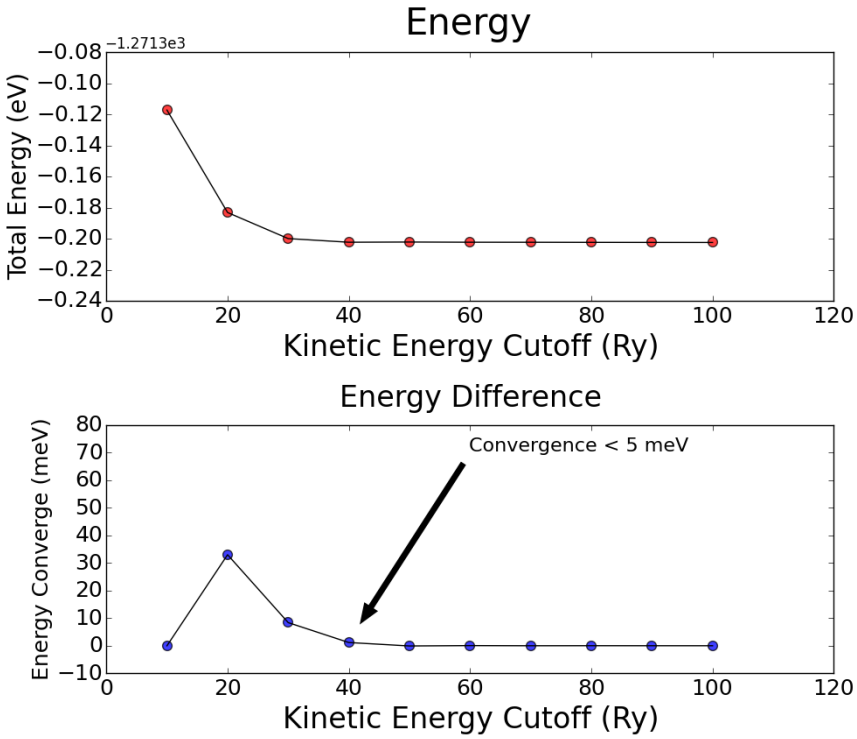
Nano 266

Lab 2 Report

Chen Zheng

A53048780

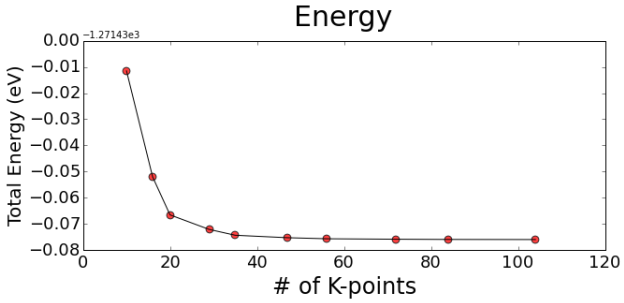
Q1:

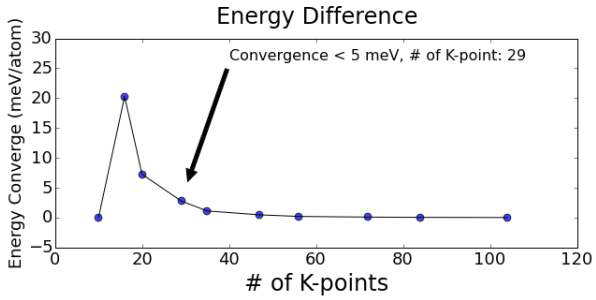


When the energy cutoff increases to higher than 40 Ry, we reached the level of convergence below 5 meV/atom. We see the calculated energy difference drops rapidly initially with increasing of kinetic energy cutoff and than flattened after the energy cut off passes 40 Ry.

