MS 4023 : Electronic Structures and Atomistic Modeling

LAB EXERCISE - III

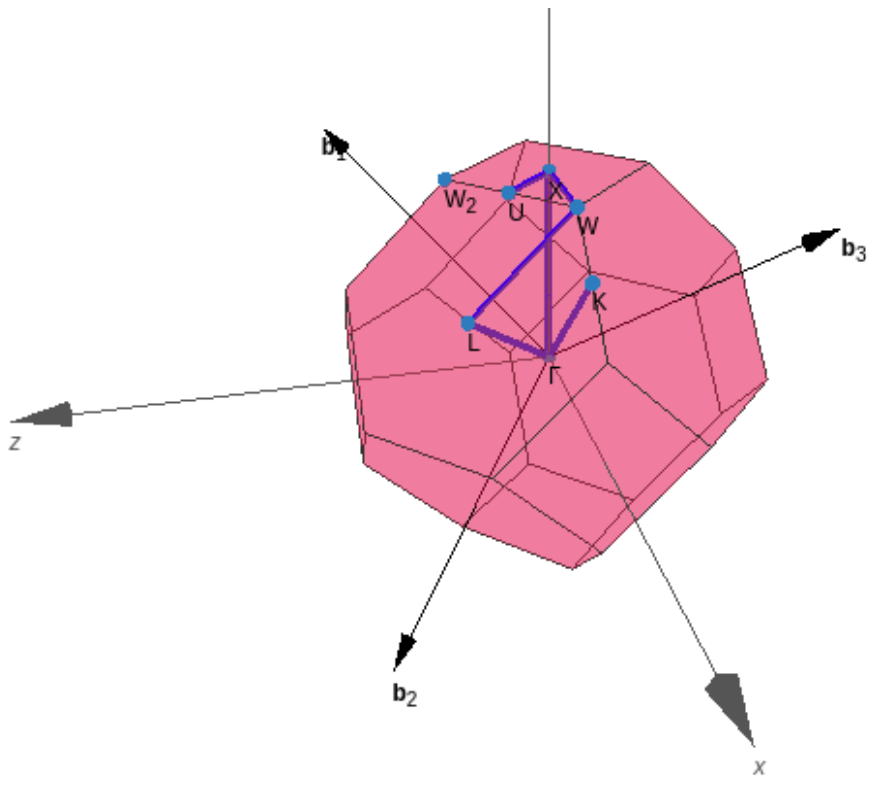
CO23BTECH11021

pwd: /home/co23btech11021/testDIrectory/Jan2025/hw3/

Si

1. Brillouin Zone and K points

The Brillouin Zone figure and the high symmetry K points are :



The high symmetry K points and the reciprocal coordinates in scaled units are :

Suggested path

Γ—X—U|K—Γ—L—W—X

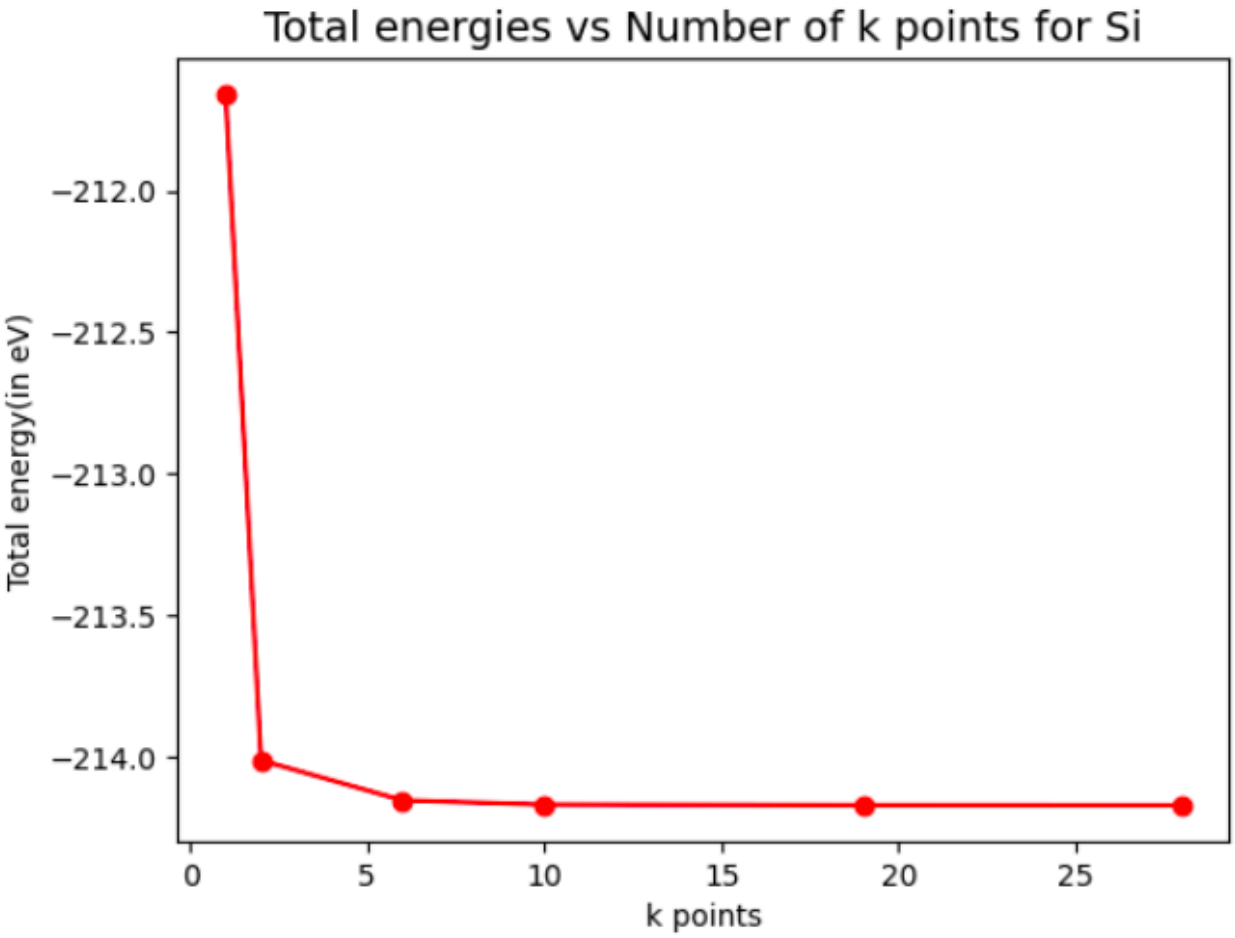
High-symmetry points (scaled units)

