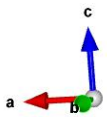
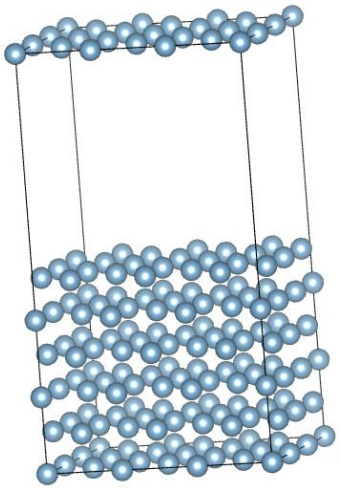
Assignment 3
Bhuvanesh P - MM19B027

1. Al-(100)





2.

New structure
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0.0000000000 12.1199998856 0.0000000000
0.0000000000 0.0000000000 22.1199998856
Al
108
Cartesian
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0.000000000 2.020000041 2.020000041
2.020000041 0.000000000 2.020000041
2.020000041 2.020000041 0.000000000
0.000000000 0.000000000 4.040000082
0.000000000 0.000000000 8.080000165
4.040000082 0.000000000 0.000000000
8.080000165 0.000000000 0.000000000
0.000000000 4.040000082 0.000000000
0.000000000 8.080000165 0.000000000
0.000000000 2.020000041 6.059999943
0.000000000 2.020000041 10.099999664
4.040000082 2.020000041 2.020000041
8.080000165 2.020000041 2.020000041
0.000000000 6.059999943 2.020000041
0.000000000 10.099999664 2.020000041
2.020000041 0.000000000 6.059999943
2.020000041 0.000000000 10.099999664
6.059999943 0.000000000 2.020000041

10.099999664	0.000000000	2.020000041
2.020000041	4.040000082	2.020000041
2.020000041	8.080000165	2.020000041
2.020000041	2.020000041	4.040000082
2.020000041	2.020000041	8.080000165
6.059999943	2.020000041	0.000000000
10.099999664	2.020000041	0.000000000
2.020000041	6.059999943	0.000000000
2.020000041	10.099999664	0.000000000
0.000000000	4.040000082	4.040000082
0.000000000	8.080000165	8.080000165
0.000000000	8.080000165	4.040000082
0.000000000	4.040000082	8.080000165
4.040000082	0.000000000	4.040000082
8.080000165	0.000000000	8.080000165
4.040000082	0.000000000	8.080000165
8.080000165	0.000000000	4.040000082
4.040000082	4.040000082	0.000000000
8.080000165	8.080000165	0.000000000
8.080000165	4.040000082	0.000000000
4.040000082	8.080000165	0.000000000
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0.000000000	10.099999664	10.099999664
0.000000000	10.099999664	6.059999943
0.000000000	6.059999943	10.099999664
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8.080000165	2.020000041	10.099999664
4.040000082	2.020000041	10.099999664
8.080000165	2.020000041	6.059999943
4.040000082	6.059999943	2.020000041
8.080000165	10.099999664	2.020000041
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4.040000082	10.099999664	2.020000041
2.020000041	4.040000082	6.059999943
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2.020000041	8.080000165	6.059999943
2.020000041	4.040000082	10.099999664
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6.059999943	0.000000000	10.099999664
10.099999664	0.000000000	6.059999943
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10.099999664	4.040000082	2.020000041
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2.020000041	6.059999943	4.040000082
2.020000041	10.099999664	8.080000165
2.020000041	10.099999664	4.040000082
2.020000041	6.059999943	8.080000165

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6.059999943	10.099999664	0.000000000
4.040000082	4.040000082	4.040000082
8.080000165	8.080000165	8.080000165
8.080000165	8.080000165	4.040000082
4.040000082	4.040000082	8.080000165
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8.080000165	6.059999943	10.099999664
4.040000082	10.099999664	6.059999943
4.040000082	10.099999664	10.099999664
8.080000165	6.059999943	6.059999943
6.059999943	4.040000082	6.059999943
10.099999664	8.080000165	10.099999664
10.099999664	8.080000165	6.059999943
6.059999943	4.040000082	10.099999664
10.099999664	4.040000082	10.099999664
6.059999943	8.080000165	6.059999943
6.059999943	8.080000165	10.099999664
10.099999664	4.040000082	6.059999943
6.059999943	6.059999943	4.040000082
10.099999664	10.099999664	8.080000165
10.099999664	10.099999664	4.040000082
6.059999943	6.059999943	8.080000165
10.099999664	6.059999943	8.080000165
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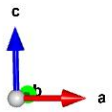
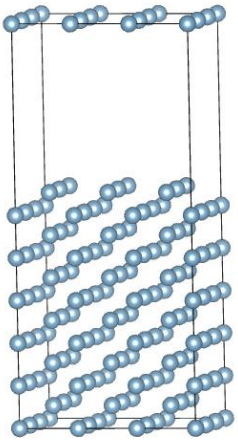
Al – (110)





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0.0000000000 0.0000000000 27.1402683258
Al
108
Cartesian
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0.000000000 0.000000000 2.856711473
0.000000000 0.000000000 5.713422946
0.000000000 0.000000000 8.570134163
0.000000000 0.000000000 11.426845891
0.000000000 0.000000000 14.283556598
0.000000000 2.856711473 0.000000000
0.000000000 2.856711473 2.856711473
0.000000000 2.856711473 5.713422946
0.000000000 2.856711473 8.570134163
0.000000000 2.856711473 11.426845891
0.000000000 2.856711473 14.283556598
0.000000000 5.713422946 0.000000000
0.000000000 5.713422946 2.856711473
0.000000000 5.713422946 5.713422946
0.000000000 5.713422946 8.570134163
0.000000000 5.713422946 11.426845891
0.000000000 5.713422946 14.283556598
4.040000082 0.000000000 0.000000000
4.040000082 0.000000000 2.856711473
4.040000082 0.000000000 5.713422946
4.040000082 0.000000000 8.570134163
4.040000082 0.000000000 11.426845891
4.040000082 0.000000000 14.283556598

4.040000082	2.856711473	0.000000000
4.040000082	2.856711473	2.856711473
4.040000082	2.856711473	5.713422946
4.040000082	2.856711473	8.570134163
4.040000082	2.856711473	11.426845891
4.040000082	2.856711473	14.283556598
4.040000082	5.713422946	0.000000000
4.040000082	5.713422946	2.856711473
4.040000082	5.713422946	5.713422946
4.040000082	5.713422946	8.570134163
4.040000082	5.713422946	11.426845891
4.040000082	5.713422946	14.283556598
8.080000165	0.000000000	0.000000000
8.080000165	0.000000000	2.856711473
8.080000165	0.000000000	5.713422946
8.080000165	0.000000000	8.570134163
8.080000165	0.000000000	11.426845891
8.080000165	0.000000000	14.283556598
8.080000165	2.856711473	0.000000000
8.080000165	2.856711473	2.856711473
8.080000165	2.856711473	5.713422946
8.080000165	2.856711473	8.570134163
8.080000165	2.856711473	11.426845891
8.080000165	2.856711473	14.283556598
8.080000165	5.713422946	0.000000000
8.080000165	5.713422946	2.856711473
8.080000165	5.713422946	5.713422946
8.080000165	5.713422946	8.570134163
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8.080000165	5.713422946	14.283556598
2.020000041	1.428355736	1.428355736
2.020000041	1.428355736	4.285067081
2.020000041	1.428355736	7.141778299
2.020000041	1.428355736	9.998489516
2.020000041	1.428355736	12.855201244
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2.020000041	4.285067081	1.428355736
2.020000041	4.285067081	4.285067081
2.020000041	4.285067081	7.141778299
2.020000041	4.285067081	9.998489516
2.020000041	4.285067081	12.855201244
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2.020000041	7.141778299	7.141778299
2.020000041	7.141778299	9.998489516
2.020000041	7.141778299	12.855201244
2.020000041	7.141778299	15.711912973
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6.059999943	1.428355736	4.285067081
6.059999943	1.428355736	7.141778299
6.059999943	1.428355736	9.998489516
6.059999943	1.428355736	12.855201244
6.059999943	1.428355736	15.711912973
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6.059999943	4.285067081	7.141778299
6.059999943	4.285067081	9.998489516
6.059999943	4.285067081	12.855201244
6.059999943	4.285067081	15.711912973
6.059999943	7.141778299	1.428355736
6.059999943	7.141778299	4.285067081
6.059999943	7.141778299	7.141778299
6.059999943	7.141778299	9.998489516
6.059999943	7.141778299	12.855201244
6.059999943	7.141778299	15.711912973
10.099999664	1.428355736	1.428355736
10.099999664	1.428355736	4.285067081
10.099999664	1.428355736	7.141778299
10.099999664	1.428355736	9.998489516
10.099999664	1.428355736	12.855201244
10.099999664	1.428355736	15.711912973
10.099999664	4.285067081	1.428355736
10.099999664	4.285067081	4.285067081
10.099999664	4.285067081	7.141778299
10.099999664	4.285067081	9.998489516
10.099999664	4.285067081	12.855201244
10.099999664	4.285067081	15.711912973
10.099999664	7.141778299	1.428355736
10.099999664	7.141778299	4.285067081
10.099999664	7.141778299	7.141778299
10.099999664	7.141778299	9.998489516
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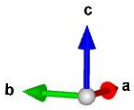
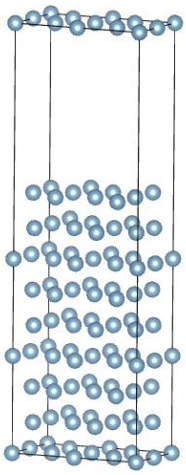
Al – (111)





New structure
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0.0000000000	0.0000000000	30.9924545288

Al
72
Cartesian

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0.000000000	0.000000000	6.997485051
0.000000000	0.000000000	13.994970103
0.000000000	4.947969437	0.000000000
0.000000000	4.947969437	6.997485051
0.000000000	4.947969437	13.994970103
2.856711388	0.000000000	0.000000000
2.856711388	0.000000000	6.997485051
2.856711388	0.000000000	13.994970103
2.856711388	4.947969437	0.000000000
2.856711388	4.947969437	6.997485051
2.856711388	4.947969437	13.994970103
1.428355694	0.824661597	2.332494965
1.428355694	0.824661597	9.329979860
1.428355694	0.824661597	16.327464912
1.428355694	5.772630813	2.332494965
1.428355694	5.772630813	9.329979860
1.428355694	5.772630813	16.327464912
4.285067081	0.824661597	2.332494965
4.285067081	0.824661597	9.329979860
4.285067081	0.824661597	16.327464912
4.285067081	5.772630813	2.332494965
4.285067081	5.772630813	9.329979860
4.285067081	5.772630813	16.327464912

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0.000000000	3.298646389	9.329979860
0.000000000	3.298646389	16.327464912
0.000000000	8.246616121	2.332494965
0.000000000	8.246616121	9.329979860
0.000000000	8.246616121	16.327464912
2.856711388	3.298646389	2.332494965
2.856711388	3.298646389	9.329979860
2.856711388	3.298646389	16.327464912
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2.856711388	8.246616121	16.327464912
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0.000000000	1.649323195	18.659959720
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0.000000000	6.597292779	11.662475294
0.000000000	6.597292779	18.659959720
2.856711388	1.649323195	4.664989930
2.856711388	1.649323195	11.662475294
2.856711388	1.649323195	18.659959720
2.856711388	6.597292779	4.664989930
2.856711388	6.597292779	11.662475294
2.856711388	6.597292779	18.659959720
1.428355694	4.123307766	4.664989930
1.428355694	4.123307766	11.662475294
1.428355694	4.123307766	18.659959720
1.428355694	9.071276907	4.664989930
1.428355694	9.071276907	11.662475294
1.428355694	9.071276907	18.659959720
4.285067081	4.123307766	4.664989930
4.285067081	4.123307766	11.662475294
4.285067081	4.123307766	18.659959720
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4.285067081	9.071276907	11.662475294
4.285067081	9.071276907	18.659959720
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1.428355694	2.473984718	6.997485051
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1.428355694	7.421954155	6.997485051
1.428355694	7.421954155	13.994970103
4.285067081	2.473984718	0.000000000
4.285067081	2.473984718	6.997485051
4.285067081	2.473984718	13.994970103
4.285067081	7.421954155	0.000000000
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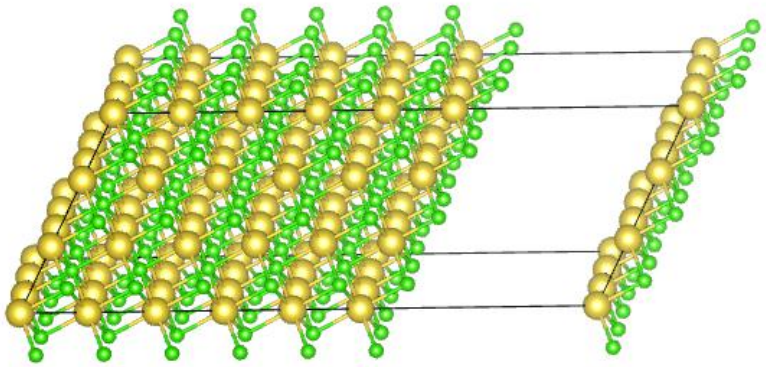
2.Nacl - {111}



New structure
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6.0457623186 10.4715691163 0.0000000000
-6.0457630157 -3.4905231729 9.8726895680
Na Cl
54 54
Cartesian
0.000000000 0.000000000 0.000000000
-2.015254399 -1.163507759 3.290896621
-4.030508797 -2.327015518 6.581793242
2.015254166 3.490523143 0.000000000
-0.000000232 2.327015384 3.290896621
-2.015254631 1.163507625 6.581793242
4.030508332 6.981046286 0.000000000
2.015253934 5.817538527 3.290896621
-0.000000465 4.654030768 6.581793242
4.030508797 0.000000000 0.000000000
2.015254399 -1.163507759 3.290896621
0.000000000 -2.327015518 6.581793242
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2.015254166 1.163507625 6.581793242
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4.030508797 -2.327015518 6.581793242
10.076271761 3.490523143 0.000000000

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10.076271528	5.817538527	3.290896621
8.061017130	4.654030768	6.581793242
12.091526031	0.000000000	0.000000000
10.076271633	-1.163507759	3.290896621
8.061017234	-2.327015518	6.581793242
14.106780198	3.490523143	0.000000000
12.091525799	2.327015384	3.290896621
10.076271400	1.163507625	6.581793242
16.122034364	6.981046286	0.000000000
14.106779965	5.817538527	3.290896621
12.091525567	4.654030768	6.581793242
16.122035189	0.000000000	0.000000000
14.106780790	-1.163507759	3.290896621
12.091526392	-2.327015518	6.581793242
18.137289355	3.490523143	0.000000000
16.122034957	2.327015384	3.290896621
14.106780558	1.163507625	6.581793242
20.152543522	6.981046286	0.000000000
18.137289123	5.817538527	3.290896621
16.122034724	4.654030768	6.581793242
20.152542905	0.000000000	0.000000000
18.137288507	-1.163507759	3.290896621
16.122034108	-2.327015518	6.581793242
22.167797072	3.490523143	0.000000000
20.152542673	2.327015384	3.290896621
18.137288274	1.163507625	6.581793242
24.183051238	6.981046286	0.000000000
22.167796839	5.817538527	3.290896621
20.152542441	4.654030768	6.581793242
2.015254282	1.163507692	1.645448310
-0.000000026	-0.000000015	4.936344784
-2.015254245	-1.163507670	8.227241111
4.030508359	4.654030679	1.645448310
2.015254050	3.490522972	4.936344784
-0.000000168	2.327015317	8.227241111
6.045762345	8.144553509	1.645448310
4.030508036	6.981045802	4.936344784
2.015253818	5.817538147	8.227241111
6.045762900	1.163507692	1.645448310
4.030508591	-0.000000015	4.936344784
2.015254373	-1.163507670	8.227241111
8.061016976	4.654030679	1.645448310
6.045762667	3.490522972	4.936344784
4.030508449	2.327015317	8.227241111
10.076270962	8.144553509	1.645448310
8.061016653	6.981045802	4.936344784

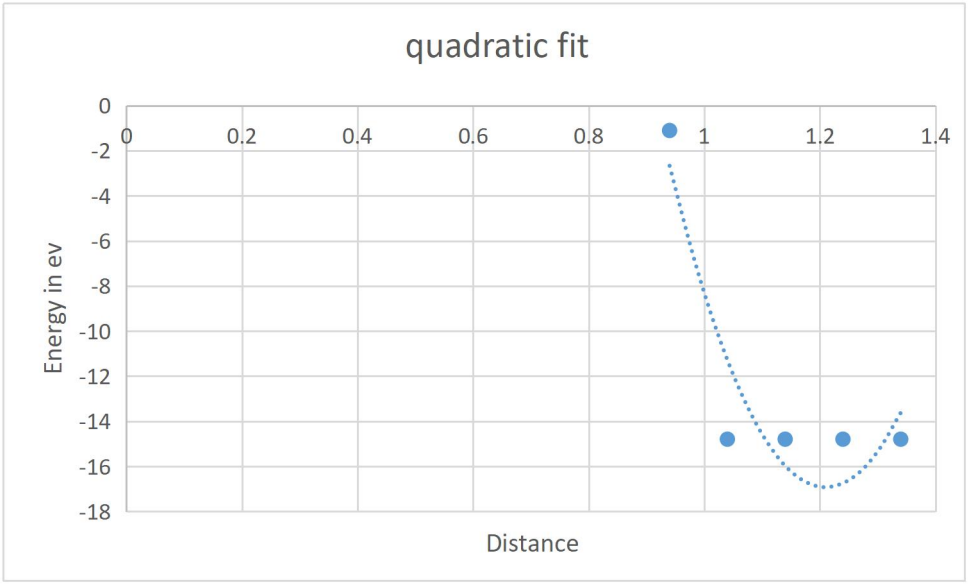
6.045762435	5.817538147	8.227241111
10.076271336	1.163507692	1.645448310
8.061017028	-0.000000015	4.936344784
6.045762809	-1.163507670	8.227241111
12.091525413	4.654030679	1.645448310
10.076271104	3.490522972	4.936344784
8.061016886	2.327015317	8.227241111
14.106779399	8.144553509	1.645448310
12.091525090	6.981045802	4.936344784
10.076270872	5.817538147	8.227241111
14.106779773	1.163507692	1.645448310
12.091525465	-0.000000015	4.936344784
10.076271246	-1.163507670	8.227241111
16.122033850	4.654030679	1.645448310
14.106779541	3.490522972	4.936344784
12.091525323	2.327015317	8.227241111
18.137287836	8.144553509	1.645448310
16.122033527	6.981045802	4.936344784
14.106779309	5.817538147	8.227241111
18.137288931	1.163507692	1.645448310
16.122034622	-0.000000015	4.936344784
14.106780404	-1.163507670	8.227241111
20.152543007	4.654030679	1.645448310
18.137288699	3.490522972	4.936344784
16.122034480	2.327015317	8.227241111
22.167796993	8.144553509	1.645448310
20.152542685	6.981045802	4.936344784
18.137288466	5.817538147	8.227241111
22.167798089	1.163507692	1.645448310
20.152543780	-0.000000015	4.936344784
18.137289562	-1.163507670	8.227241111
24.183052165	4.654030679	1.645448310
22.167797856	3.490522972	4.936344784
20.152543638	2.327015317	8.227241111
26.198306151	8.144553509	1.645448310
24.183051842	6.981045802	4.936344784
22.167797624	5.817538147	8.227241111

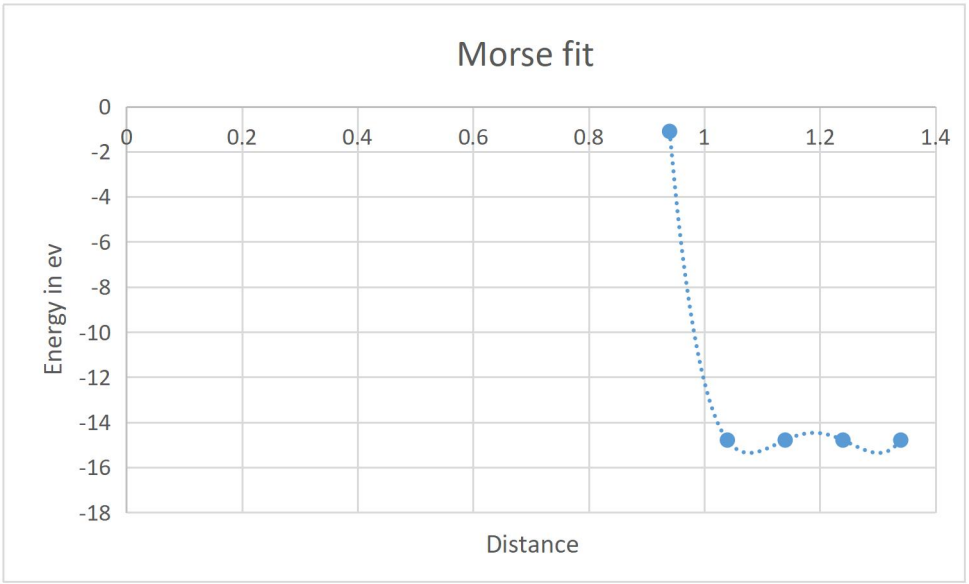
Question 5

The energy values are

Distance in Angstrom	Energy in eV
0.94	-1.10404755
1.04	-14.79347335
1.14	-14.7934226

1.24	-14.79371015
1.24	-14.79367252





The Morse potential fits better because the atom are also vibrating in addition to the potential energy it has. Only electrostatic energy will have quadratic equation as a better fit.

3) The most stable phase is Diamond cubic which has the lowest energy

On applying hydrostatic compressive stress, volume will decrease hence Diamond cubic gets transformed to β tin

4) For {1,1,1}

No of broken bonds - 3

No of atoms per unit area - $\frac{4}{\sqrt{3}a^2}$

No of broken bonds per unit area $= 3 + \frac{4}{\sqrt{3}a^2}$

$a = \sqrt{2}\,(4.04)\,A^{\circ}$ $= \frac{4.25 \times 10^{19}}{2}$

$= 2.125 \times 10^{19}$

For {1,1,0}

No of broken bonds per atom - 5

Atoms per unit area $= \frac{\sqrt{2}}{a^2}$

No of broken bonds per unit area

$= 5 \times \frac{\sqrt{2}}{a^2} = 4.3325 \times 10^{19} = 2.16 \times 10^{19}$

for (1,0,0)

- No of broken bonds = 1

- Atoms per unit area = $\frac{2}{a^2}$

- No of broken bonds per unit area

= $4.9 \times 10^{19} / 2$

= 2.15×10^{19}

6) The stopping criteria is if energy diff is less than 1meV

- The k point convergence is 12 for Al atom beyond which the diff is less than 1meV

7) Primitive unit cell of Al - 13 electron

CO molecule - 6 + 8 - 14 electrons

8) Surface energy $= \frac{1}{2A}\left[E_{slab} - n E_{bulk}\right]$

for Al (0 0 1) surface

E_{bulk} = Energy per atom

E_{slab} = Energy per atom of entire supercell

A = Surface area of (0 0 1) ~~plan~~ face

$= 4 \times 4 \times 10^{-20} = 16 \times 10^{-20}\ m^2$

$S.E = \frac{1}{2 \times 16 \times 10^{-20}}\left[-450 + n(3)\right] \times 1.6 \times 10^{-19}$

$n = 10 \times 2 = 20$ atoms

$= 10 \times 1.6 \times 10^{-19} / 32 \times 10^{-20}$

$= 5\ J/m^2$

9) The exchange correlation used is GGA
- Generalized Gradient Approximation

10) $E = 0.05x^2 - x - 200$

$B = V\left(\frac{d^2E}{dV^2}\Big|_{V_0}\right)$

To find V_0 $\frac{dE}{dx} = 0 = 0.1x - 1$

$x = 10\ A^{\circ 3}$

$a^3 = V = 10\ A^{\circ 3}$

$a = \sqrt[3]{V} = 2.154\ A^{\circ}$ — Lattice parameter

$B = V\left(\frac{d^2E}{dx^2}\right) = 10 \times 0.1$ $eV/A^{\circ 3}$

$= \frac{1.6 \times 10^{-19}}{10^{-30}} = 1.6 \times 10^{11}\ J/m^3$

$= 160$ GPa