Homework of Day 1

1. Calculate the lattice constant by minimization of stress and energy of W and Ni.
2. Calculate the density of states and local density of states of W and Ni.
3. Calculate the band structure and partial band structure of W and Ni.
We demo the results of Au (fcc) and Fe (bcc). However, the W has a bcc crystal structure and Ni has a fcc crystal structure.

Element/Struc.	POTCAR	Lattice constant A^0
Au fcc	PAW LDA	4.06
Fe bcc	PAW GGA	2.82
Ni fcc	PAW GGA	3.52
W bcc	PAW LDA	3.13

Homework of Day 2

1. **Calculate the Surface Relaxation, Surface Energy and Work Function for W(100) and Ni(100) Surfaces using 1, 3 and 5 layers.**
2. **Calculate the Bond Length and Binding Energy of O2 Molecule.**

How to submit your homework ?

In the example, we use Au, Fe and CO.
In your homework, replaced its by W, Ni and O_2.

1. After you finish your homework, use homework.sh to copy your working directory (work-vasp) to /work/u50tcl00/spring-school-2021/homework

- cdw
- ls
- work-vasp result_VASPspring_school
- homework.sh

In order to save space, homework.sh will remove the WAVCAR and CHG in your working directory

2. And upload your pdf file with name : site_number-name-hw-spring-school-2021

Site number : 1-a12 or 2-a12
其中第一個數字代表課程的梯次
1 代表第一梯次 ; 2 代表第二梯次

1-a12-tcleung-hw-spring-school.pdf

or

1-a12-梁贊全-hw-spring-school.pdf

T1-93

參加第一原理暑期課程需繳交的作業範本

Homework-spring-school-2021

Name:_____ Site number : 1-a25

Username in NCHC _____

(A) Au-bulk

1. Use the method of minimization of the stress

Lattice constant = 4.056A (PREC = high in INCAR) according to the OUTCAR.

external pressure = -4.86 kB Pullay stress = 0.00 kB

VOLUME and BASIS-vectors are now :

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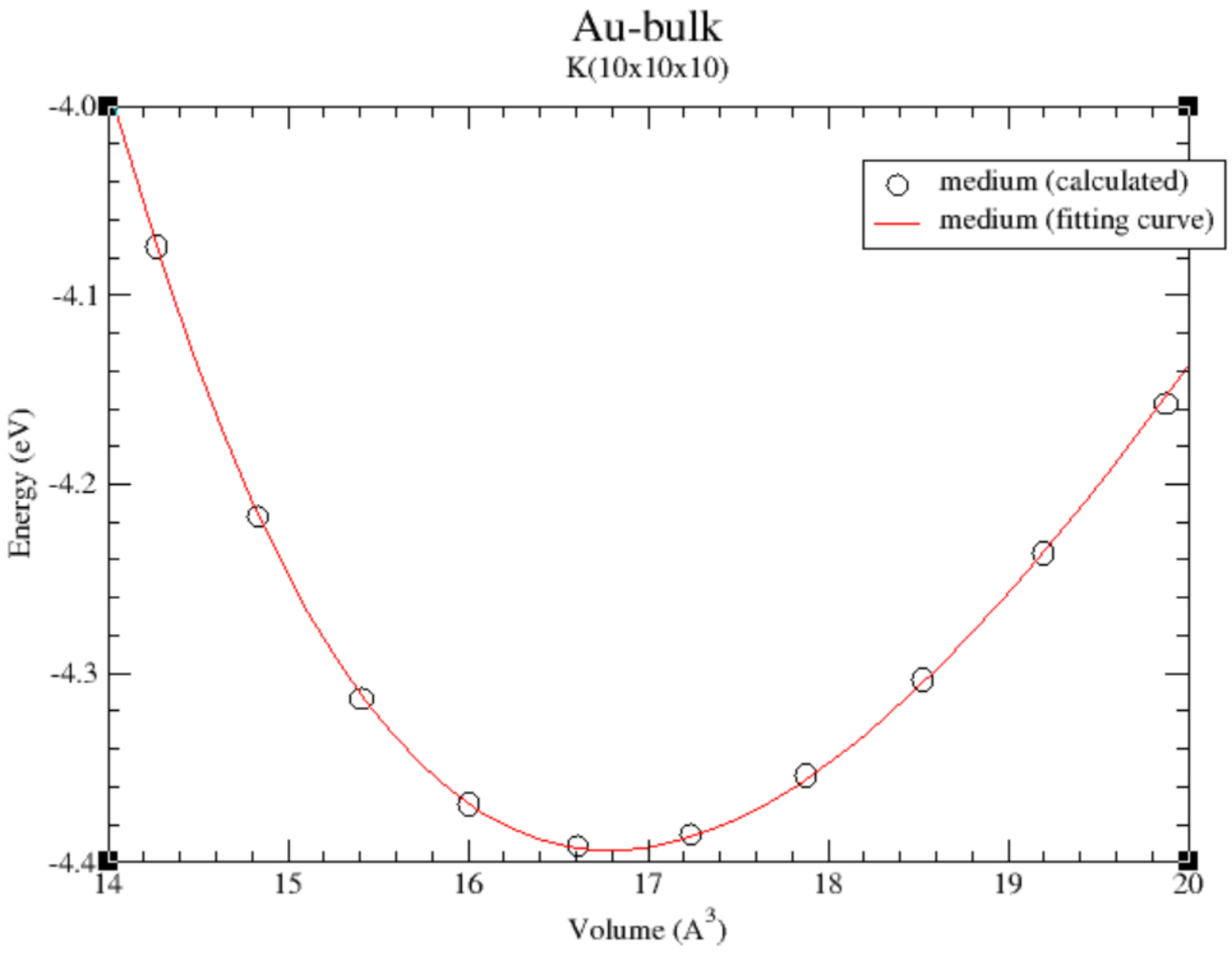
energy-cutoff : 287.34

