Material Modeling Homework 3 Report

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November 7, 2025

1 Introduction

In this homework, we focus on discovering the usage of VASP and Aflow, and we also writing Python script to simulate the ising model an d find out what is it inner properties.

2 PART I: DFT AND VASP

2.1 Static energy vs. plane-wave cutoff(Si, diamond)

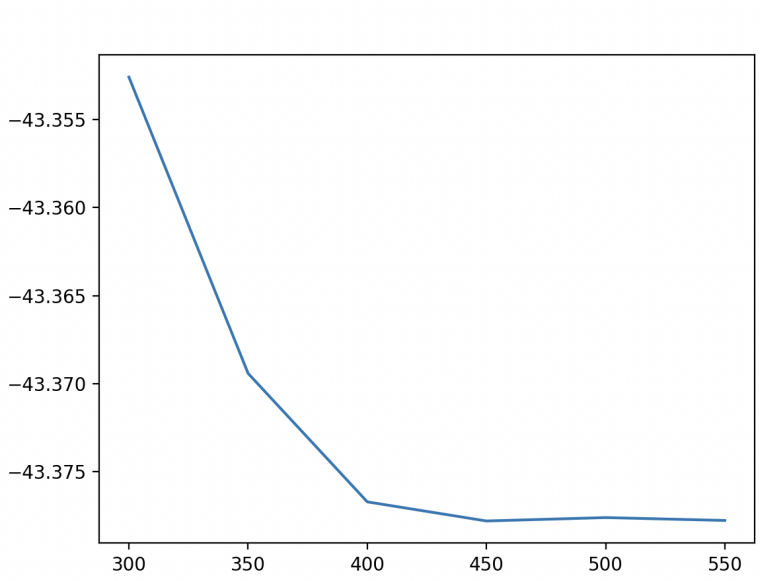

Figure 1: Static energy vs. plane-wave cutoff

The static energy change as plane-wave cutoff increase shows in the figure 1, and this shows us that 400 in cutoff is sufficient for tolerance.

2.2 Hand-building a POSCAR for Cu_3Au ($L1_2$)

In a valid POSCAR contains the title line, global scale, lattice vectors, element line, counts and the coordinate block. The title line is for comment so VASP will ignore this line. The real lattice vectors are global scale time lattice vectors. Element line contains the elements that in the structure. The counts are the numbers of atoms for each elements. The coordinate block describe the location of atoms in the lattice, in this section we have two different coordinate systems (direct and cartesian). Direct coordinates are defined relative to the cell's lattice vectors. And Cartesian coordinates are defined relative to a standard orthogonal coordinate system.

A valid POSCAR for Cu_3Au is shown below.

```
POSCAR for AuCu3
3.80
    1.0  0.0  0.0
    0.0  1.0  0.0
    0.0  0.0  1.0
Au Cu
1 3
Direct
    0.0  0.0  0.0
    0.5  0.5  0.0
    0.5  0.0  0.5
    0.0  0.5  0.5
```

POSCAR for a $2 \times 1 \times 1$ supercell of Cu_3Au is shown below.

```
AuCu3 2x1x1
3.80
    2.0  0.0  0.0
    0.0  1.0  0.0
    0.0  0.0  1.0
Au Cu
2 6
Direct
    0.00  0.00  0.00
    0.50  0.00  0.00
    0.25  0.50  0.00
    0.75  0.50  0.00
    0.25  0.00  0.50
    0.75  0.00  0.50
```

```
    0.00  0.50  0.50
    0.50  0.50  0.50
```

2.3 Do relaxations find the same final structure

The table below shows the free energies and other data in different type of POSCAR.

Type of perturbation	Free Energy (TOTEN)	Initial a	Final optimized a	Cell shape cubic
Slight expansion	-17.76349444 eV	3.7485	3.6374	Yes
Slight compression + jiggle	-16.62687075 eV	3.9015	3.5652	Yes
Light shear	-17.26420957 eV	3.8250	3.6024	Yes

2.4 Prototype identification and decoration

2.4.1 Generate $L1_2$ automatically

In aflow.in generated by aflow automatically, we structure block shown below.

```
AuCu_pv/AB3_cP4_221_a_c.AB params=-1 SG=221 [ANRL doi: 10.1016/j.commatsci.2017.01.017 (
-54.238100
   1.00000000000000   0.00000000000000   0.00000000000000
   0.00000000000000   1.00000000000000   0.00000000000000
   0.00000000000000   0.00000000000000   1.00000000000000
1 3
Direct(4) [A1B3]
   0.00000000000000   0.00000000000000   0.00000000000000  Au
   0.00000000000000   0.50000000000000   0.50000000000000  Cu_pv
   0.50000000000000   0.00000000000000   0.50000000000000  Cu_pv
   0.50000000000000   0.50000000000000   0.00000000000000  Cu_pv
```

Compare this structure block with POSCAR from Q2, we found the lattice is cubic and the coordinate format is same.

