

Calculating electronic structure using density functional theory

- Band structures and Density of states

2024

Krishnaraj K



Recap

Density functional theory calculations using Vienna Ab-initio Simulations Package (VASP)

Inputs:

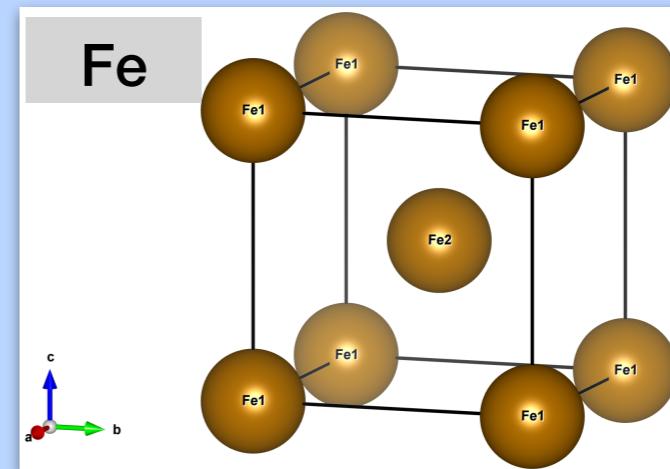
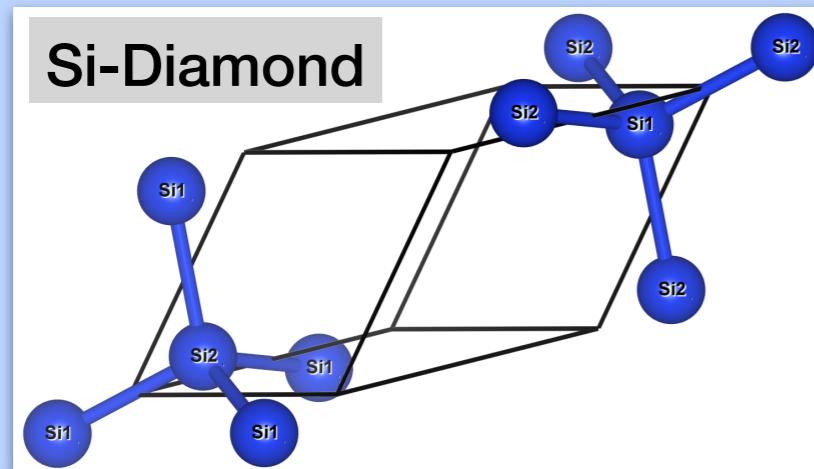
POSCAR

POTCAR

KPOINTS

INCAR

1. Selected two compounds and performed lattice convergence (ISIF=2; IBRION=2)



2. Performed k-point convergence by varying the k-mesh in KPOINTS file

11 x 11 x 11

11 x 11 x 11

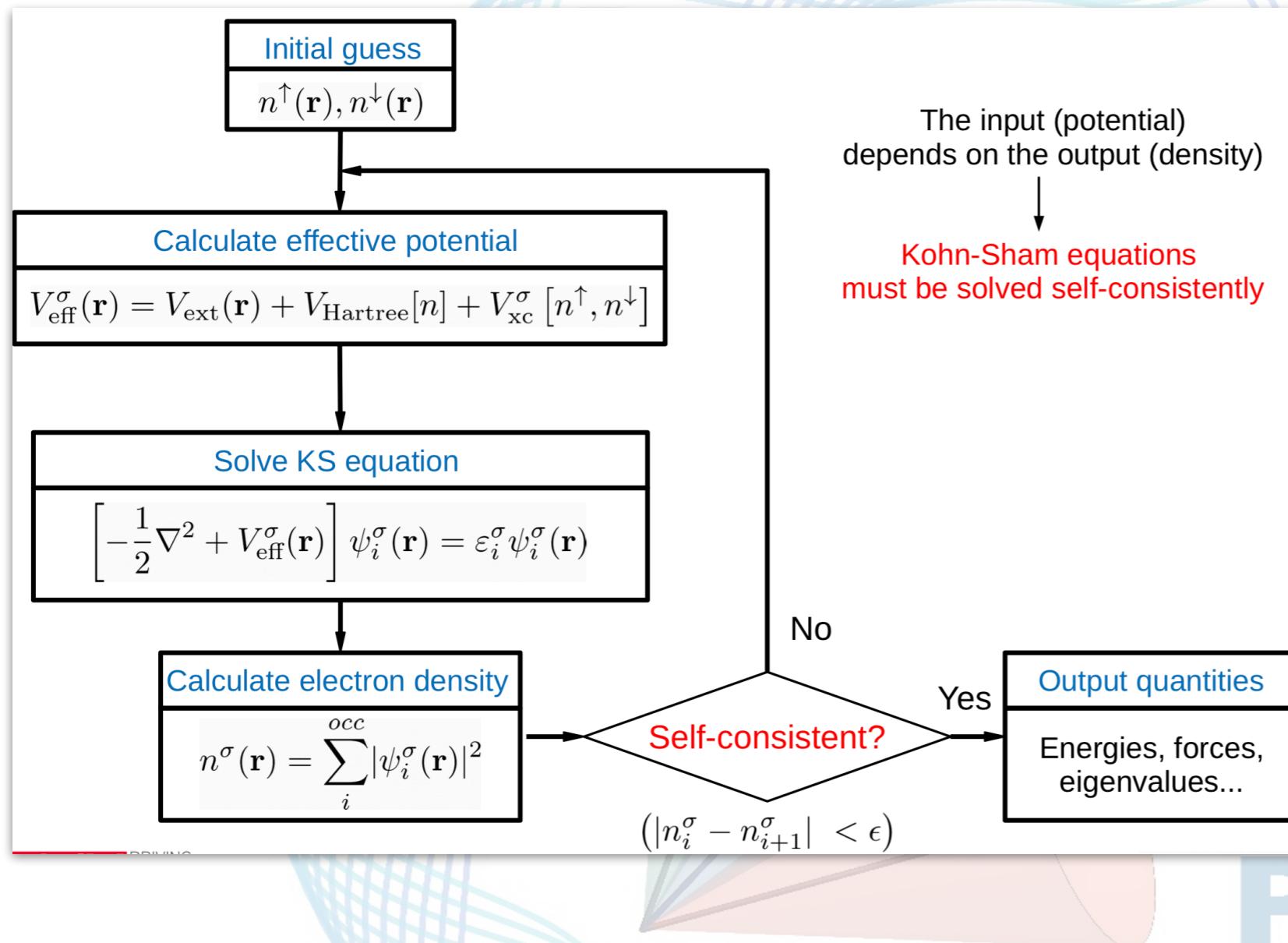
3. Performed ENCUT convergence by varying the ENCUT value in INCAR file