volume of cell : 16.69

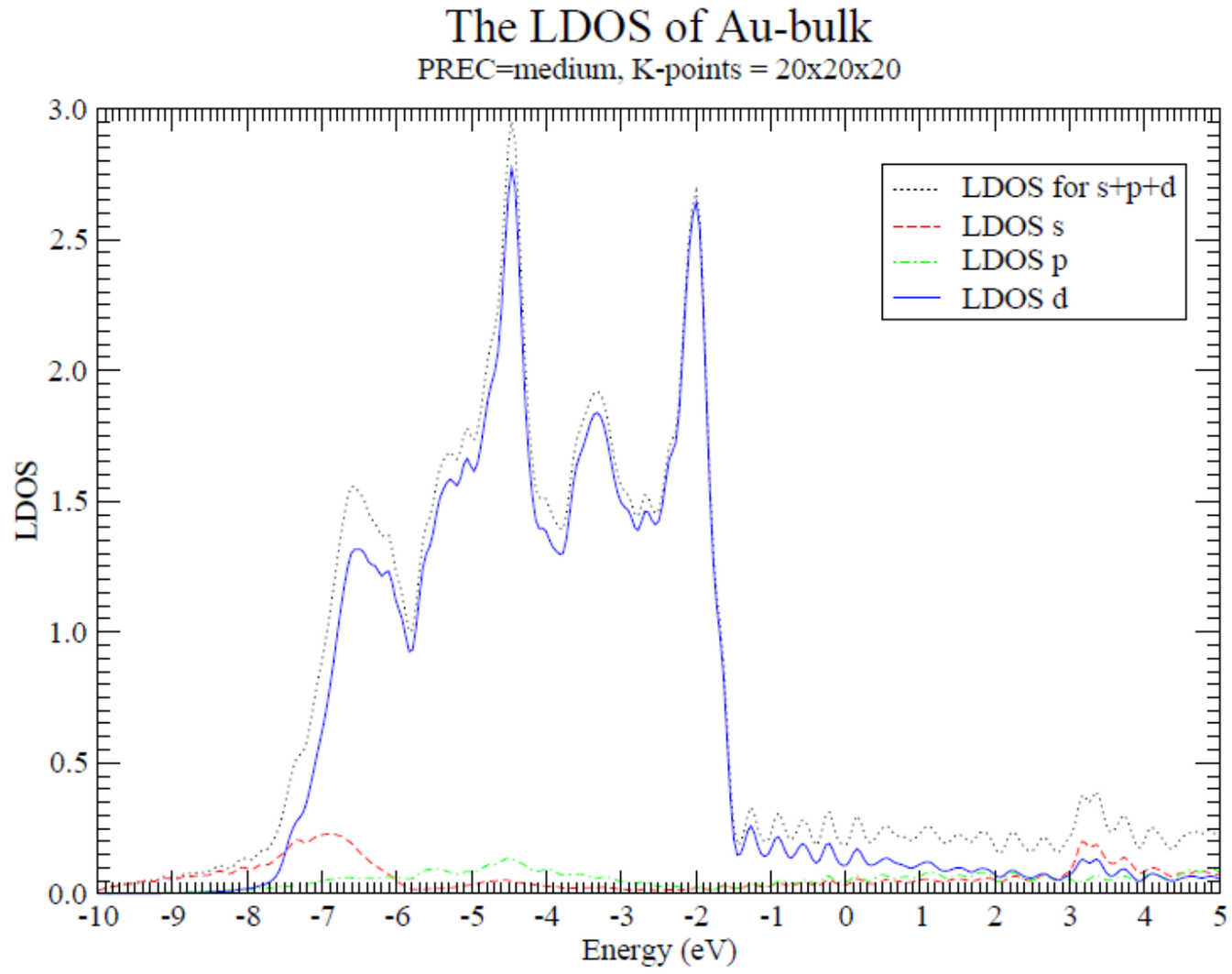
direct lattice vectors			reciprocal lattice vectors		
0.000000000	2.028440663	2.028440663	-0.246494763	0.246494763	0.246494763
2.028440663	0.000000000	2.028440663	0.246494763	-0.246494763	0.246494763
2.028440663	2.028440663	0.000000000	0.246494763	0.246494763	-0.246494763