Label	k_1	k_2	k_3
Γ	0.0000000000	0.0000000000	0.0000000000
K	0.3750000000	0.3750000000	0.7500000000
L	0.5000000000	0.5000000000	0.5000000000
U	0.6250000000	0.2500000000	0.6250000000
W	0.5000000000	0.2500000000	0.7500000000
W_2	0.7500000000	0.2500000000	0.5000000000
X	0.5000000000	0.0000000000	0.5000000000

2. Table

Grid Size	**Cutoff Energy** (in eV)	**Total Energy** (in eV)	**No. of K points**	**No. of G vectors**	**SCF iterations**
1x1x1	340.1426	-211.6588	1	4573	6
2x2x2	340.1426	-214.0114	2	4573	5
3x3x3	340.1426	-214.1528	6	4573	5
4x4x4	340.1426	-214.1677	10	4573	5
5x5x5	340.1426	-214.1698	19	4573	5
6x6x6	340.1426	-214.1702	28	4573	5

3. Graph



As evident from the graph, the total energy is **converging** with an increase in the number of k points.

4. Total Energy vs K points

The convergence of total energy with respect to the number of k points is **monotonic**.

5. Runtime vs K points

No. of K Points	**Runtime (WALL)** (in s)
1	0.39
2	0.41
6	0.5
10	0.59
19	0.8
28	1

The time required to run the SCF calculations (**WALL runtime**) **increased** with an increase in the number of K points.

6. Symmetry

Yes, symmetry was used to reduce the number of K points. In the cases when the K point grid was 2x2x2 to 6x6x6, the number of K points observed in the output were less than the total number of grid points provided in the input. This is due to the symmetry present.

In all the cases, a total of **48 symmetry operations** were performed.