400

400

4. Performed geometry relaxation using ISIF=3 and IBRION=2 with converged parameters

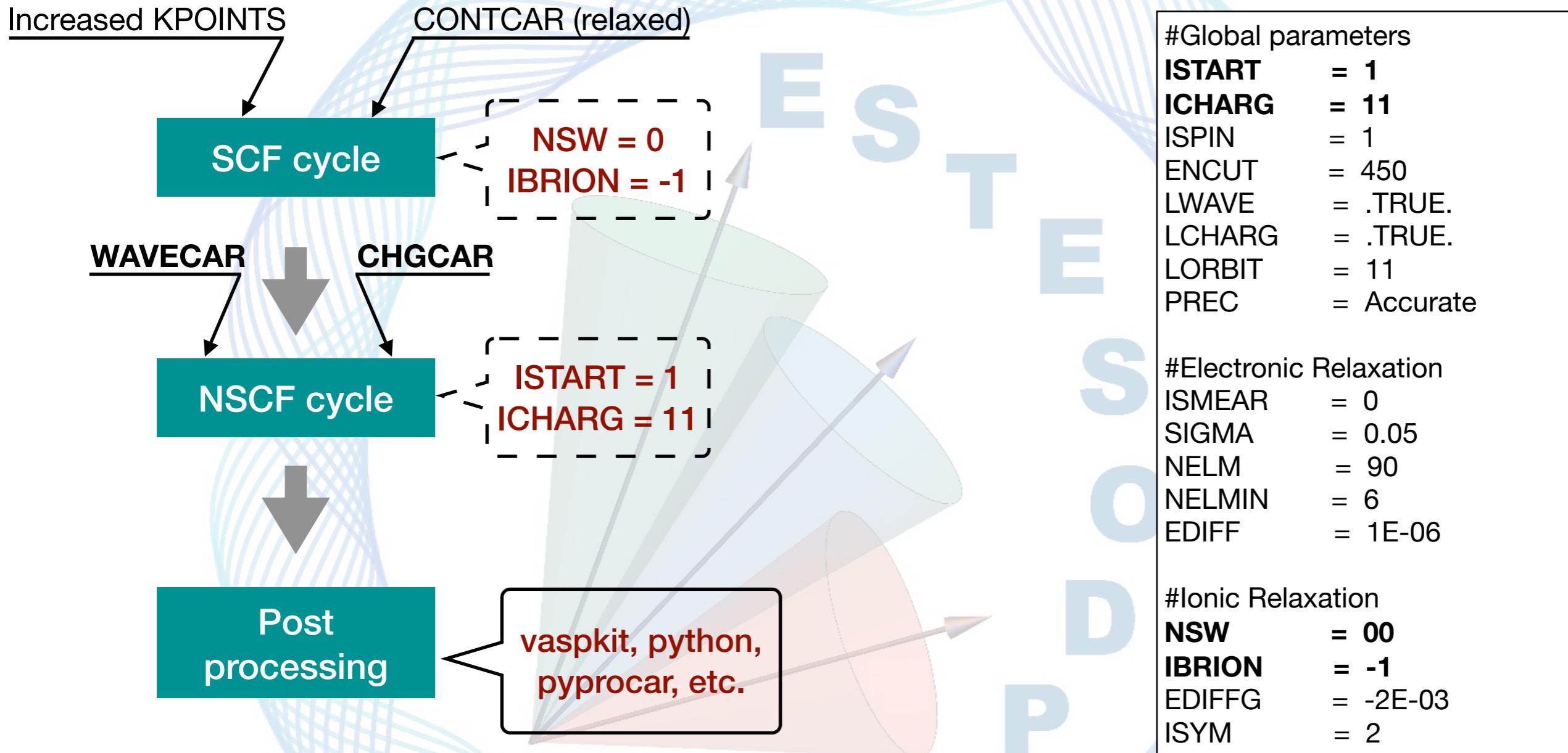
Self Consistent Field (SCF) calc.



#Global parameters	
ISTART	= 0
#ICHARG	= 11
ISPIN	= 1
ENCUT	= 450
LWAVE	= .TRUE.
LCHARG	= .TRUE.
LORBIT	= 11
PREC	= Accurate
#Electronic Relaxation	
ISMEAR	= 0
SIGMA	= 0.05
NELM	= 90
NELMIN	= 6
EDIFF	= 1E-06
#Ionic Relaxation	
NSW	= 00
IBRION	= -1
EDIFFG	= -2E-03
ISYM	= 2

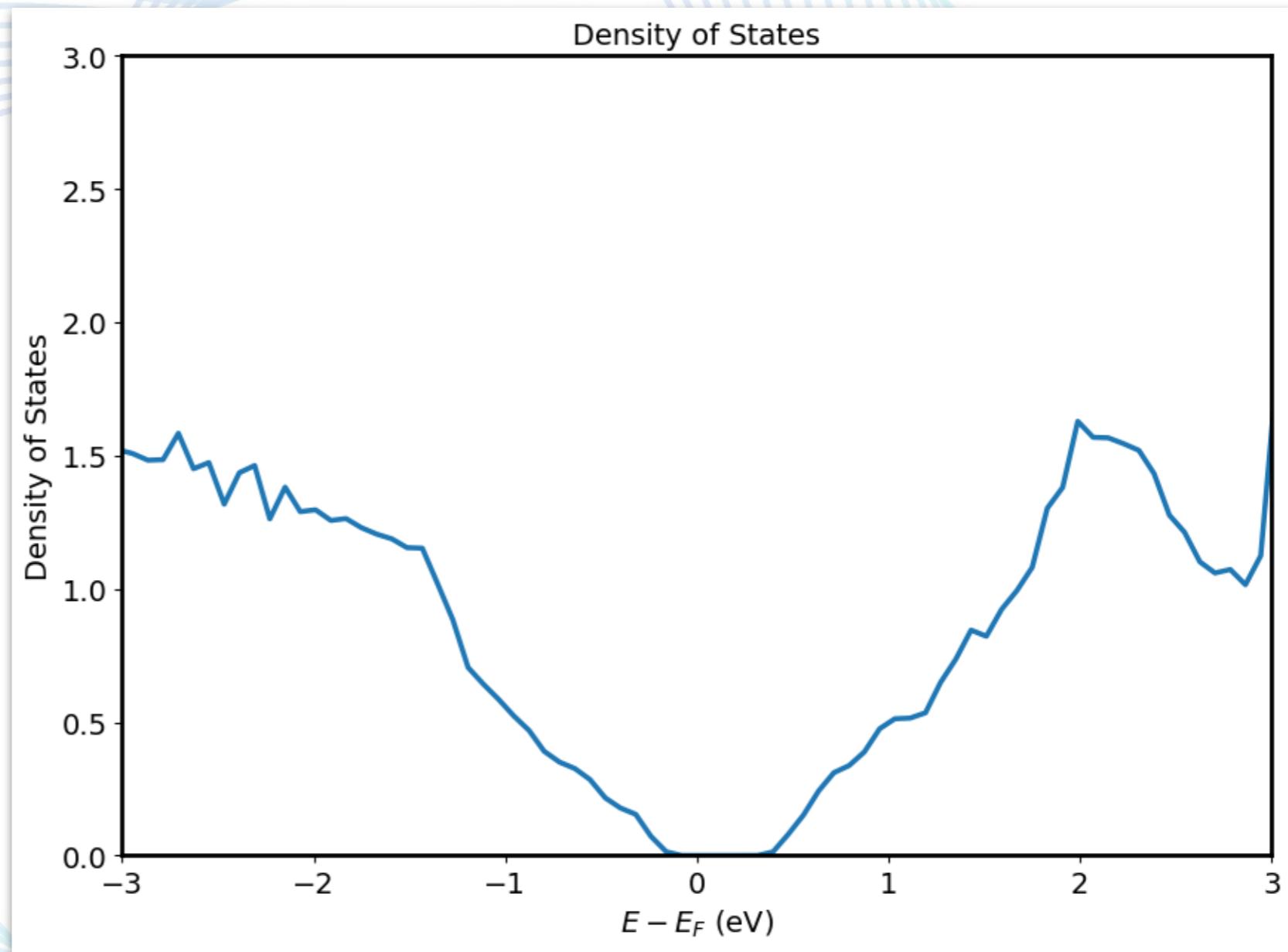
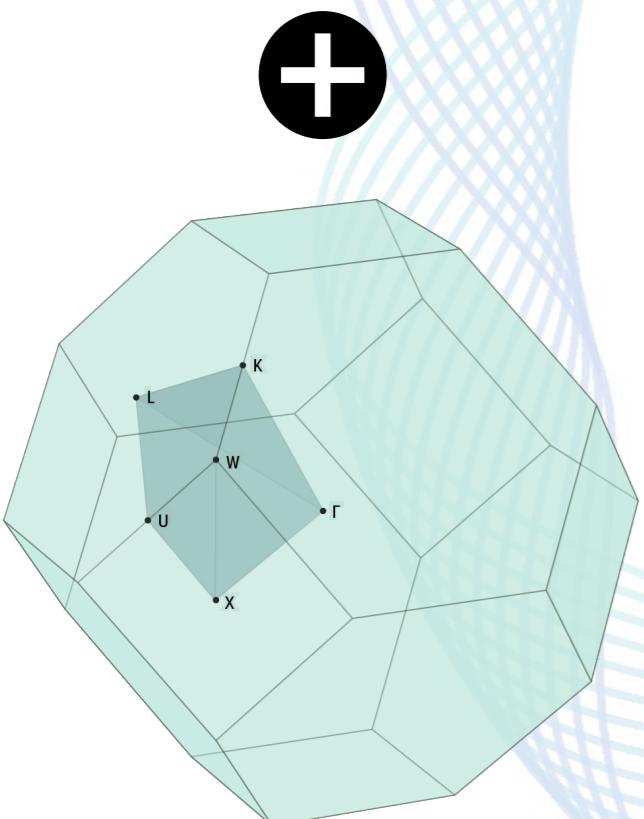
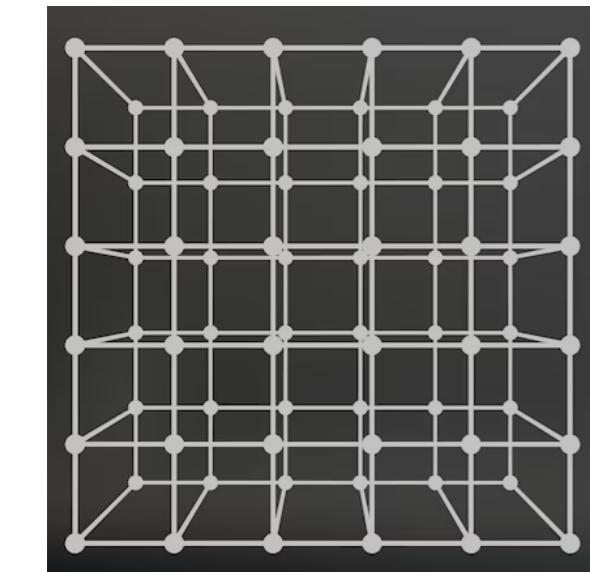
- No change in the geometry of the system (**IBRION = -1**)
- Only one cycle of electronic optimisation is done (**NSW = 00**)

Non-Self Consistent Field (NSCF) calc.