T1-94

2. Find the lattice constant by Energy-volume relation :

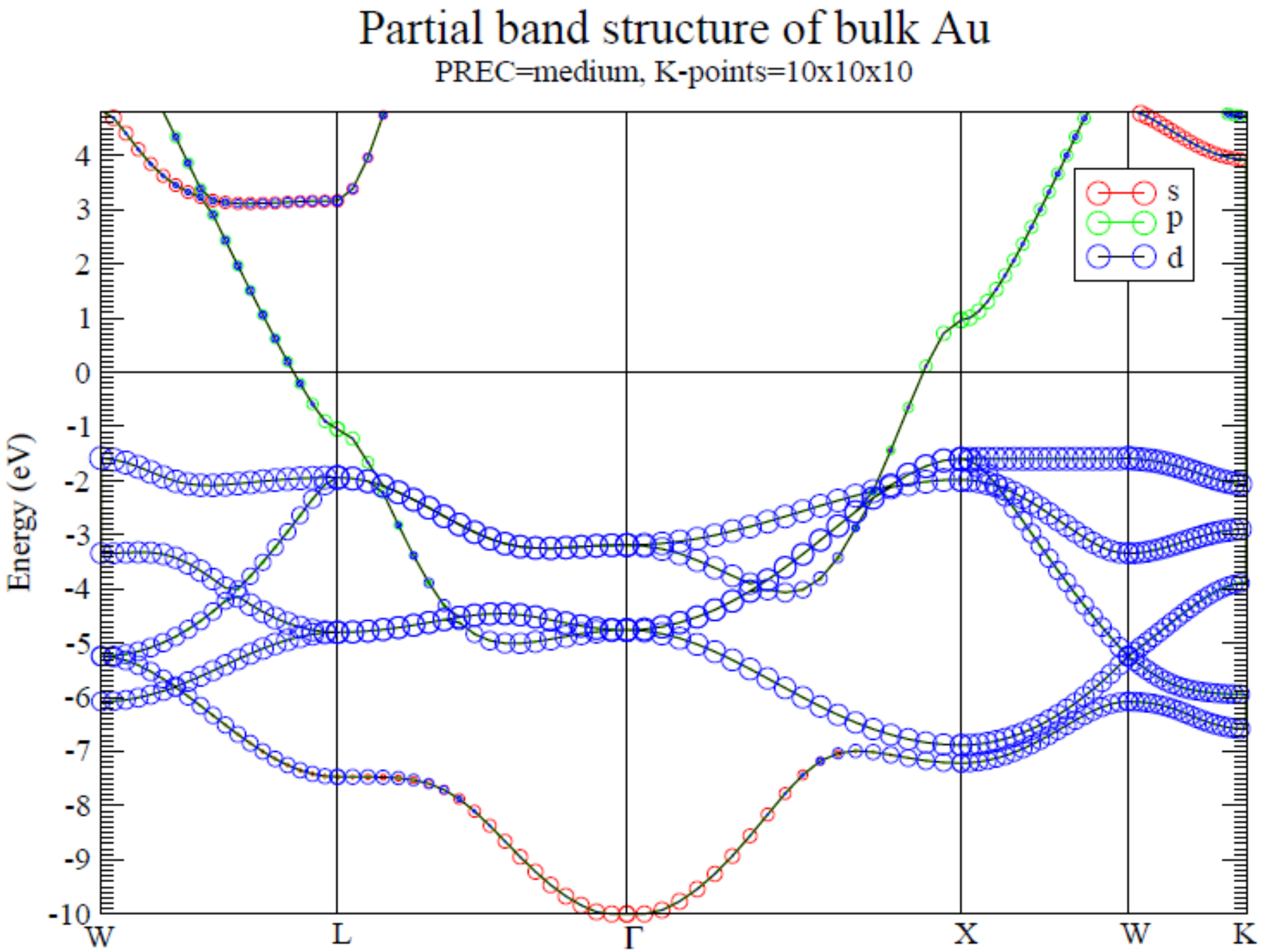


3. Density of states



T1-96

4. Partial band structure



T1-97

(B) Fe-bulk

1. Use the method of minimization of the stress

Lattice constant = 2.835A (PREC = high in INCAR) according to the OUTCAR.

external pressure = -3.95 kB Pullay stress = 0.00 kB

VOLUME and BASIS-vectors are now :