Al

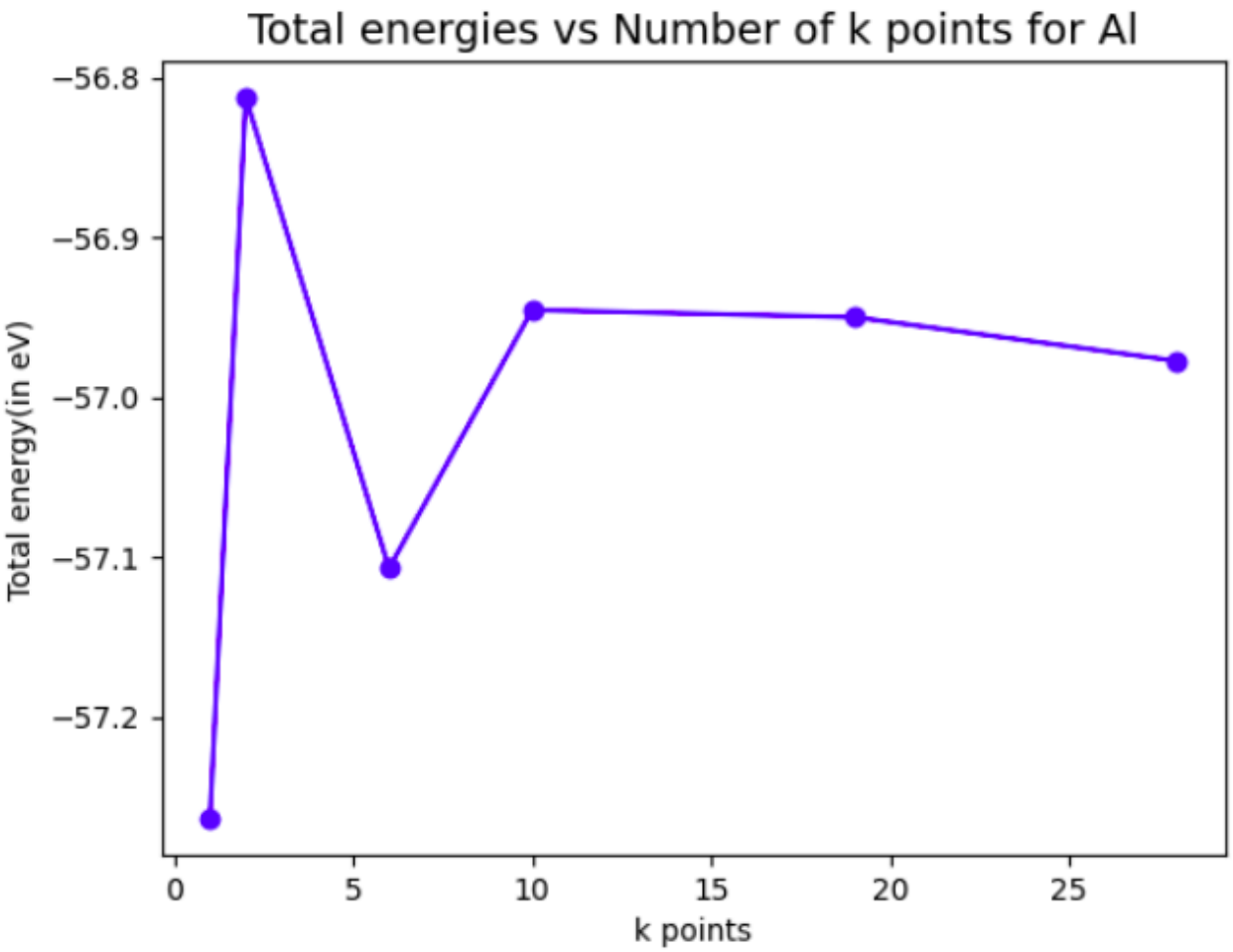
1. Brillouin Zone and K points

The figure obtained for the Brillouin Zone and the coordinates of high symmetry K points are the same as the case of Si.

2. Table

Grid Size	**Cutoff Energy** (in eV)	**Total Energy** (in eV)	**No. of K points**	**No. of G vectors**	**SCF iterations**
1x1x1	340.1426	-57.2636	1	1917	4
2x2x2	340.1426	-56.8126	2	1917	3
3x3x3	340.1426	-57.1072	6	1917	3
4x4x4	340.1426	-56.9456	10	1917	3
5x5x5	340.1426	-56.9501	19	1917	3
6x6x6	340.1426	-56.9775	28	1917	3

3. Graph



The total energy is **converging** with an increase in the number of K points.

4. Total Energy vs Convergence

The total energy **doesn't converge monotonically**.

5. Runtime vs K points

No. of K Points	**Runtime (WALL)** (in s)
1	0.22
2	0.24
6	0.31
10	0.34
19	0.43
28	0.52

The time required to run the SCF calculations (**WALL runtime**) **increased** with an increase in the number of K points.

6. Symmetry

Yes, symmetry was used to reduce the number of K points. In the cases when the K point grid was 2x2x2 to 6x6x6, the number of K points observed in the output were less than the total number of grid points provided in the input. This is due to the symmetry present.

In all the cases, a total of **48 symmetry operations** were performed.