- Self Consistent Field calculations to get optimised charge density (CHGCAR) and Kohn-Sham wave functions (WAVECAR) for the relaxed geometry
- These are then taken as input to run Non-Self Consistent Field calculations

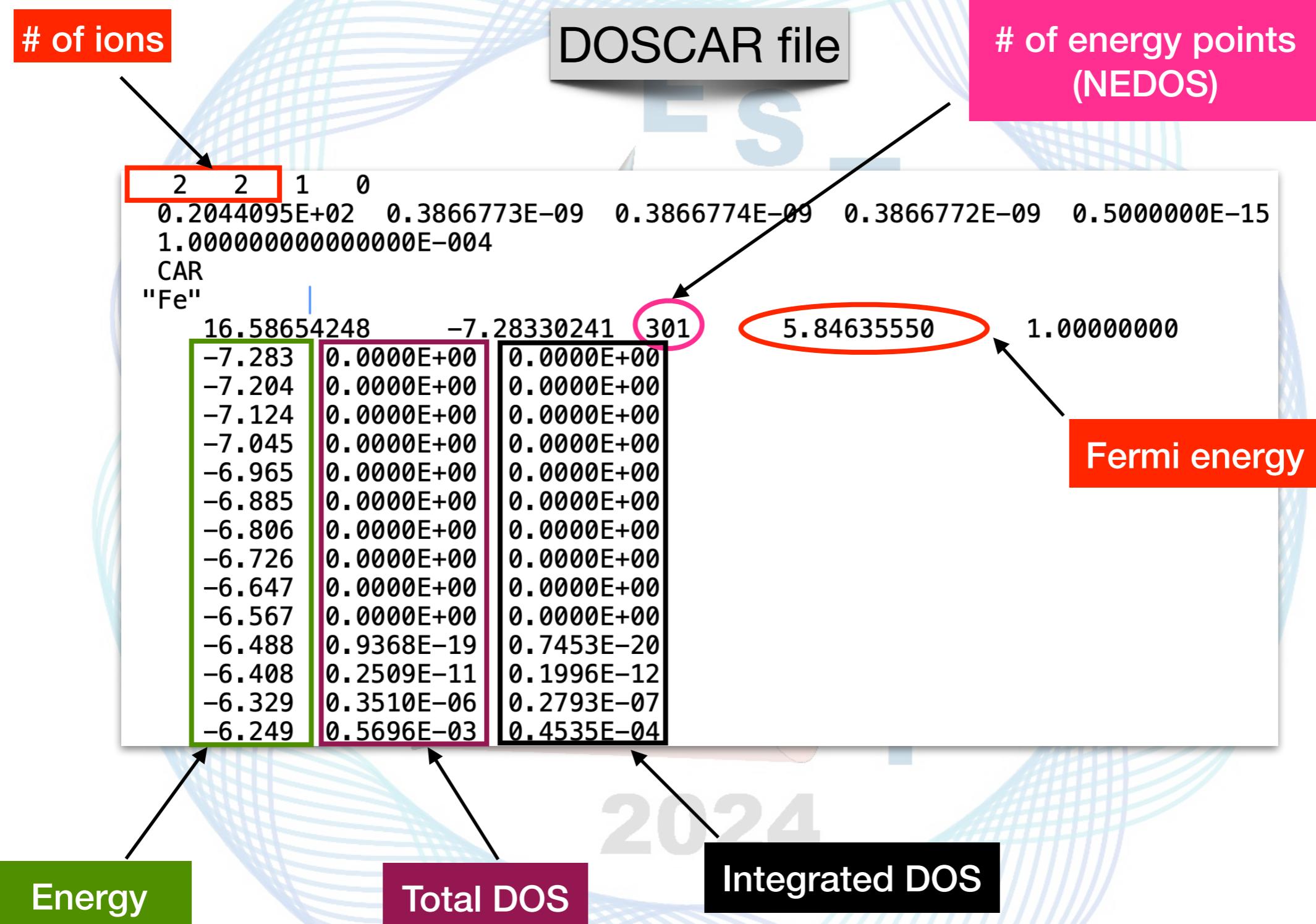
Calculating density of states (DOS)



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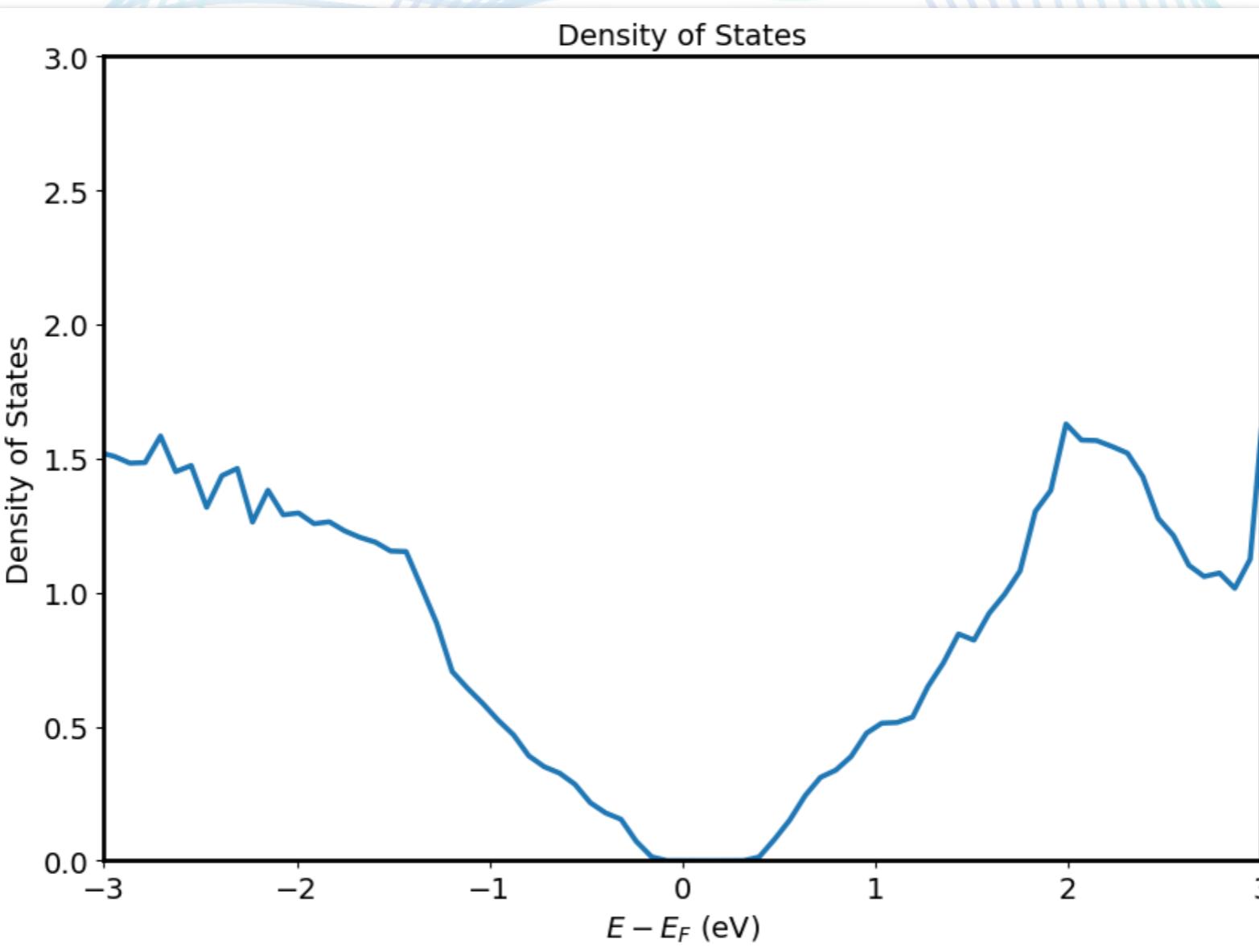
- 📌 Take a finer mesh of k-points for better accuracy of density of states

DOSCAR



- Take a finer mesh of k-points for better accuracy of density of states

Plotting DOS



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- Extract DOS details using “vaspkit” software
- Plot the DOS using python in google collab

Partial DOS (PDOS)

DOSCAR file									
ion index									
16.109	0.0000E+00	0.1600E+02							
16.189	0.0000E+00	0.1600E+02							
16.268	0.0000E+00	0.1600E+02							
16.348	0.0000E+00	0.1600E+02							
16.427	0.0000E+00	0.1600E+02							
16.507	0.0000E+00	0.1600E+02							
16.587	0.0000E+00	0.1600E+02							
16.58654248	-7.28330241	301	5.84635550	1.00000000					
-7.283	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
-7.204	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
-7.124	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
-7.045	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
-6.965	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
-6.885	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
-6.806	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
-6.726	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
-6.647	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
-6.567	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
-6.488	0.1986E-19	0.1347E-32	0.1347E-32	0.1347E-32	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
-6.408	0.5317E-12	0.6766E-16	0.6766E-16	0.6766E-16	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
-6.329	0.7439E-07	0.1516E-10	0.1516E-10	0.1516E-10	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
-6.249	0.1207E-03	0.4121E-07	0.4121E-07	0.4121E-07	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
-6.169	0.4758E-02	0.3221E-05	0.3221E-05	0.3221E-05	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
-6.090	0.1843E-01	0.2639E-04	0.2639E-04	0.2639E-04	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
-6.010	0.2857E-01	0.7478E-04	0.7478E-04	0.7478E-04	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
-5.931	0.3592E-01	0.1410E-03	0.1410E-03	0.1410E-03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
-5.851	0.4162E-01	0.2187E-03	0.2187E-03	0.2187E-03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
-5.772	0.4624E-01	0.3017E-03	0.3017E-03	0.3017E-03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00

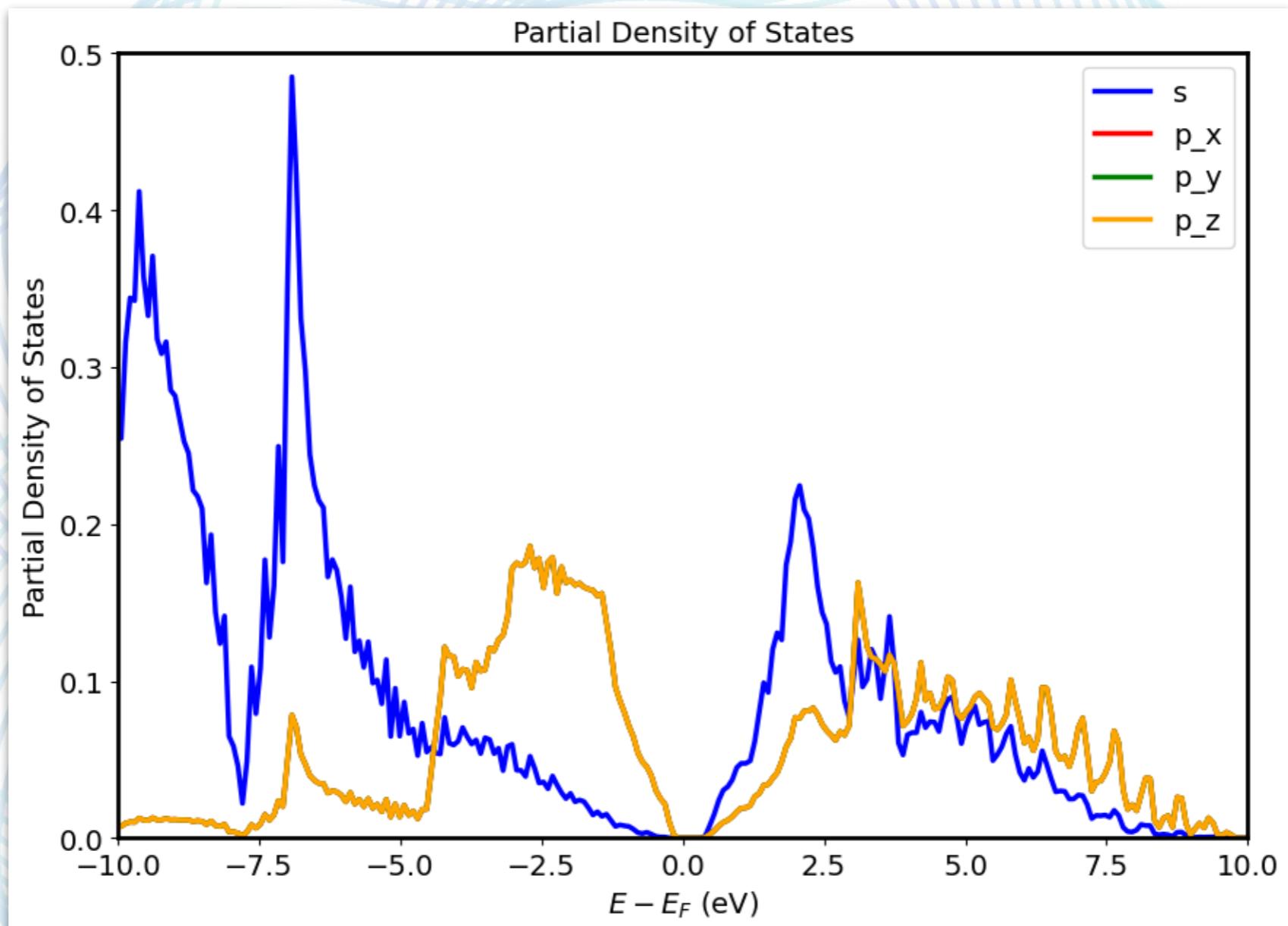
Energy

s orbital

p orbital

d orbital

Plotting PDOS



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- Extract PDOS details using “vaspkit” software
- Plot the PDOS using python in google collab

Spin-polarised DOS

DOSCAR file

2	2	1	0	0.1133275E+02	0.2830013E-09	0.2830013E-09	0.2830013E-09	0.5000000E-15
1.000000000000000E-004								
CAR								
unknown system								
46.37405141	-4.929	0.0000E+00	-4.92901603	301	5.84667741	1.00000000		
-4.929	0.0000E+00		0.0000E+00		0.0000E+00	0.0000E+00		
-4.758	0.0000E+00		0.0000E+00		0.0000E+00	0.0000E+00		
-4.587	0.0000E+00		0.0000E+00		0.0000E+00	0.0000E+00		
-4.416	0.0000E+00		0.0000E+00		0.0000E+00	0.0000E+00		
-4.245	-0.3552E-32		0.0000E+00		-0.6075E-33	0.0000E+00		
-4.074	-0.2351E-26		-0.5825E-32		-0.4020E-27	-0.9962E-33		
-3.903	-0.3643E-21		-0.3661E-26		-0.6230E-22	-0.6260E-27		
-3.732	-0.1281E-16		-0.5389E-21		-0.2191E-17	-0.9215E-22		
-3.561	-0.1084E-12		-0.1806E-16		-0.1854E-13	-0.3089E-17		
-3.390	-0.2137E-09		-0.1446E-12		-0.3657E-10	-0.2473E-13		
-3.219	-0.9818E-07		-0.2707E-09		-0.1683E-07	-0.4632E-10		