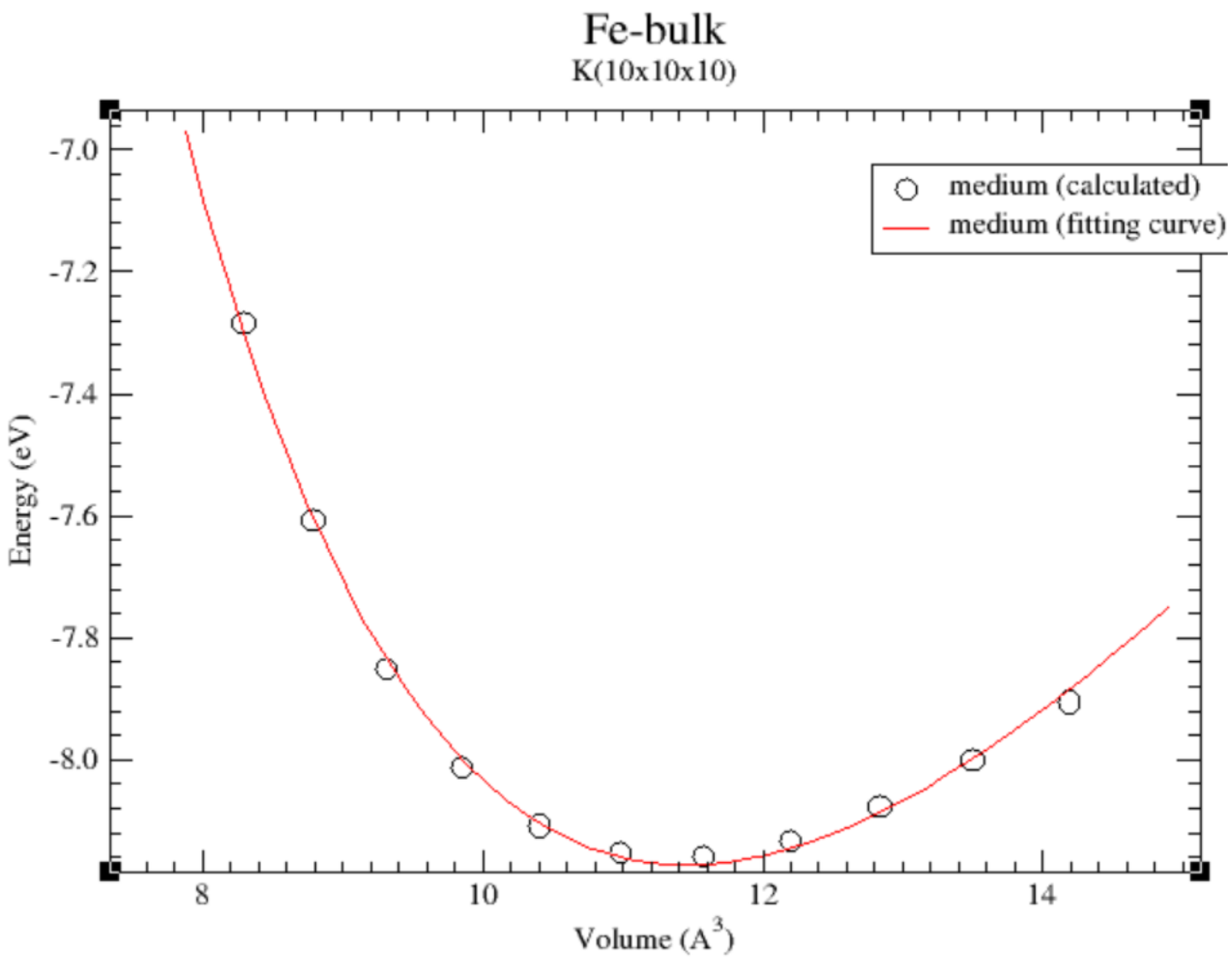
---

energy-cutoff : 334.88

volume of cell : 11.39

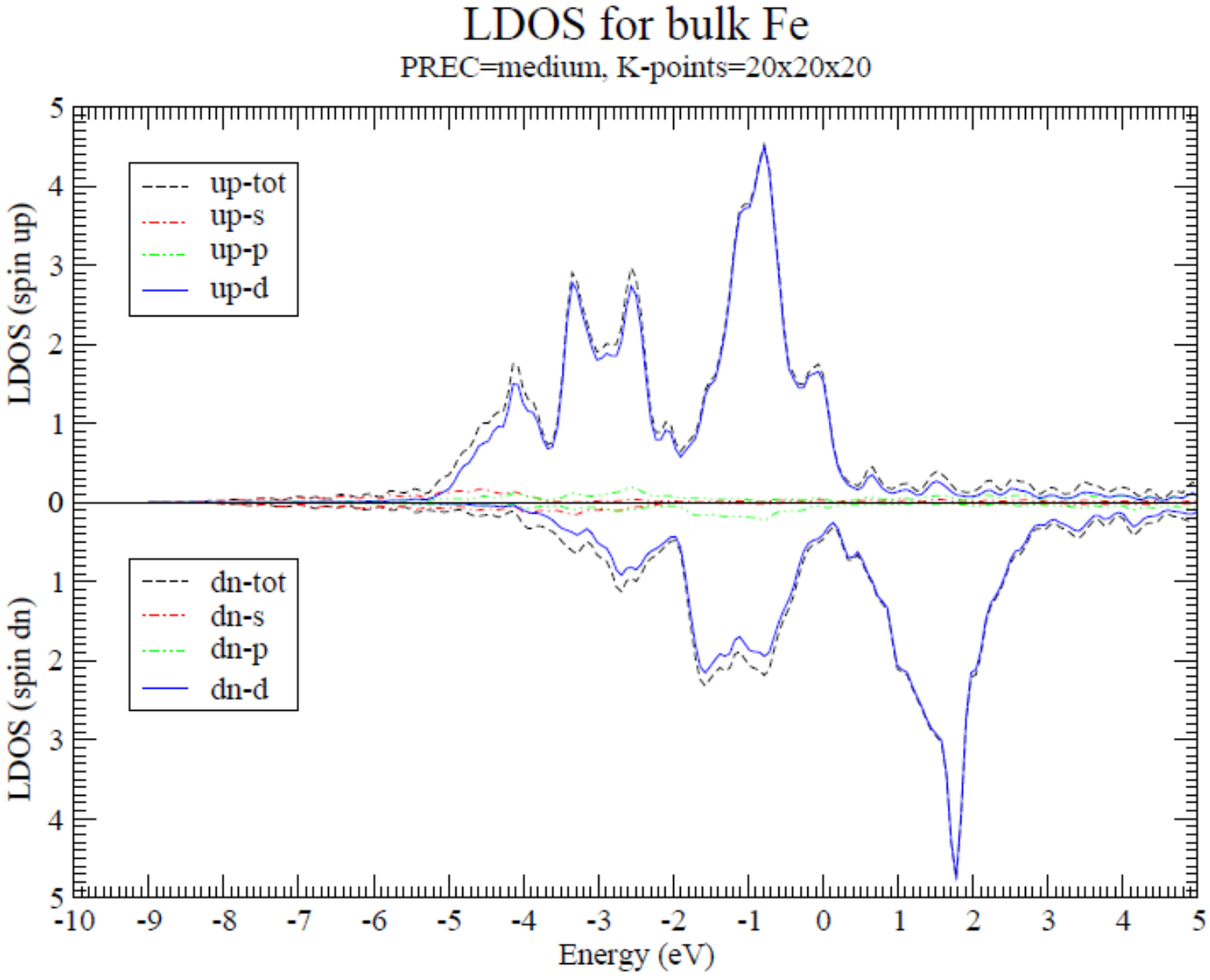
direct lattice vectors			reciprocal lattice vectors		
-1.417328818	1.417328818	1.417328818	0.000000000	0.352776289	0.352776289
1.417328818	-1.417328818	1.417328818	0.352776289	0.000000000	0.352776289
1.417328818	1.417328818	-1.417328818	0.352776289	0.352776289	0.000000000