NaCl

1. Brillouin Zone and K points

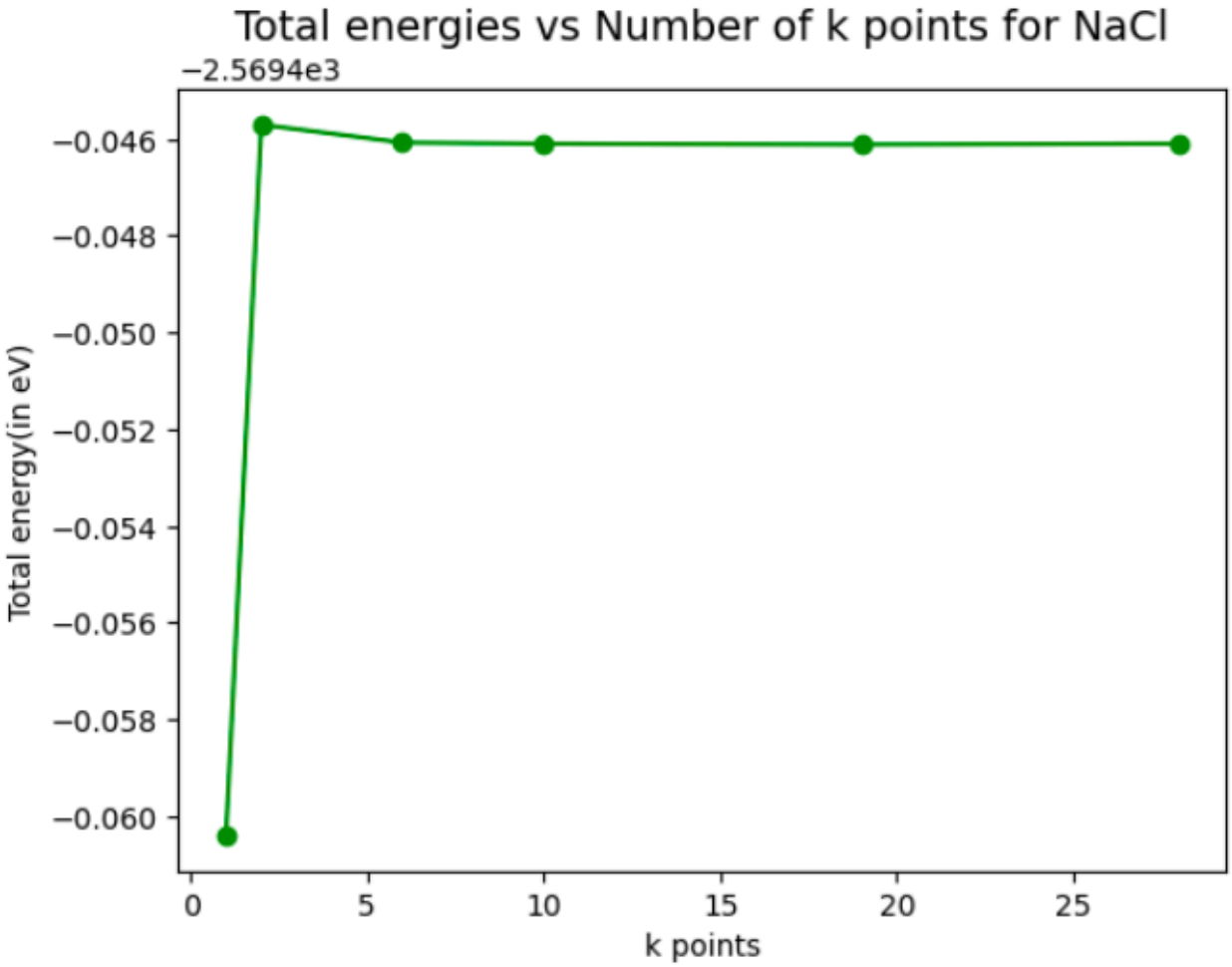
The Brillouin Zone obtained is the same as the Si case. The high symmetry K points are also the same.

The Brillouin Zone shape and the K points are same for all the three cases possibly because all the **primitive cells of NaCl, Al and Si belong to the same type of Bravais lattice** (i.e) the Face Centred Cubic type.

2. Table

Grid Size	**Cutoff Energy** (in eV)	**Total Energy** (in eV)	**No. of K points**	**No. of G vectors**	**SCF iterations**
1x1x1	476.1996	-2569.4604	1	8363	7
2x2x2	476.1996	-2569.4457	2	8363	7
3x3x3	476.1996	-2569.44607	6	8363	5
4x4x4	476.1996	-2569.4460942	10	8363	7
5x5x5	476.1996	-2569.44611	19	8363	7
6x6x6	476.1996	-2569.4460927	28	8363	7

3. Graph



The total energy is **converging** with an increase in the number of K points.

4. Total Energy vs Convergence

The total energy **doesn't converge monotonically**.

5. Runtime vs K points

No. of K Points	**Runtime (WALL)** (in s)
1	1.50
2	1.67
6	1.84
10	3.23
19	5.07
28	5.38

The time required to run the SCF calculations (**WALL runtime**) **increased** with an increase in the number of K points.

6. Symmetry

Yes, symmetry was used to reduce the number of K points. In the cases when the K point grid was 2x2x2 to 6x6x6, the number of K points observed in the output were less than the total number of grid points provided in the input. This is due to the symmetry present.

In all the cases, a total of **48 symmetry operations** were performed.