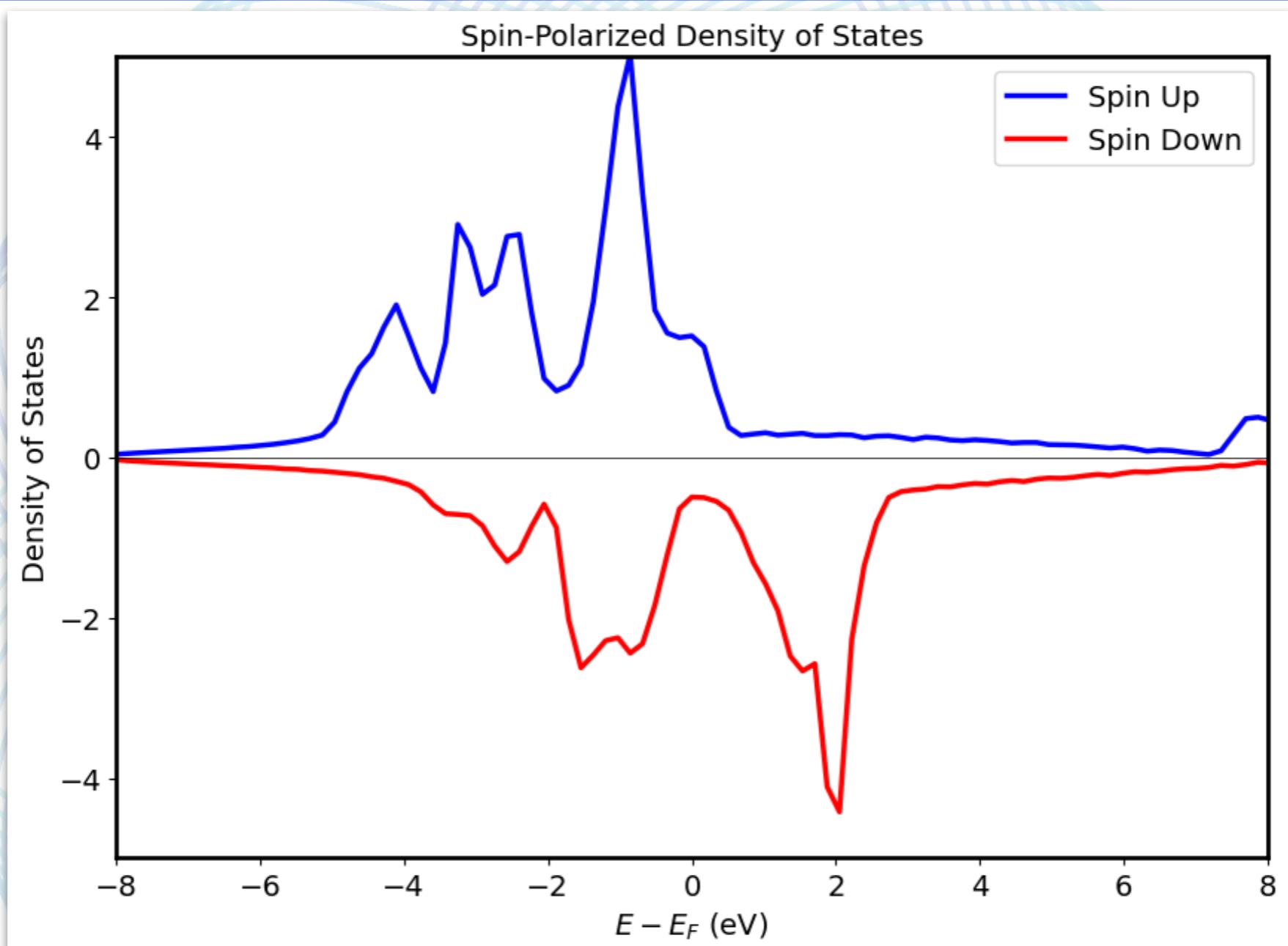
Energy

Total spin up DOS

Total spin down DOS

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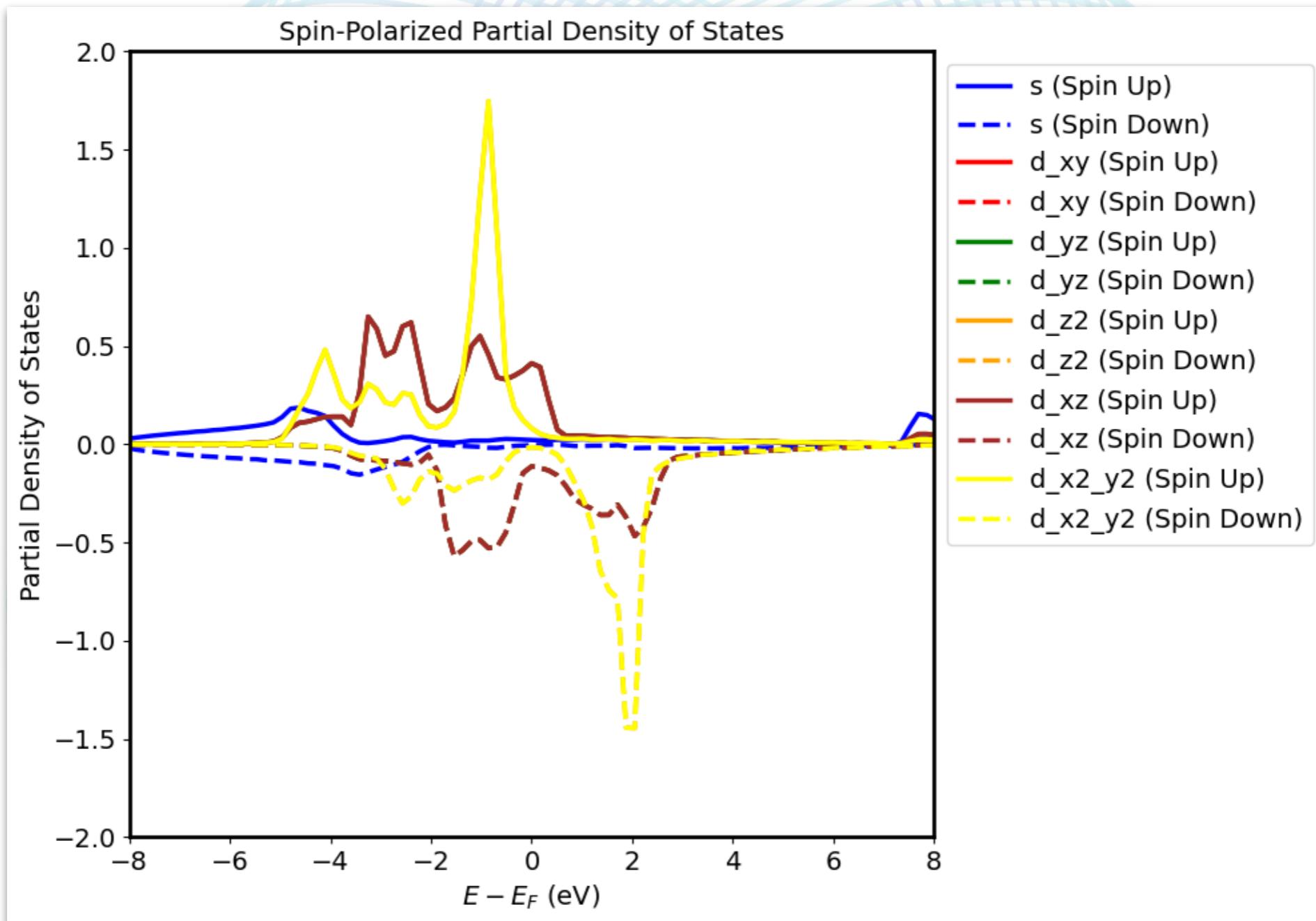
Spin-polarised DOS



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- Extract DOS details using “vaspkit” software
- Plot the DOS using python in google collab