2. Find the lattice constant by Energy-volume relation :



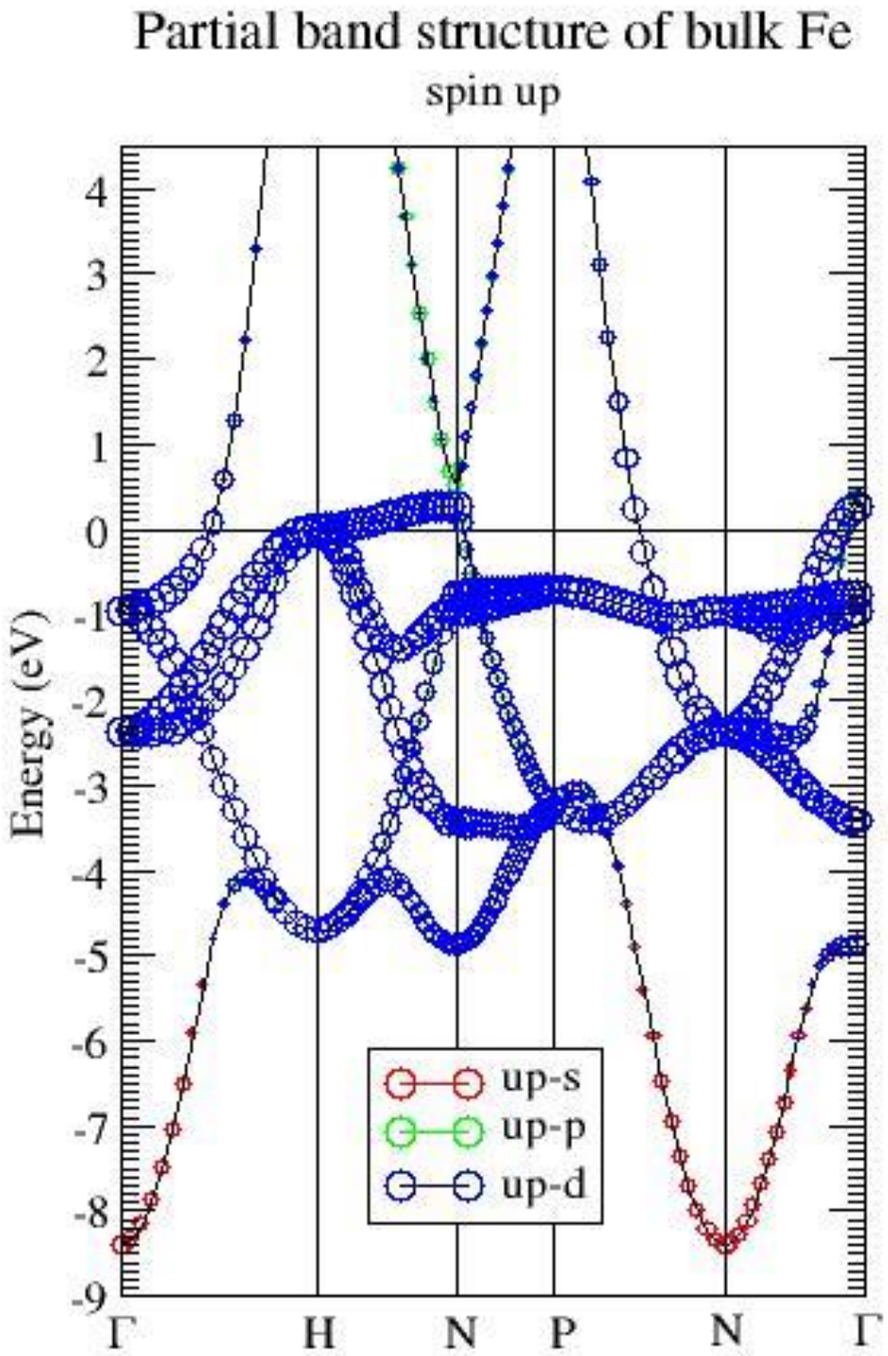
T1-99

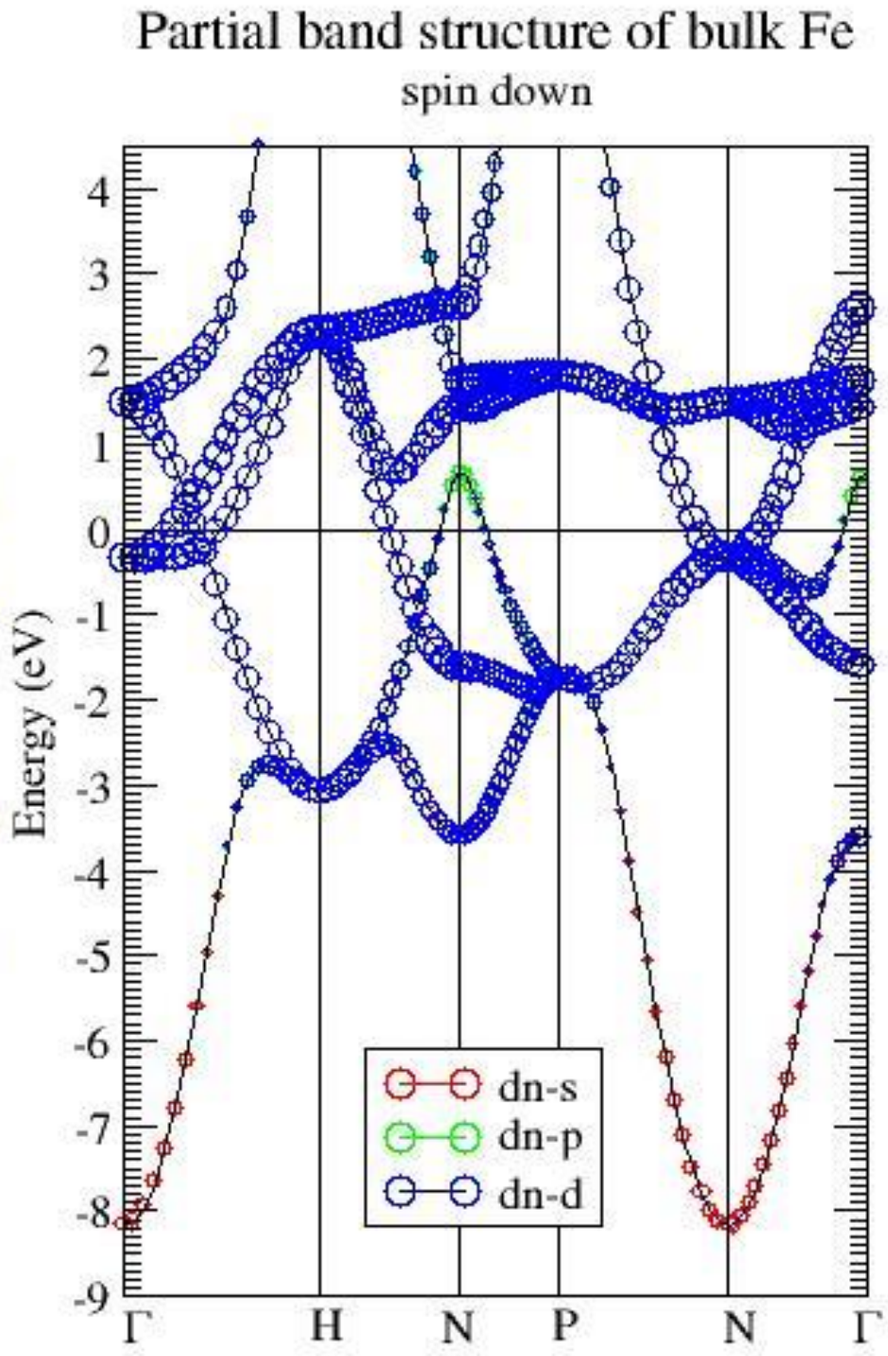
3. Density of states



T1-100

4. Partial band structure





(C) Surface Calculation for Au(100)

relax.out

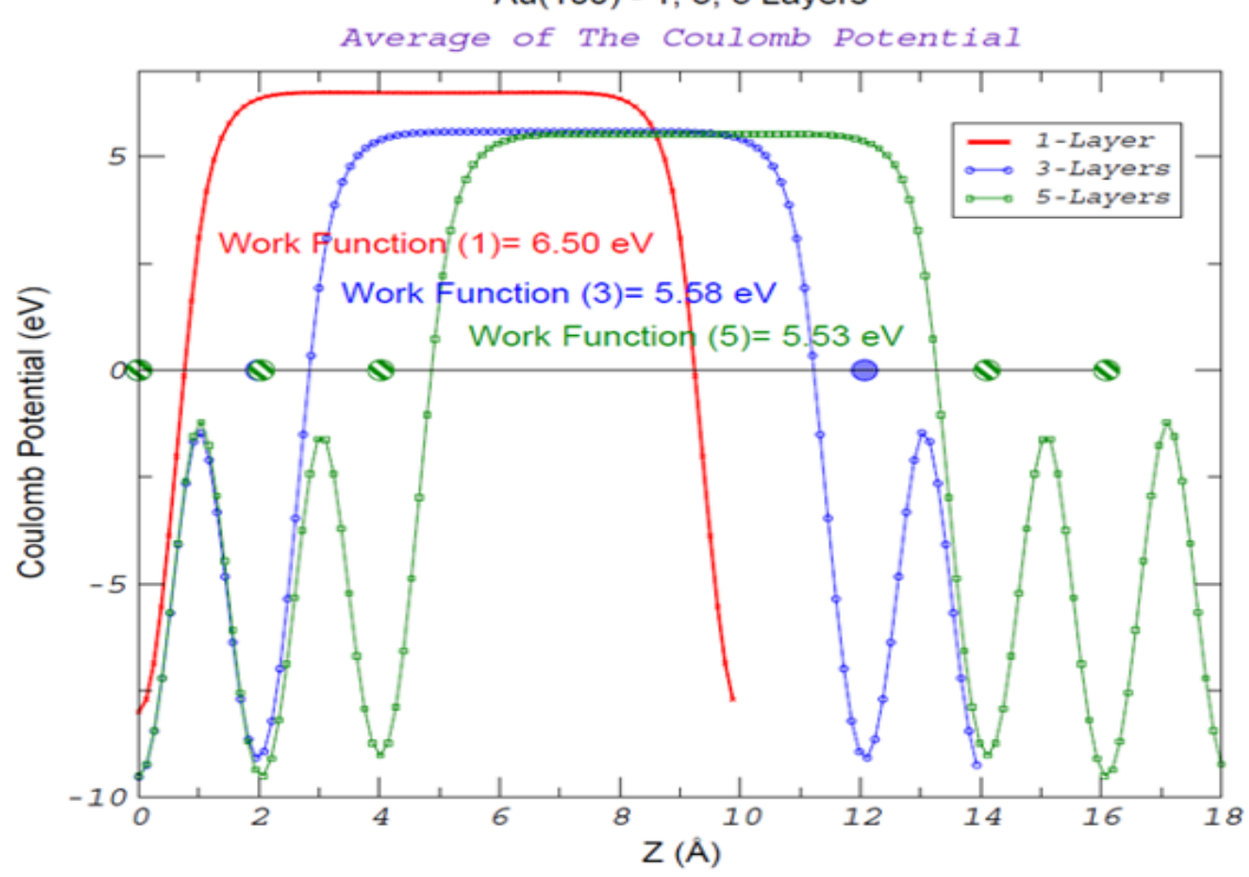
del	del(angstrom)	del(%)
0.10963	1.98752	-2.20234
0.11243	2.03822	0.29249
0.11243	2.03822	0.29251
0.10963	1.98752	-2.20237

Relaxation S ≒ −2.20 %
Relaxation S–1 ≒ 0.29 %

$$Surface\ Energy = \frac{1}{2}(E_{Slab} - NE_{Bulk}) = \frac{1}{2}[-21.955766 - 3\times(-8.1584718)] \approx 1.2636\ eV$$

Au(100) - 1, 3, 5 Layers

Average of The Coulomb Potential



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(D) Surface Calculation for Fe(100)

relax.out

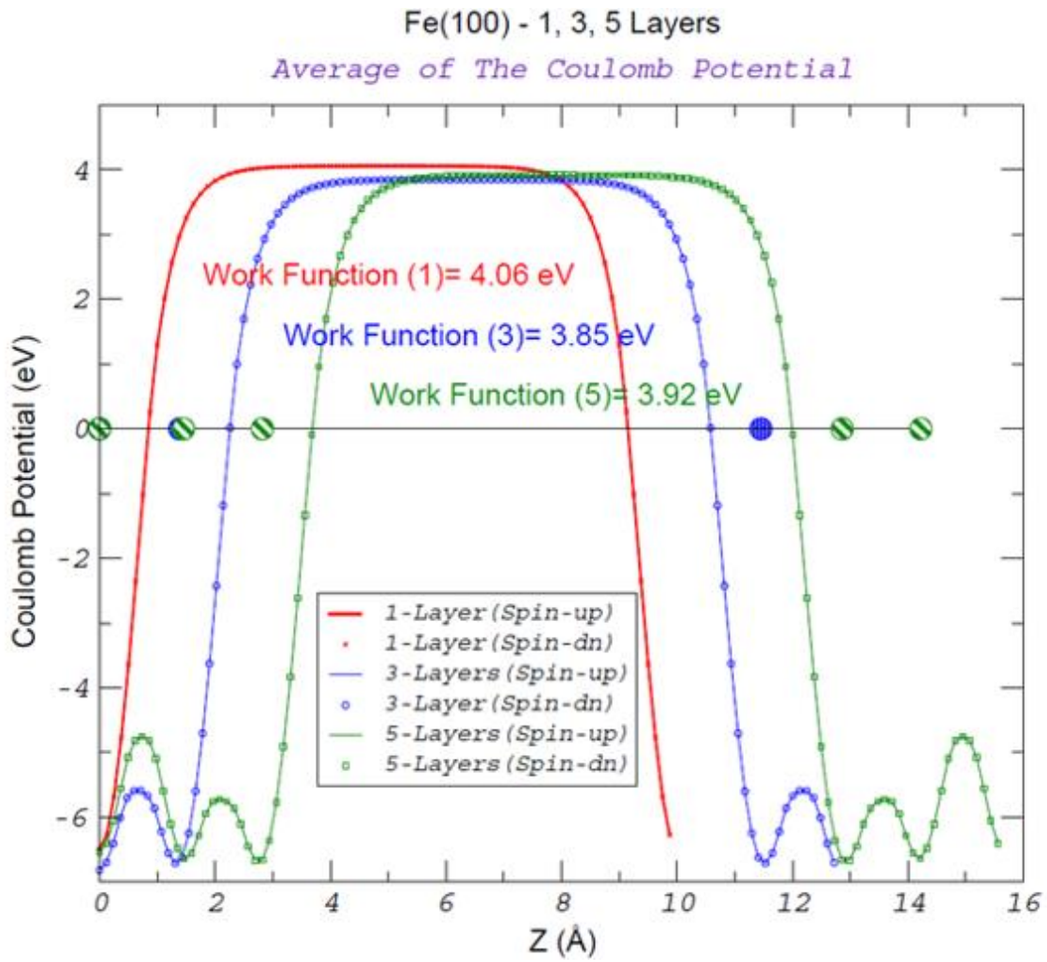
del	del(angstrom)	del(%)
0.08689	1.36248	-4.04993
0.09278	1.45475	2.44792
0.09278	1.45475	2.44792
0.08689	1.36248	-4.04989

