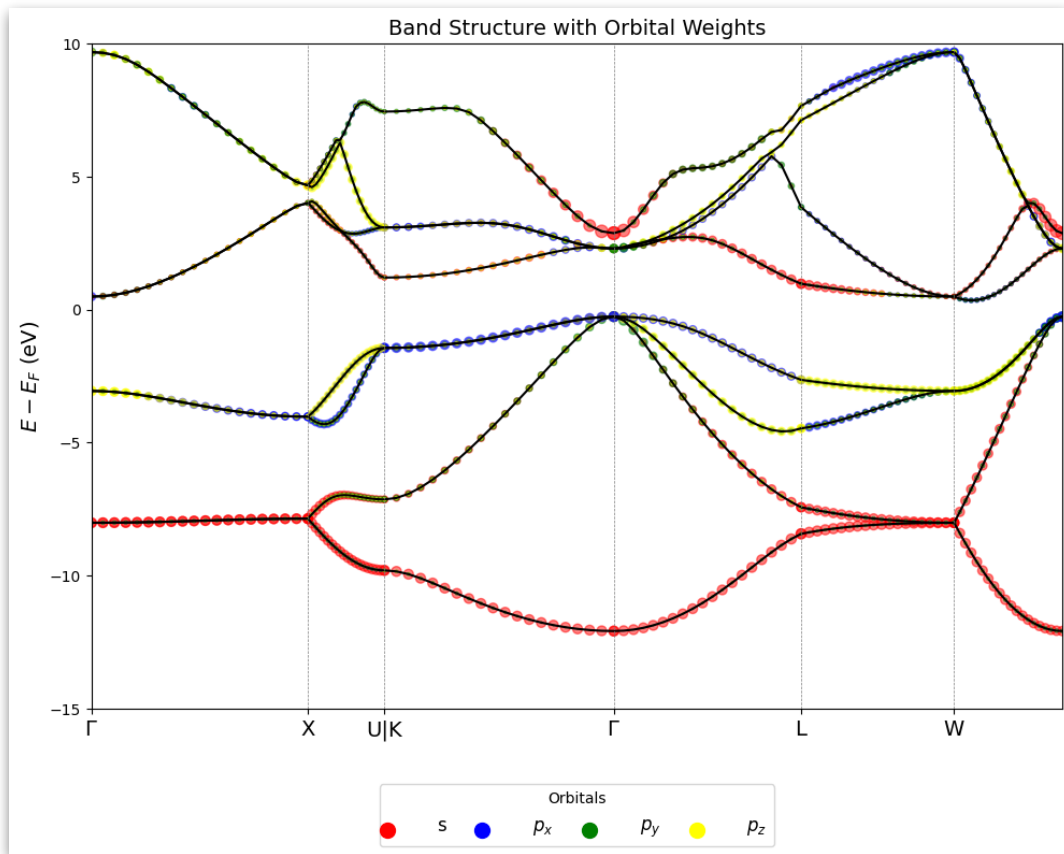


6. Plotting fat band structure using python in google collab

- **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:

Plot_Band.ipynb - Colab

https://colab.research.google.com/drive/1CTvxEngXWoCSK

Plot_Band.ipynb

File Edit View Insert Runtime Tools Help Last saved at 10:35 PM

Files

- sample_data
- BAND.dat
- KLABELS

75.40 GB available

Connected to Python 3 Google Compute Engine backend

Spin polarised band

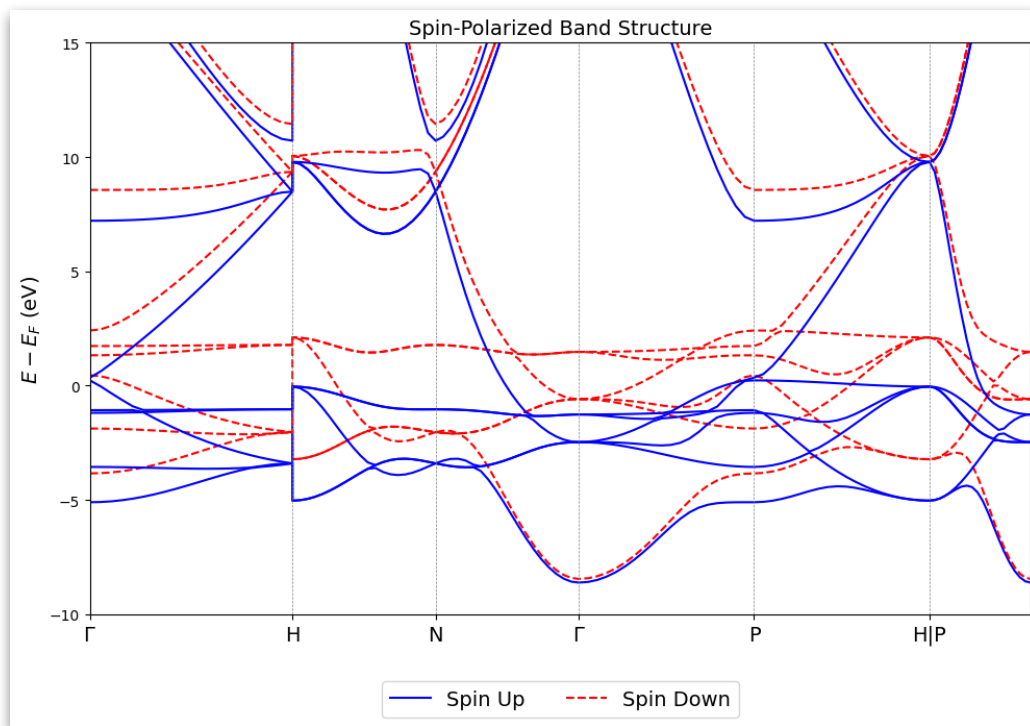
```
import numpy as np
import matplotlib.pyplot as plt

# Function to read spin-polarized band structure data from a .dat
def read_spin_polarized_band_structure(filename):
    k_points = []
    energies_up = []
    energies_down = []

    try:
        with open(filename, 'r') as file:
            lines = file.readlines()

        # Read the second line for NKPTS and NBANDS
        nkpts = 0
        nbands = 0
```

- 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:

