MS4023 : Electronic Structures and Atomistic Modeling

LAB EXERCISE - IV

CO23BTECH11021

Question 1 :

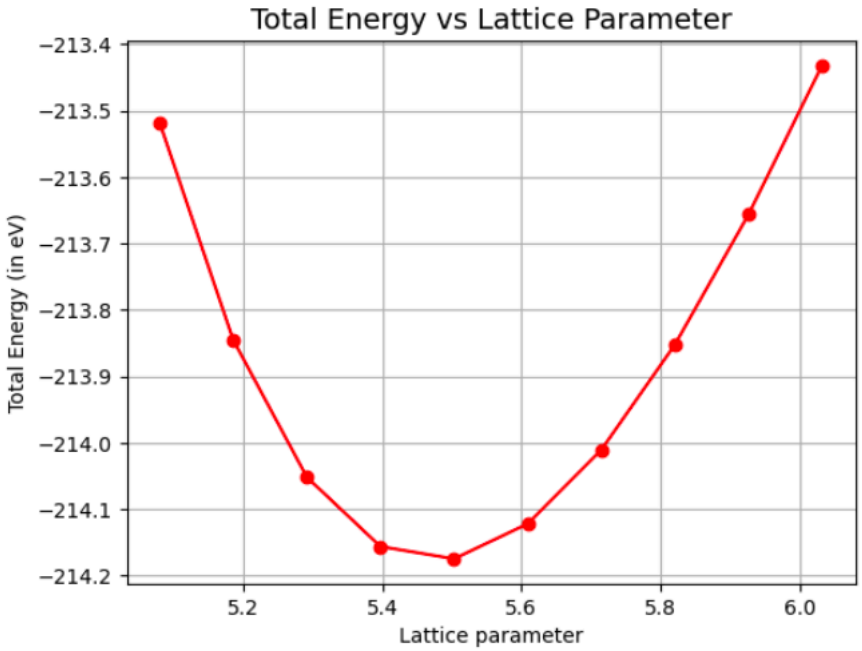
Si

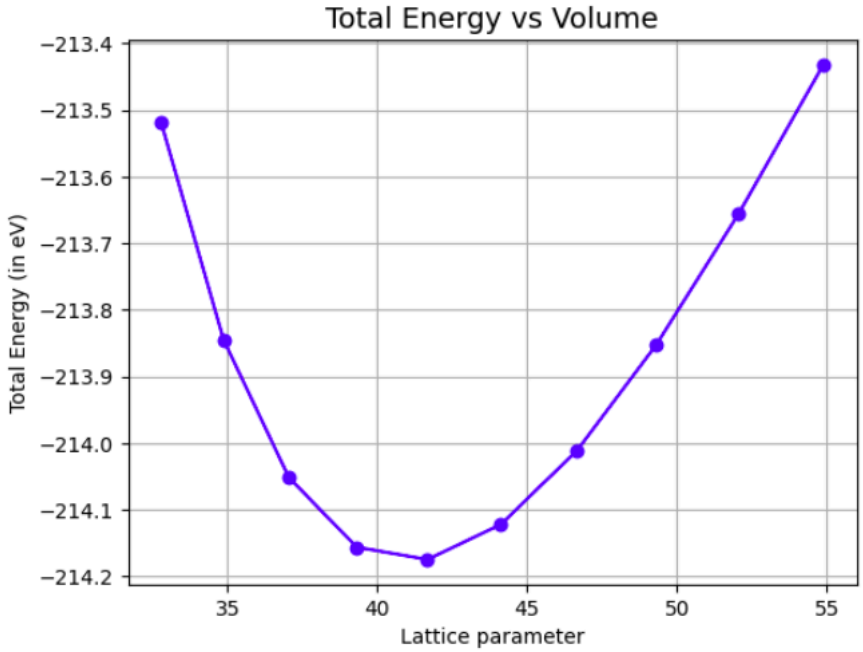
For **GGA approximation** the results obtained were as follows :

1. **Table**

Pseudopotential	**Celldm(1)** (in Bohr radii)	**Lattice Parameter** (in Å)	**Volume** (in $Å^3$)	**Total Energy** (in eV)
Si.pbe-rrkj.UPF	9.6	5.0801	32.7760	-213.5184
Si.pbe-rrkj.UPF	9.8	5.1859	34.8675	-213.8453
Si.pbe-rrkj.UPF	10	5.29177	37.0461	-214.0517
Si.pbe-rrkj.UPF	10.2	5.3976	39.3137	-214.156
Si.pbe-rrkj.UPF	**10.4**	**5.5034**	**41.6719**	**-214.1745**
Si.pbe-rrkj.UPF	10.6	5.6093	44.1225	-214.1218
Si.pbe-rrkj.UPF	10.8	5.7151	46.6675	-214.0107
Si.pbe-rrkj.UPF	11	5.82095	49.3084	-213.8524
Si.pbe-rrkj.UPF	11.2	5.9268	52.0472	-213.6567
Si.pbe-rrkj.UPF	11.4	6.0326	54.8855	-213.4324

2. Plots


Total Energy vs Lattice Parameter
Total Energy (in eV)
−213.4
−213.5
−213.6
−213.7
−213.8
−213.9
−214.0
−214.1
−214.2
5.2
5.4
5.6
5.8
6.0
Lattice parameter


Total Energy vs Volume
Total Energy (in eV)
−213.4
−213.5
−213.6
−213.7
−213.8
−213.9
−214.0
−214.1
−214.2
35
40
45
50
55
Lattice parameter

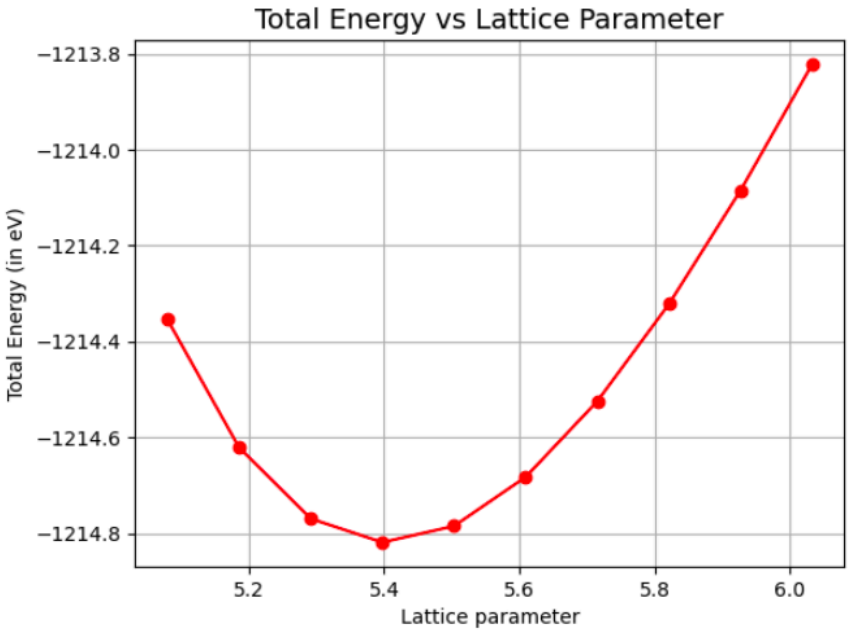
For **LDA approximation** the results obtained were as follows :

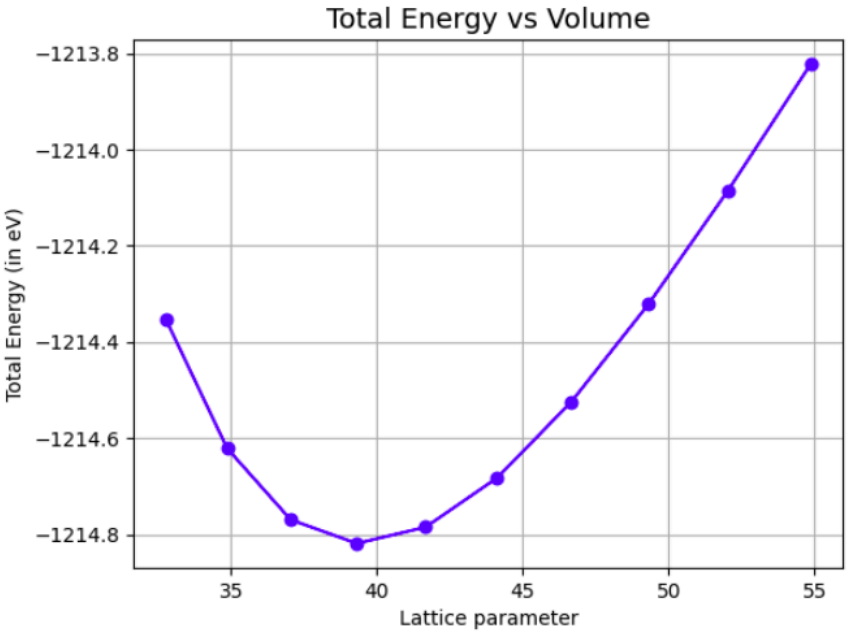
1. Table

The convergence in this case was observed for **ecutwfc = 20 Ry** and **k point grid size - 4x4x4**.

Pseudopotential	**Celldm(1)** (in Bohr radii)	**Lattice Parameter** (in Å)	**Volume** (in $Å^3$)	**Total Energy** (in eV)
Si.pz-n-kjpaw_psl.0.1.UPF	9.6	5.0801	32.7760	-1214.3543
Si.pz-n-kjpaw_psl.0.1.UPF	9.8	5.1859	34.8675	-1214.6212
Si.pz-n-kjpaw_psl.0.1.UPF	10	5.29177	37.0461	-1214.7695
Si.pz-n-kjpaw_psl.0.1.UPF	**10.2**	**5.3976**	**39.3137**	**-1214.8188**
Si.pz-n-kjpaw_psl.0.1.UPF	10.4	5.5034	41.6719	-1214.7849
Si.pz-n-kjpaw_psl.0.1.UPF	10.6	5.6093	44.1225	-1214.6825
Si.pz-n-kjpaw_psl.0.1.UPF	10.8	5.7151	46.6675	-1214.5246
Si.pz-n-kjpaw_psl.0.1.UPF	11	5.82095	49.3084	-1214.322
Si.pz-n-kjpaw_psl.0.1.UPF	11.2	5.9268	52.0472	-1214.0849
Si.pz-n-kjpaw_psl.0.1.UPF	11.4	6.0326	54.8855	-1213.8219

2. Plots


Total Energy vs Lattice Parameter
−1213.8
−1214.0
−1214.2
−1214.4
−1214.6
−1214.8
Total Energy (in eV)
5.2
5.4
5.6
5.8
6.0
Lattice parameter


Total Energy vs Volume
−1213.8
−1214.0
−1214.2
−1214.4
−1214.6
−1214.8
Total Energy (in eV)
35
40
45
50
55
Lattice parameter

Answers

1. Using GGA approximation, the value of equilibrium lattice constant is 10.4 bohr radii. The volume of unit cell is 41.6719 Å^3.

   Using LDA approximation, the value of equilibrium lattice constant is 10.2 bohr radii. The volume of unit cell is 39.3137 Å^3.