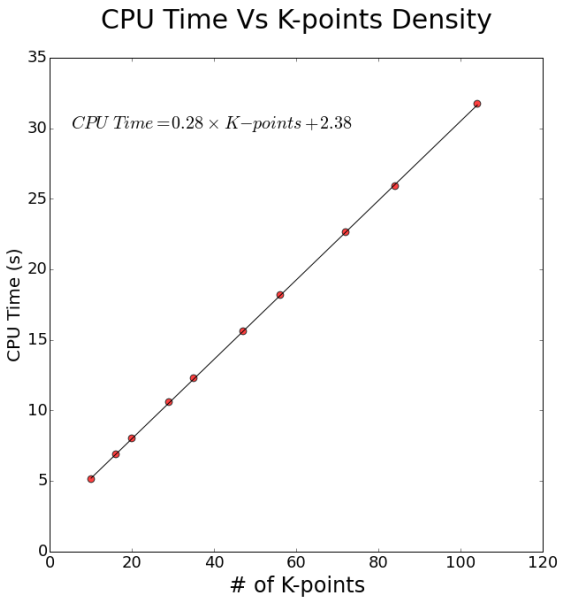
Q2

b) With increasing of k-points number, the total energy decreases rapidly at the beginning, and then become stable when the unique K-point number reach 29 (8*8*8 K-point grid setting in input file). Since K-points number is related to number of integrals we need to consider during evaluating the energy in the space, higher density of K-points means we have more points for sampling, and have more accurate results.

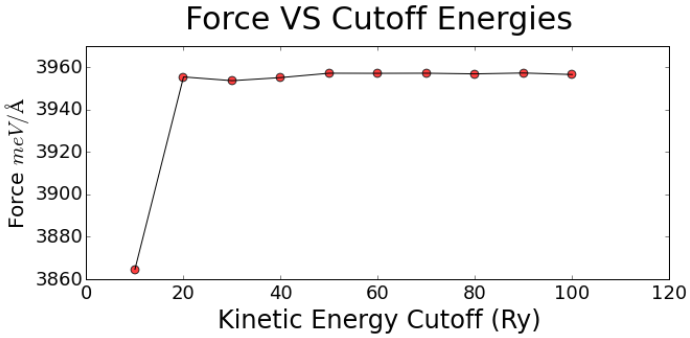


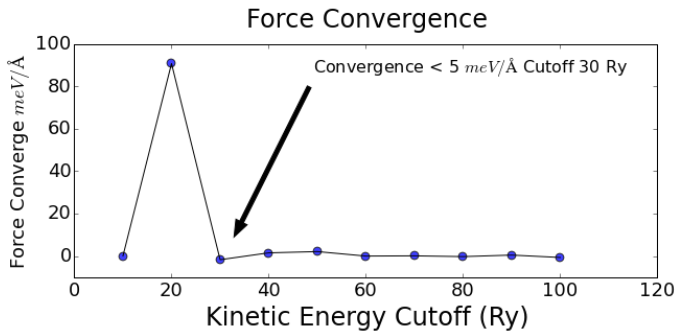


c) The relationship between number of K-points and calculation time is linear as we could see from the below plot, and linear regression model fit their relationship pretty well with slope equals to 0.28 and intercept equals 2.38.