2.4.2 Identify a prototype from a CIF

By running code `cat MgSiO3.cif | aflow --prototype`, the output is shown as follow, based on this we could know the prototype is `AB3C_oC20_63_a_cf_c`

```
AFLOW label      : AB3C_oC20_63_a_cf_c
params           : a,b/a,c/a,y2,y3,y4,z4
params values    : 3.1003,3.27443,2.48086,0.077,0.747,0.631,0.936
```

Then running code `aflow --proto=<AFLOW_LABEL>.ABC:Mg:O:Si --params=<params_values>` we could get the POSCAR for this structure.

```
MgOSi/AB3C_oC20_63_a_cf_c.ABC params=3.1003,3.27443,2.48086,0.077,0.747,0.631,0.936 SG=6
1.000000
   1.55015000000000   -5.07585766450000    0.00000000000000
   1.55015000000000    5.07585766450000    0.00000000000000
   0.00000000000000    0.00000000000000    7.69141025800000
2 6 2
Direct(10) [A2B6C2]
   0.00000000000000    0.00000000000000    0.00000000000000  Mg
   0.00000000000000    0.00000000000000    0.50000000000000  Mg
   0.92300000000000    0.07700000000000    0.25000000000000  O
   0.07700000000000    0.92300000000000    0.75000000000000  O
   0.36900000000000    0.63100000000000    0.93600000000000  O
   0.63100000000000    0.36900000000000    0.43600000000000  O
   0.36900000000000    0.63100000000000    0.56400000000000  O
   0.63100000000000    0.36900000000000    0.06400000000000  O
   0.25300000000000    0.74700000000000    0.25000000000000  Si
   0.74700000000000    0.25300000000000    0.75000000000000  Si
```

2.4.3 Decorate a related hypothetical compound

We cannot replace the elements Ca or Mg with Al, Nb and Rh, and that is because they have different oxidation states.

3 PART II: STABILITY AND DISORDER: CHULL AND POCC

3.1 Constructing a Convex Hull

I choose a binary system $\mathrm{Ni-Al}$, and based on the pdf, the structures $\mathrm{Al_3Ni}$, $\mathrm{Al_3Ni_2}$, $\mathrm{Al_4Ni_3}$, AiNi, $\mathrm{Al_3Ni_5}$, $\mathrm{AlNi_3}$ lie on the hull, and other structures are above the hull. For $\mathrm{Al_8Ni}$, $\Delta H = 79\mathrm{meV/atom}$, and for $\mathrm{Al_7Ni}$, $\Delta H = 102\mathrm{meV/atom}$.

In the result for Part I, we know the composition should lie slightly above the hull. Because the structure of the DFT result is similar to the ground state.

3.2 Modeling Disorder with POCC

I choose the binary prototype is `AB_hP4_186_b_b-001`, and the command is `aflow --proto=AB_hP4_186_b_b-001:Ag:N:P --pocc_params=_params=S0-1xA_S1-0.5xB-0.5xC`. The elements Ag, N, P are ordered alphabetically, and the argument `S0-1xA_S1-0.5xB-0.5xC` map these elements to the two sublattices based on their alphabetical position.

In `prototypes.txt` I choose the prototype `AB2_aP12_1_4a_8a-001.{AB}`, and A, B are Fe and S respectively. Then run the command line code

```
aflow --proto=AB2_aP12_1_4a_8a-001:Fe:S --pocc_params=S0-1xA_S1-0.5xB-0.5xC_S2-0.5xB-0.5xC
```

4 (BONUS) PART III: THE ISING MODEL

The Magnetization vs. temperature is shown in figure 2, where the T_C is around 3.5.