2. Yes, the answer depends on the nature of approximation used or the type of pseudopotential used.

3. Yes. The total energy is roughly symmetric about the minima/ equilibrium lattice constant.

Al

For **GGA approximation**, the values obtained were :

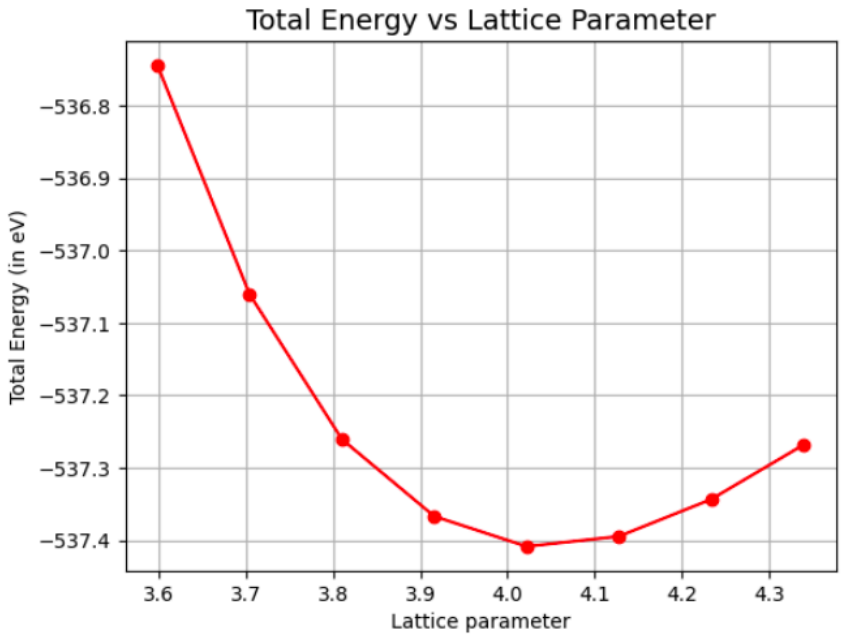
1. Table

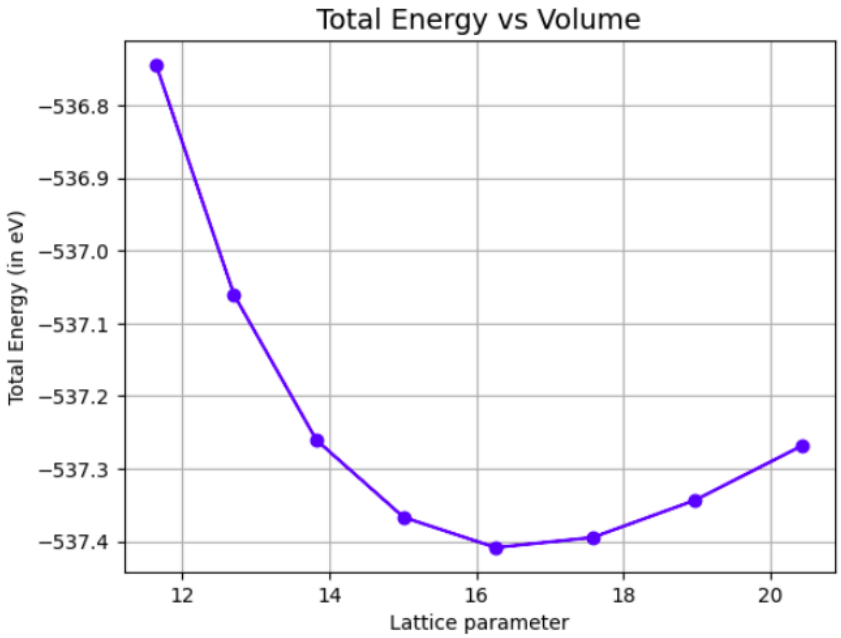
The convergence in this case was observed for **ecutwfc = 15 Ry**,

k point grid size - 5x5x5, and **degauss = 0.10**.

Pseudopotential	**Celldm(1)** (in Bohr radii)	**Lattice Parameter** (in Å)	**Volume** (in $Å^3$)	**Total Energy** (in eV)
Al.pbe-n-kjpaw_psl.1.0.0.UPF	6.8	3.5984	11.6485	-536.7443
Al.pbe-n-kjpaw_psl.1.0.0.UPF	7.0	3.7042	12.7068	-537.0607
Al.pbe-n-kjpaw_psl.1.0.0.UPF	7.2	3.8101	13.8274	-537.2608
Al.pbe-n-kjpaw_psl.1.0.0.UPF	7.4	3.9159	15.012	-537.367
Al.pbe-n-kjpaw_psl.1.0.0.UPF	**7.6**	**4.0218**	**16.2624**	**-537.4087**
Al.pbe-n-kjpaw_psl.1.0.0.UPF	7.8	4.1276	17.5803	-537.3948
Al.pbe-n-kjpaw_psl.1.0.0.UPF	8.0	4.2334	18.9676	-537.3437
Al.pbe-n-kjpaw_psl.1.0.0.UPF	8.2	4.3393	20.4261	-537.2685

2. Plots


Total Energy vs Lattice Parameter
Total Energy (in eV)
−536.8
−536.9
−537.0
−537.1
−537.2
−537.3
−537.4
3.6
3.7
3.8
3.9
4.0
4.1
4.2
4.3
Lattice parameter


Total Energy vs Volume
Total Energy (in eV)
−536.8
−536.9
−537.0
−537.1
−537.2
−537.3
−537.4
12
14
16
18
20
Lattice parameter

For **LDA approximation**, the values obtained are as follows :

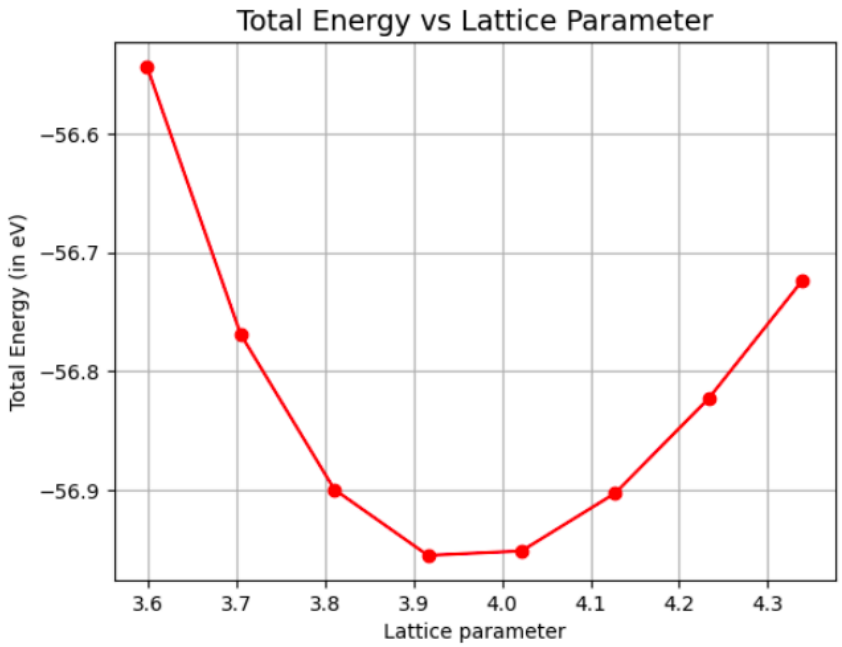
1. Table

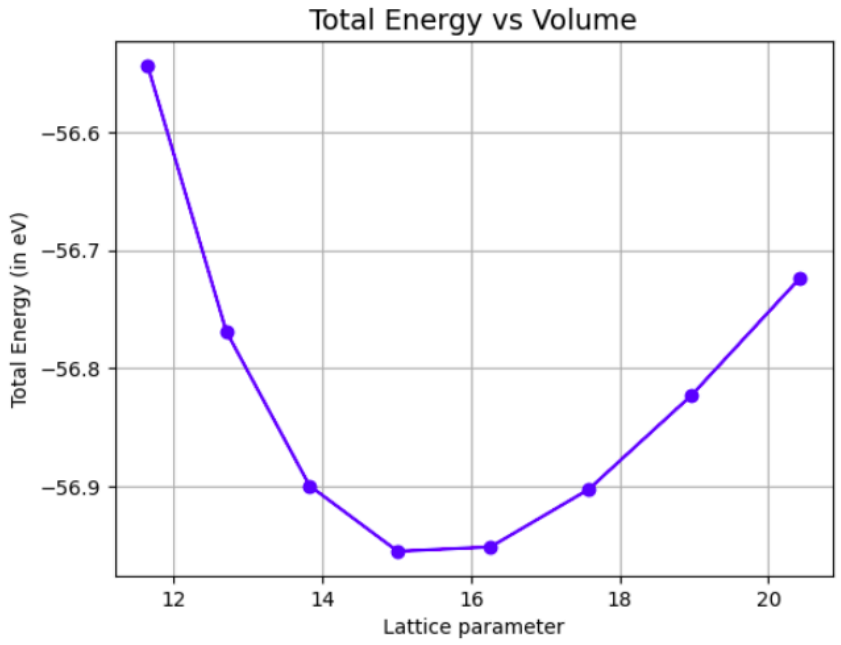
The convergence in this case was observed for **ecutwfc = 20 Ry**,

k point grid size - 5x5x5, and **degauss = 0.02**.

Pseudopotential	**Celldm(1)** (in Bohr radii)	**Lattice Parameter** (in Å)	**Volume** (in $Å^3$)	**Total Energy** (in eV)
Al.pz-vbc.UPF	6.8	3.5984	11.6485	-56.5436
Al.pz-vbc.UPF	7.0	3.7042	12.7068	-56.7686
Al.pz-vbc.UPF	7.2	3.8101	13.8274	-56.8992
Al.pz-vbc.UPF	**7.4**	**3.9159**	**15.012**	**-56.9547**
Al.pz-vbc.UPF	7.6	4.0218	16.2624	-56.951
Al.pz-vbc.UPF	7.8	4.1276	17.5803	-56.9024
Al.pz-vbc.UPF	8.0	4.2334	18.9676	-56.8226
Al.pz-vbc.UPF	8.2	4.3393	20.4261	-56.7234

2. Plots


Total Energy vs Lattice Parameter
Total Energy (in eV)
−56.6
−56.7
−56.8
−56.9
3.6
3.7
3.8
3.9
4.0
4.1
4.2
4.3
Lattice parameter


Total Energy vs Volume
Total Energy (in eV)
−56.6
−56.7
−56.8
−56.9
12
14
16
18
20
Lattice parameter

Answers

1. Using GGA approximation, the value of equilibrium lattice constant is 7.6 bohr radii. The volume of unit cell is 4.0218 $Å^3$.

   Using LDA approximation, the value of equilibrium lattice constant is 7.4 bohr radii. The volume of unit cell is 3.9159 $Å^3$.

2. Yes, the answer depends on the nature of approximation used or the type of pseudopotential used.

3. Yes. The total energy is roughly symmetric about the minima/ equilibrium lattice constant.

Question 2

1. For Si system, using GGA approximation

System	**Pseudo-potential**	**Ionic Relaxation Step**	**Total Stress Tensor** (in kbar)	**Lattice Parameter** (in Å)	**Total Energy** (in eV)
Si	GGA	First	11.74	5.451194762	-856.7016
Si	GGA	Last	0.02	5.474814653	-856.7098

2. **For all the systems, using both approximations**

System	**Pseudo-potential**	**Total No. of Ionic Relaxation steps**	**Total stress Tensor** (in kbar) **in the final relaxation step**	**Lattice Parameter** (in Å) **in the final relaxation step**	**Total energy** (in eV) **in final relaxation step**
Si	GGA	4	0.02	5.474814653	-856.7098
Si	LDA	4	-0.04	5.398237560	-4859.2779
Al	GGA	3	0.45	4.038591688	-2149.6389
Al	LDA	4	0.10	3.954930915	-227.8373
NaCl	GGA	9	0.49	5.688615428	-10277.8064
NaCl	LDA	36	-1.47	5.449119032	-10050.012

3.

The final relaxed parameter in case of Si and Al for both the approximations was close to the observed values in part 1.

The total energy in case of vc relax is nearly four times that obtained in part 1.