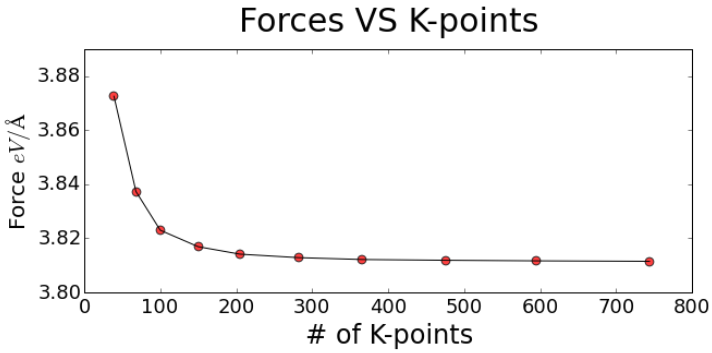


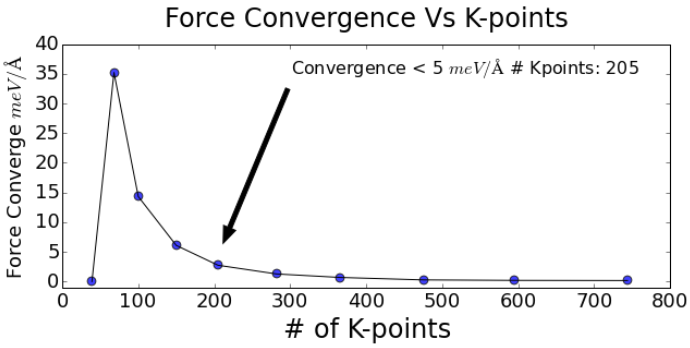
Q3: Convergence of Forces with respect to cutoff energies
From the below graph, with 30 Ry as cutoff energy, we could converged to a good force value within ~10 meV/Angstrom.



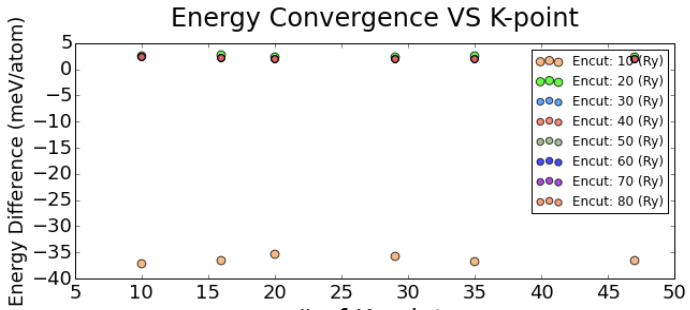


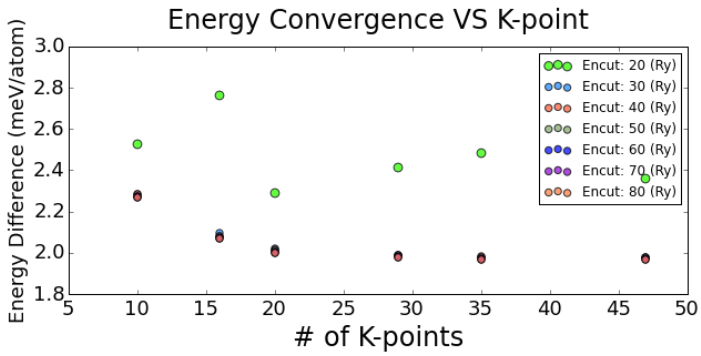
Q4: Convergence of Forces with respect to K-points
To get relative good force convergence, we need K-point grid larger than 9*9*9, with 205 unique K-points. Compared with previous energy convergence, force convergence need more unique K-point for sampling.

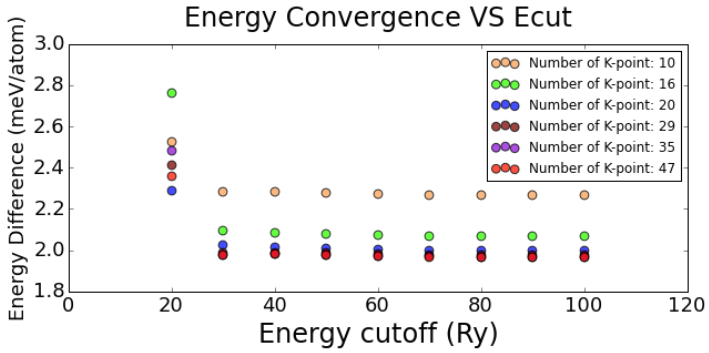




Q5: Convergence of Energy Differences with respect to energy cutoff and K-points.
1. From the below plot, we could conclude that, if we use energy cutoff as 10 Ry, the energy difference will be larger than 30 meV/atom and impossible to converge to lower than 5 meV/atom. While after we increase the energy cutoff to 20 meV/atom, the energy difference convergence much faster than the convergence of absolute energy (e.g. Q3). Low density of K-point (i.e. 6*6*6) is enough for energy difference convergence. In general, the energy difference converges much faster compared with convergence of absolute energy.