Relaxation S ≒ –4.05 %
Relaxation S–1 ≒ 2.45 %

$$Surface\ Energy = \frac{1}{2}(E_{Slab} - NE_{Bulk}) = \frac{1}{2}[-21.955766 - 3\times(-8.1584718)] \approx 1.2636\ eV$$

magnetization (x)

# of ion	s	p	d	tot
1	0.011	0.003	2.897	2.910
2	-0.012	-0.036	2.350	2.302
3	-0.001	-0.037	2.574	2.536
4	-0.012	-0.036	2.350	2.302
5	0.011	0.003	2.897	2.910
tot	0.00	-0.10	13.07	12.96



(E) CO_2 Calculation

OSZICAR

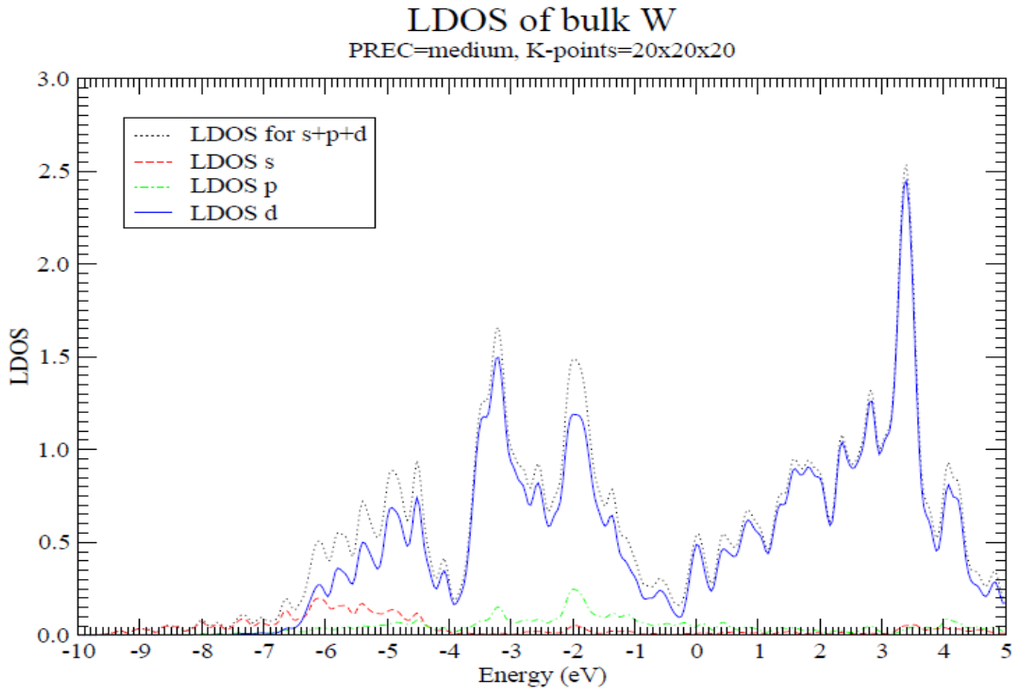
```
1 F= -.14818588E+02 E0= -.14822793E+02  d E =-.148186E+02  mag=     0.0662
2 F= -.14790401E+02 E0= -.14794603E+02  d E =0.281865E-01  mag=     0.0663
3 F= -.14818883E+02 E0= -.14823053E+02  d E =-.294836E-03  mag=     0.0659
```