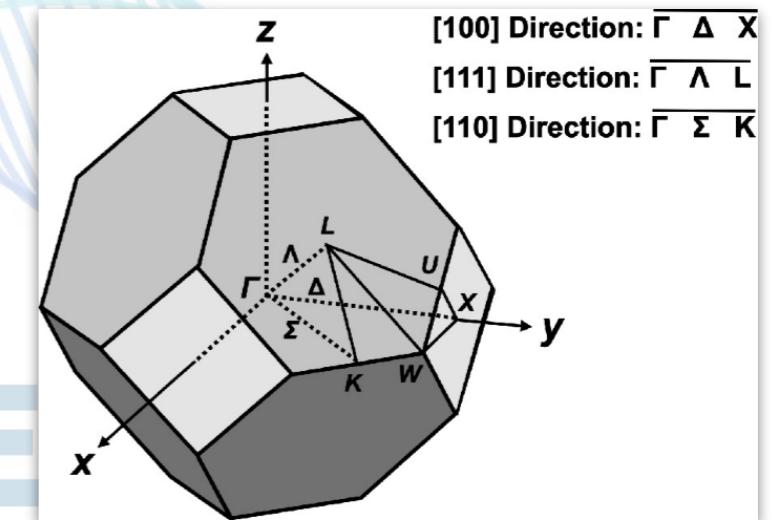
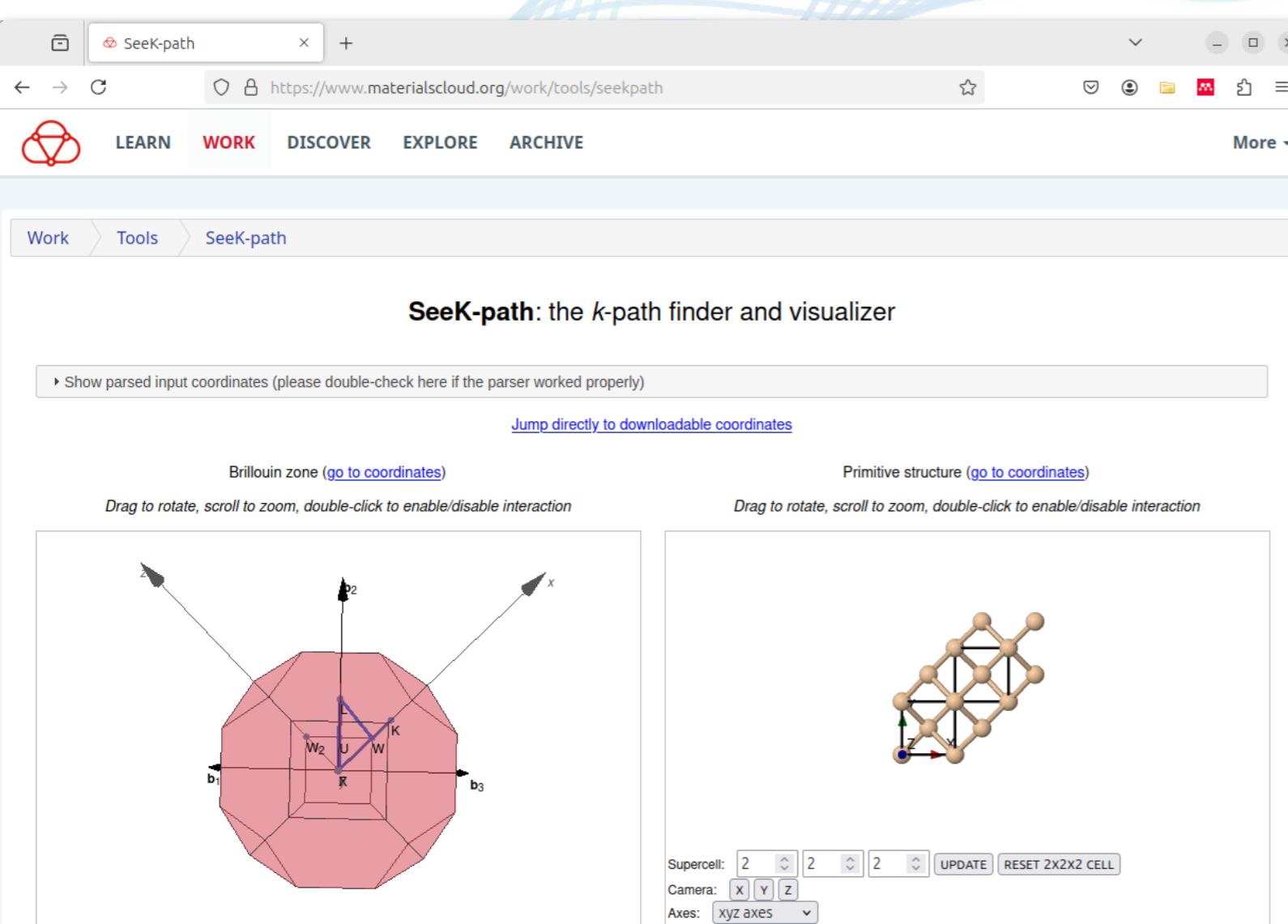
Spin-polarised PDOS



- Extract DOS details using “vaspkit” software
- Plot the DOS using python in google collab

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Calculating band structure

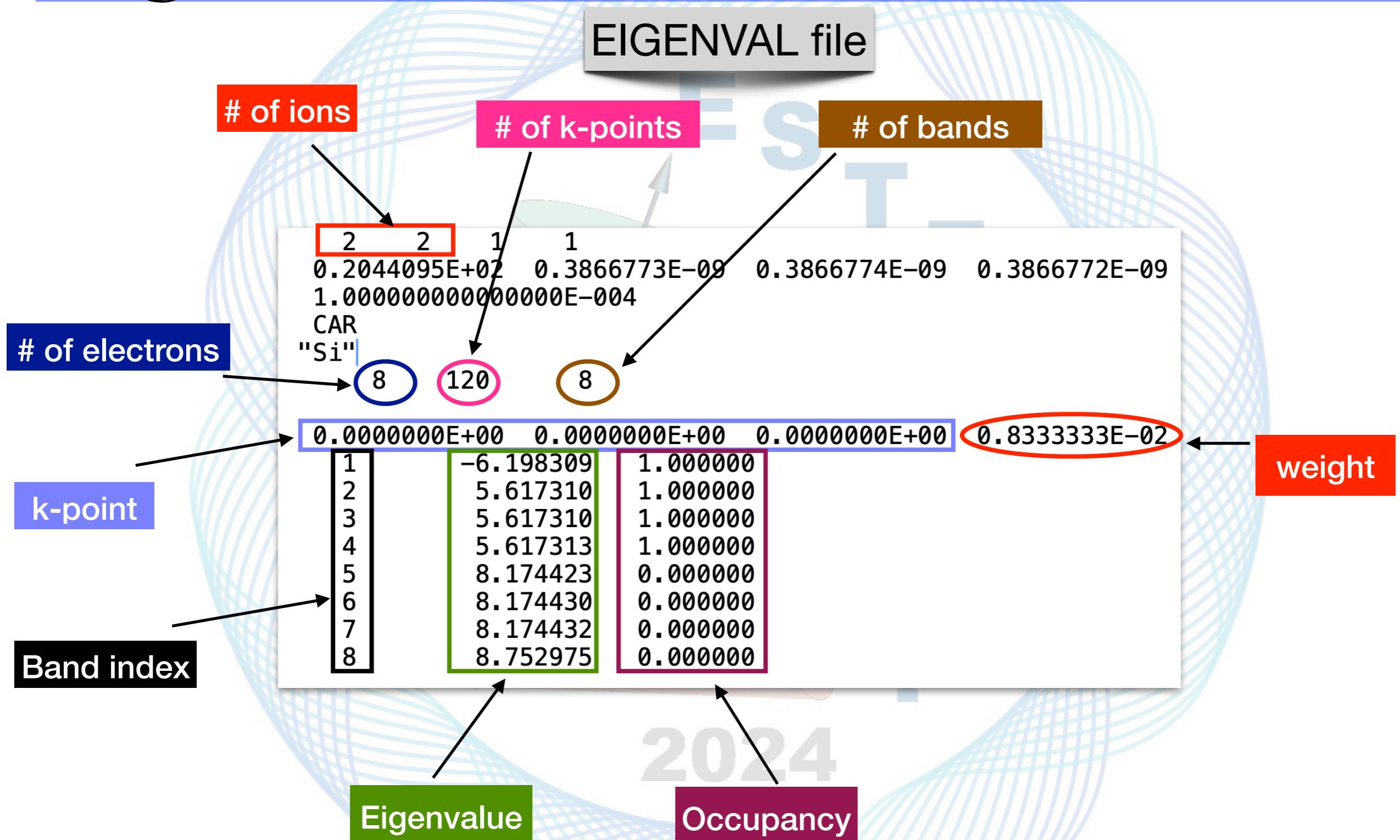


K-Path Generated by VASPKIT.

Line-Mode	Reciprocal			
20	0.0000000000	0.0000000000	0.0000000000	GAMMA
	0.5000000000	0.0000000000	0.5000000000	X
	0.5000000000	0.0000000000	0.5000000000	X
	0.6250000000	0.2500000000	0.6250000000	U
	0.3750000000	0.3750000000	0.7500000000	K
	0.0000000000	0.0000000000	0.0000000000	GAMMA
	0.0000000000	0.0000000000	0.0000000000	GAMMA
	0.5000000000	0.5000000000	0.5000000000	L
	0.5000000000	0.5000000000	0.5000000000	L
	0.5000000000	0.2500000000	0.7500000000	W
	0.5000000000	0.2500000000	0.7500000000	W
	0.5000000000	0.0000000000	0.5000000000	X