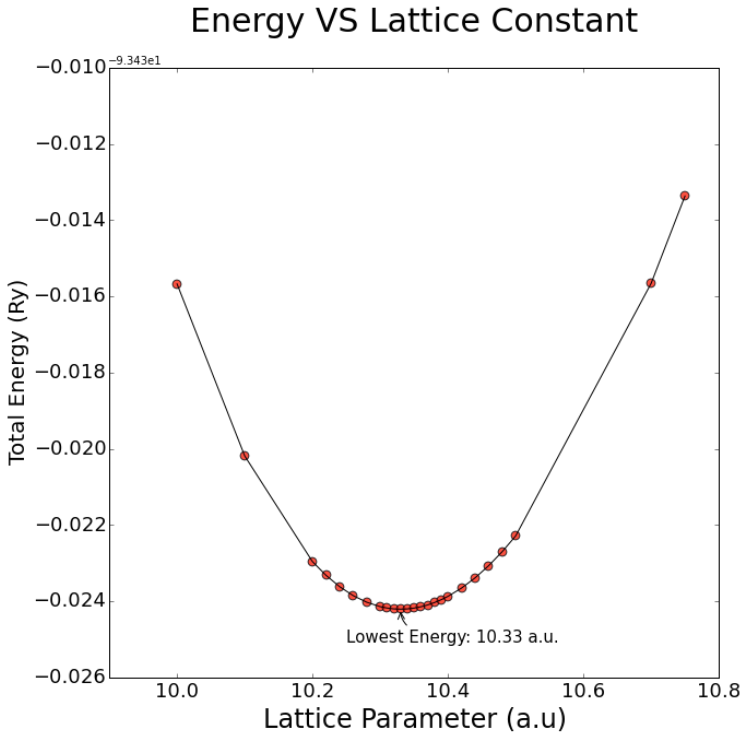




Q6:
Based on preceding question's result, for absolute energies, forces calculation, 50 Ry as kinetic energy cutoff, 9*9*9 K-points grid size might be the best parameter combinations considering both efficiency and accuracy.

For energy difference calculation, lower energy cutoff and K-point density are enough since the energy difference calculation cancelled out part of DFT systematic error.

Q7: Equilibrium structure
Using 50 Ry as energy cut off, 9*9*9 as K-point density, we obtain the below plot with difference lattice parameter in static calculation. We found that 10.33 a.u is the equilibrium structure lattice parameter which gives us the lowest total energy per primitive cell.



Q8:

Using data we got in Q7, we could use Birch Murnaghan EOS (3rd order) to find the bulk modulus of silicon at the equilibrium lattice constant.
The bulk modulus we got of silicon cell is 89.0 GPa, which is ~8.8% lower than experimental value of 97.6 GPa.