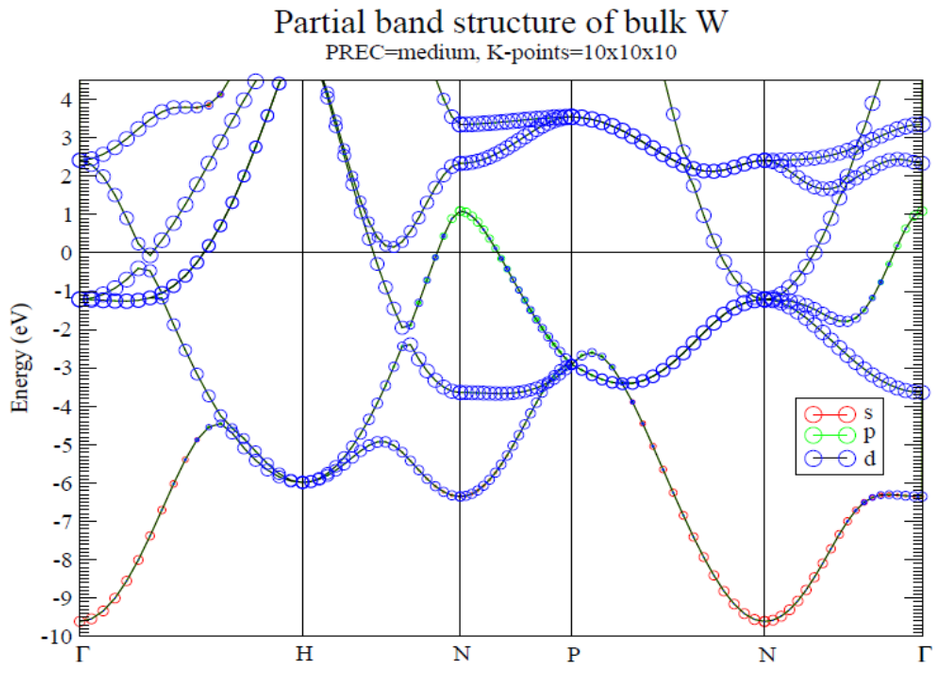
Binding Energy = *E(CO–Spin) – E(C–Spin) – E(O–Spin)* ≒ *–12. 08 eV*

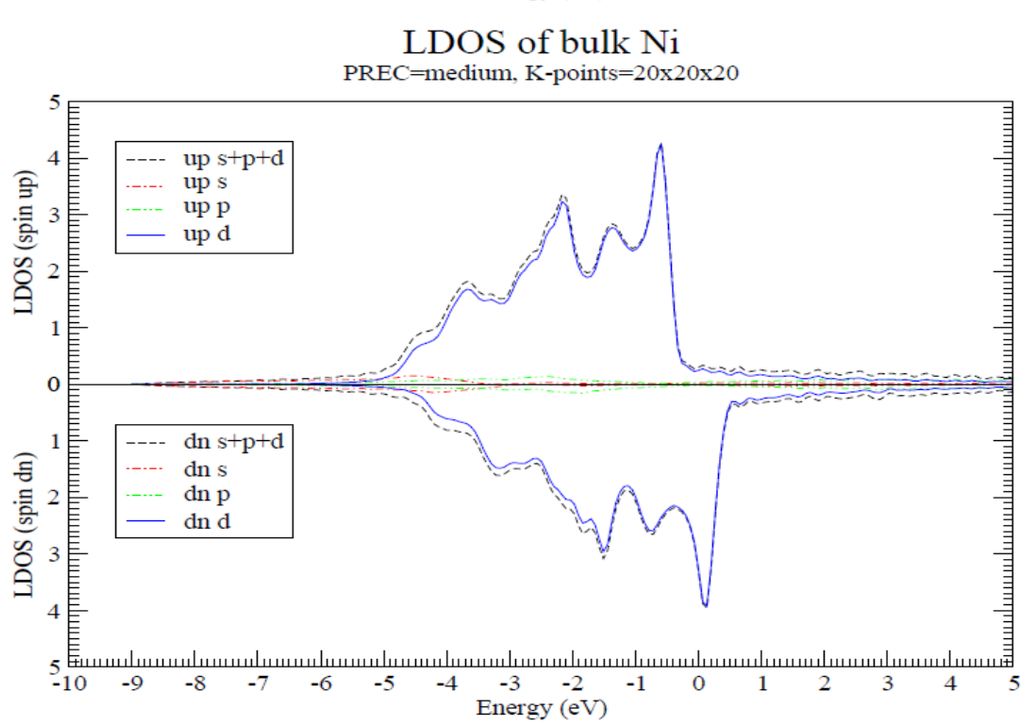
Bond Length of CO Molecule ≒ *1.142* Å

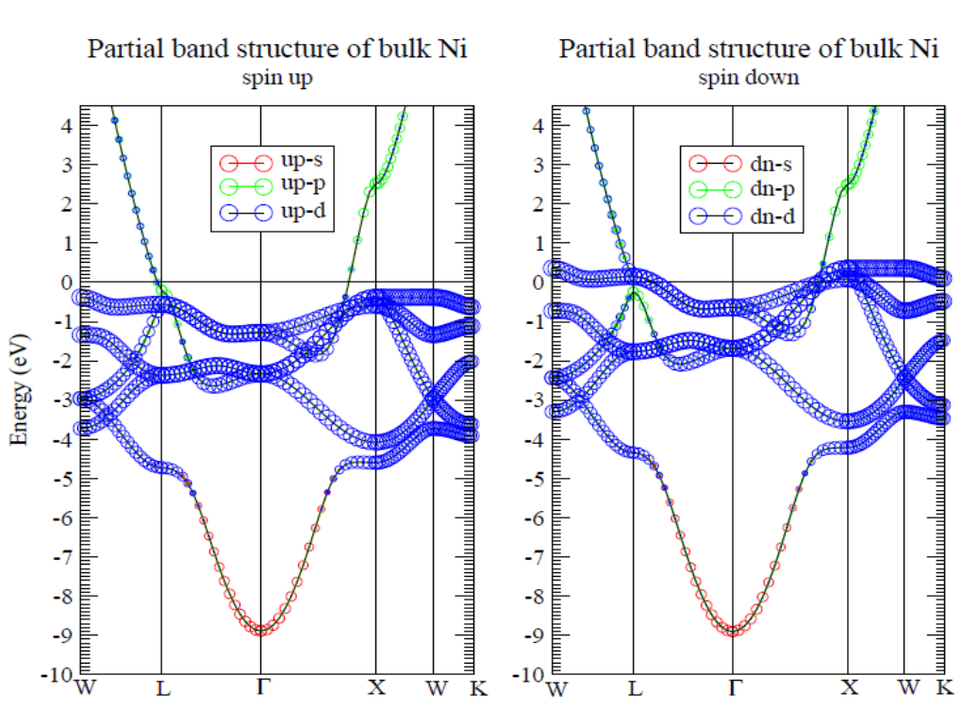
T1-104

The reference of results of homework









T1-105