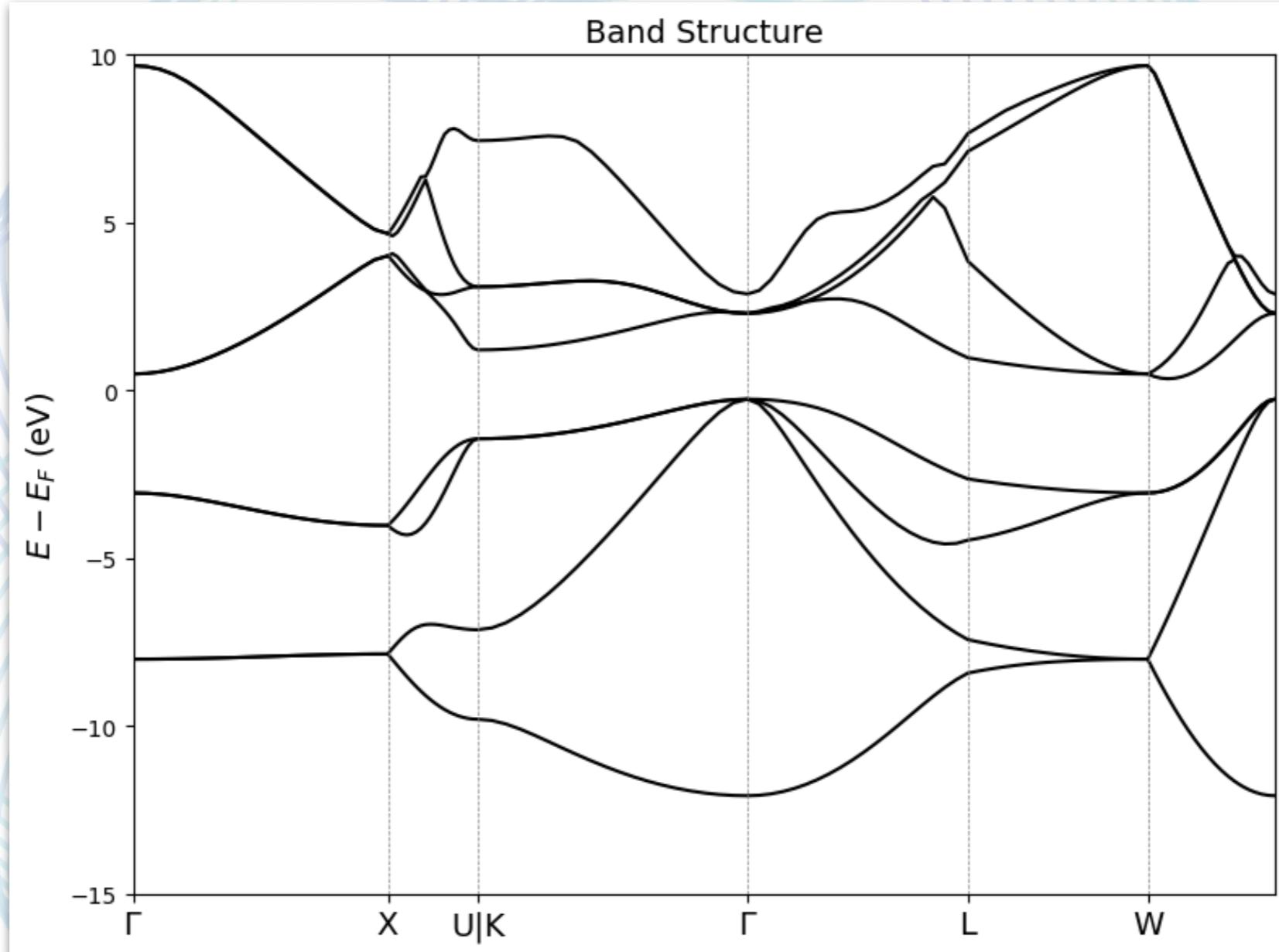
- Band structures are plotted in a 2D path joining the points corresponding to high symmetry in the first Brillouin zone
- KPOINTS file will contain special k-points on this high-symmetry path

Eigenvalues for band structure



- Occupancy of 0 signifies the conduction bands for semiconductors and insulators

Band structure plotting



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- Extract band details using “vaspkit” software
- Plot the bands using python in google collab

Orbital contributions

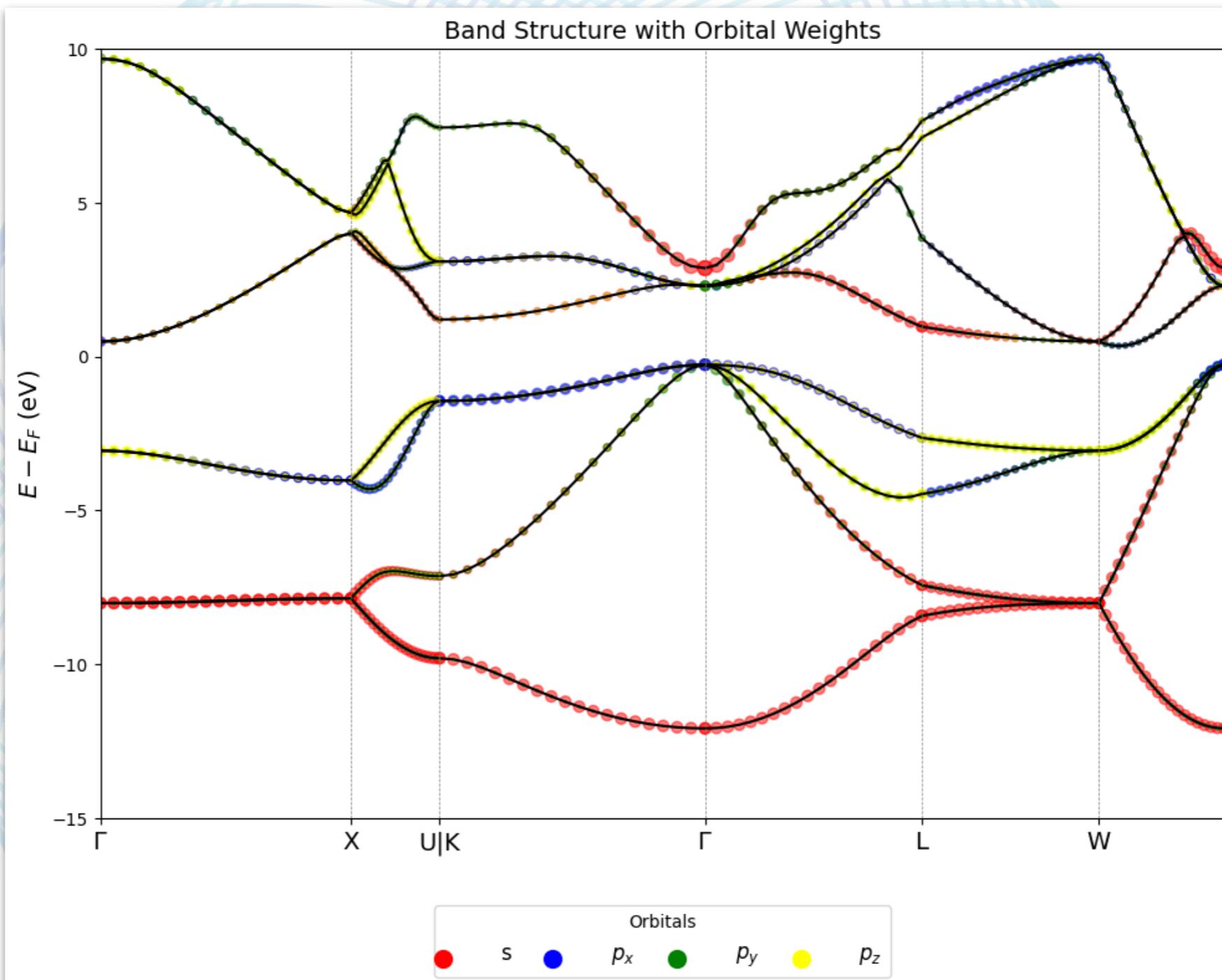
PROCAR file

PROCAR lm decomposed

		# of k-points:	120	# of bands:		8	# of ions:		2	
k-point		1 :	0.00000000 0.00000000 0.00000000							
band		1 # energy	-6.19830946	# occ.		2.00000000				
ion	s	py	pz	px	dxy	dyz	dz2	dxz	x2-y2	tot
1	0.212	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.212
2	0.212	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.212
tot	0.424	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.424
band	2 # energy	5.61730991	# occ.	2.00000000						
ion	s	py	pz	px	dxy	dyz	dz2	dxz	x2-y2	tot
1	0.000	0.000	0.205	0.009	0.000	0.000	0.000	0.000	0.000	0.214
2	0.000	0.000	0.205	0.009	0.000	0.000	0.000	0.000	0.000	0.214
tot	0.000	0.001	0.410	0.017	0.000	0.000	0.000	0.000	0.000	0.428

- Use LORBIT=11 tag in INCAR to get lm-decomposed band structure in PROCAR file
- Various combinations of contributions can be obtained from “vaspkit” software

Fat bands



- ✿ Extract band details using “vaspkit” software
- ✿ Plot the bands using python in google collab