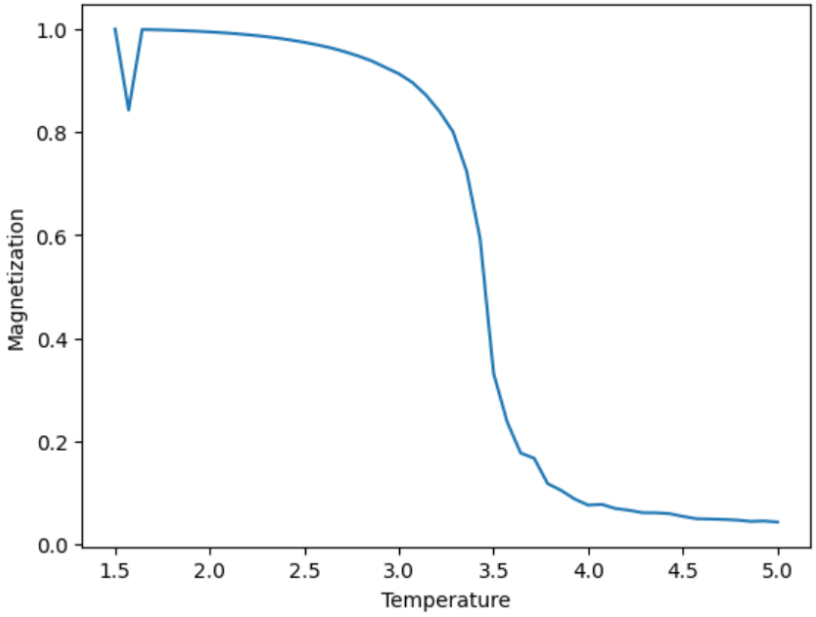

Figure 2: Magnetization vs. Temperature

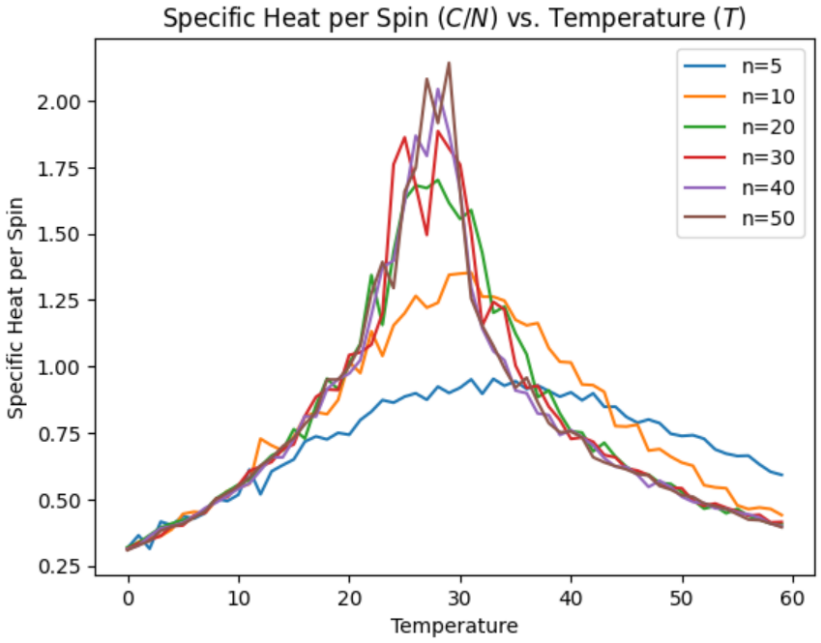

Figure 3: Specific Heat per Spin vs. Temperature

Based on the figure 4 we found that $C_{max}/N \sim \log(n)$.

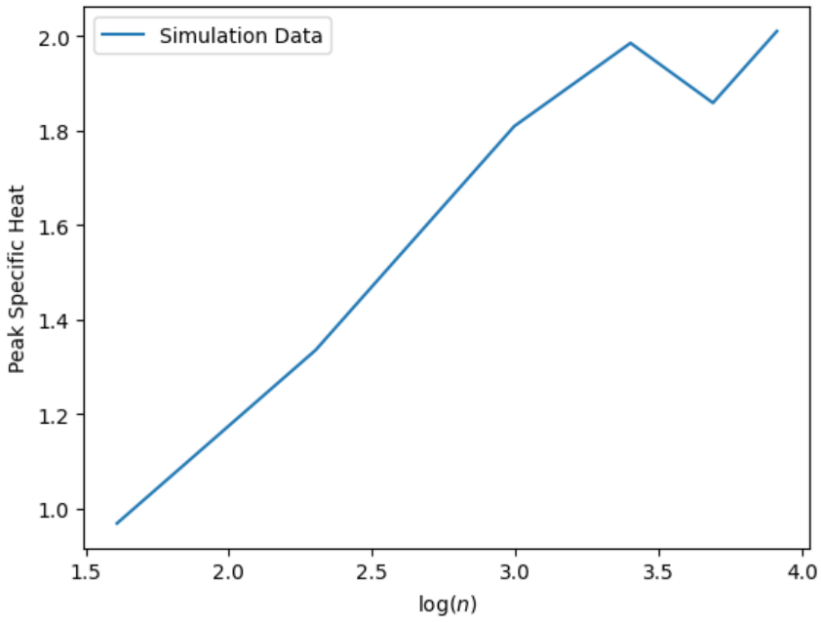

Figure 4: Specific Heat per Spin vs. Temperature

5 Contributions

In this project, I engaged in group discussion and help my group members to debug the Python code in all sections. During the project, I discussed the possibilities that may cause the difference between

our output, and also discussed how to analysis the deviation. But we finished our homework include coding and formula derivation independently.