Spin-polarised band structure

EIGENVAL file

```

1   1   1   2
0.1133275E+02  0.2450863E-09  0.2450863E-09  0.2450863E-09
1.00000000000000E-004
CAR
unknown system
8      120      12

0.0000000E+00  0.0000000E+00  0.0000000E+00  0.8333333E-02
1      -2.595340  -2.434421  1.000000  1.000000
2      3.550143   5.429079  1.000000  1.000126
3      3.550144   5.429216  1.000000  1.000127
4      3.550145   5.429227  1.000000  1.000127
5      4.758146   7.495864  1.000000  -0.000000
6      4.758147   7.496032  1.000000  -0.000000
7      30.897674  30.642588 0.000000  0.000000
8      30.897674  30.642588 0.000000  0.000000
9      30.897674  30.642588 0.000000  0.000000
10     35.995237  36.192216 0.000000  0.000000
11     35.995238  36.192224 0.000000  0.000000
12     38.318179  38.956505 0.000000  0.000000

```

Band index

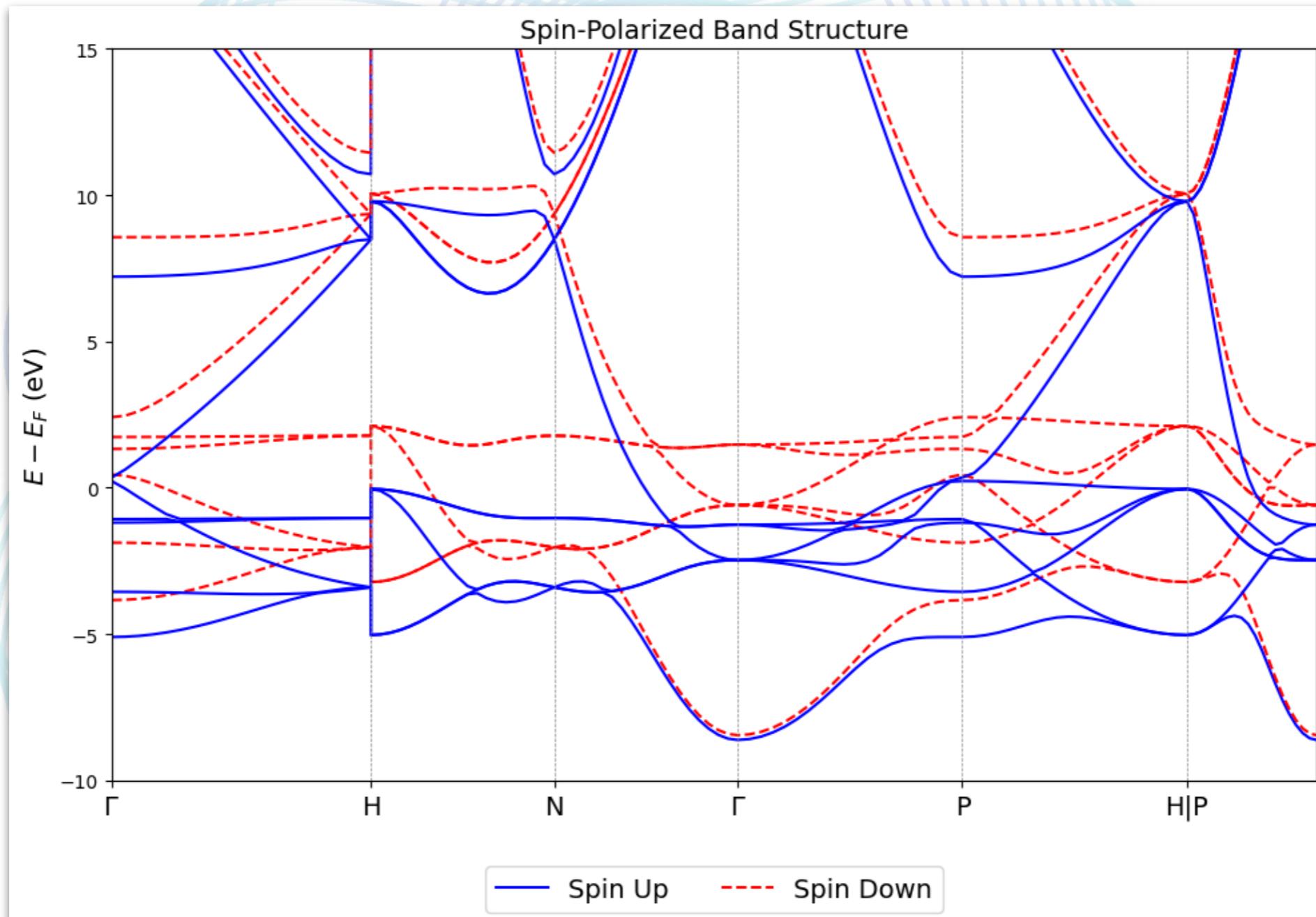
Eigenvalue spin up

Eigenvalue spin down

Occupancy spin down

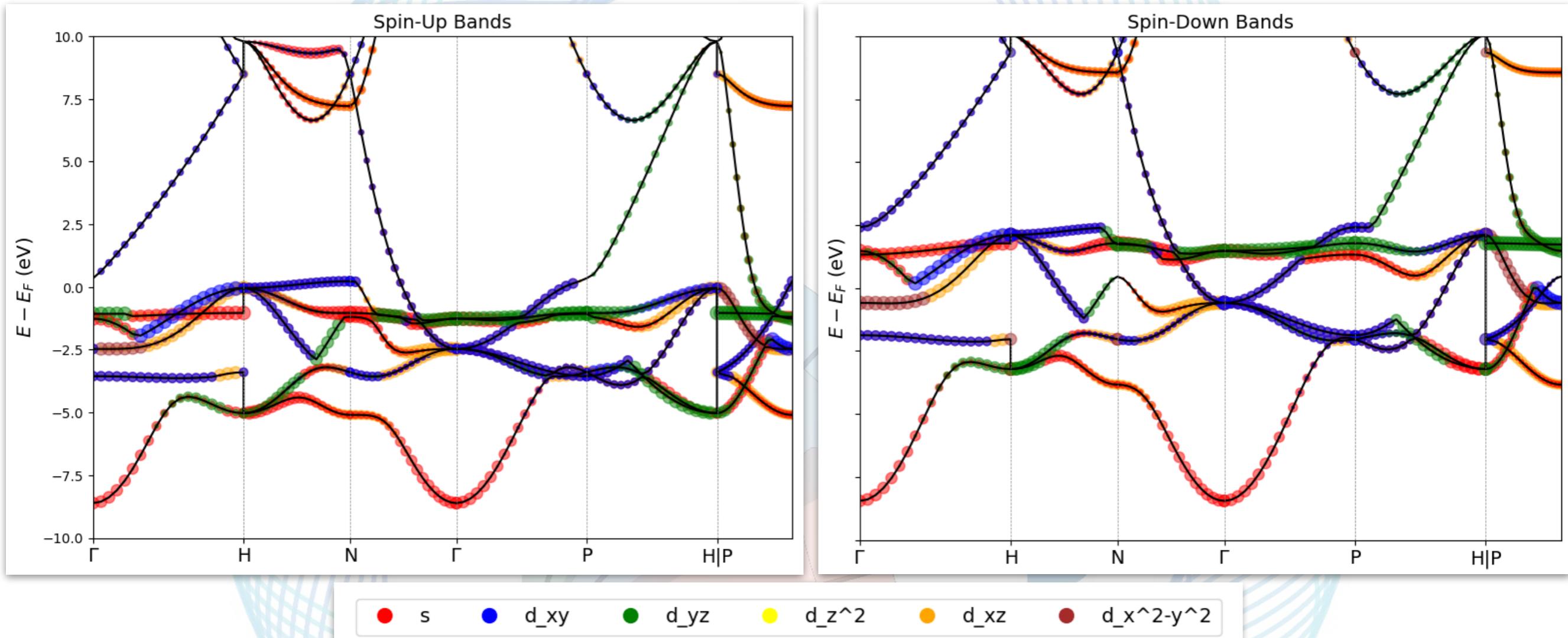
Occupancy spin up

Spin-polarised band structure



- Extract band details using “vaspkit” software
- Plot the bands using python in google collab

Spin-polarised fat band structure



- Extract band details using “vaspkit” software
- Plot the bands using python in google collab



**ESTE
S
D
P**

Thank you

2024

The background features a large, light blue circular pattern composed of many thin, curved lines forming concentric shapes. Overlaid on this are several grey arrows pointing upwards and outwards from the center. In the center of the circle, the words "ESTE", "S", "D", and "P" are arranged vertically in a light blue font. Below them, the words "Thank you" are written in a large, bold black font. At the bottom of the circle, the year "2024" is displayed in a large, light grey font.