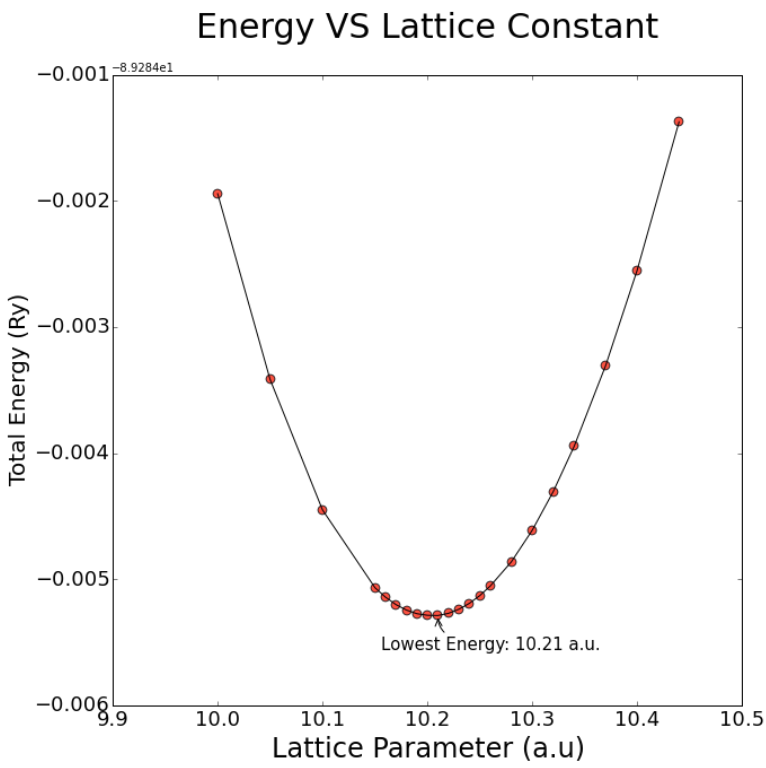
```
# equation of state: birch 3rd order.  chisq = 0.8073D-12
# a0 = 10.3303 a.u., k0 =  890 kbar, dk0 =  4.31 d2k0 = -0.007 emin =  -93.45421
# a0 =  5.46655 Ang, k0 =  89.0 GPa,  V0 = 275.598 (a.u.)^3,  V0 = 40.839 A^3
#############################################################################
# Lat.Par       E_calc        E_fit       E_diff    Pressure      Enthalpy
# a.u.            Ry           Ry           Ry        GPa           Ry
#############################################################################
  9.50000     -93.39081     -93.39081     0.00000      37.64      -92.84238
 10.00000     -93.44567     -93.44567    -0.00000      10.68      -93.26423
 10.10000     -93.45019     -93.45019     0.00000       6.96      -93.32839
 10.20000     -93.45296     -93.45296     0.00000       3.68      -93.38663
 10.22000     -93.45332     -93.45332     0.00000       3.07      -93.39760
 10.24000     -93.45362     -93.45362    -0.00000       2.48      -93.40835
 10.26000     -93.45385     -93.45385    -0.00000       1.91      -93.41888
```

10.28000	−93.45403	−93.45403	0.00000	1.34	−93.42920
10.30000	−93.45414	−93.45414	−0.00000	0.80	−93.43931
10.31000	−93.45418	−93.45418	−0.00000	0.53	−93.44428
10.32000	−93.45420	−93.45420	−0.00000	0.27	−93.44920
10.33000	−93.45421	−93.45421	−0.00000	0.01	−93.45407
10.34000	−93.45420	−93.45420	−0.00000	−0.25	−93.45889
10.35000	−93.45418	−93.45418	−0.00000	−0.50	−93.46366
10.36000	−93.45415	−93.45415	−0.00000	−0.75	−93.46838
10.37000	−93.45410	−93.45410	−0.00000	−1.00	−93.47305
10.38000	−93.45404	−93.45404	−0.00000	−1.24	−93.47766
10.39000	−93.45396	−93.45396	0.00000	−1.48	−93.48223
10.40000	−93.45387	−93.45387	−0.00000	−1.72	−93.48675
10.42000	−93.45366	−93.45366	0.00000	−2.18	−93.49564
10.44000	−93.45339	−93.45339	0.00000	−2.63	−93.50434
10.46000	−93.45307	−93.45307	0.00000	−3.07	−93.51284
10.48000	−93.45270	−93.45271	0.00000	−3.50	−93.52116
10.50000	−93.45229	−93.45229	0.00000	−3.91	−93.52929
10.70000	−93.44566	−93.44566	0.00000	−7.46	−93.60091
10.75000	−93.44337	−93.44337	−0.00000	−8.19	−93.61623

Q9:

Using LDA pseudopotential and redo the equilibrium calculation Q7, we found that the equilibrium lattice parameter changed with lower overall total energy. The equilibrium lattice parameter now becomes 10.21 a.u. The equilibrium lattice parameter predicted to be lower than in GGA due to LDA's well-known overbinding problem with lead to lower bond length, lattice parameter and atomization energies prediction. The overbinding also leads to an energy overestimating by 4% compared with GGA.

While we could conclude that evaluating bulk modulus using LDA give better agreement with experimental data.



We could use Birch Murnaghan EOS (3rd order) to fit the data. The bulk modulus of silicon at the equilibrium lattice constant.
The bulk modulus we got of silicon cell is 96.9 GPa and very close to the experimental value 97.6 GPa, and is only ~0.72% lower.

```
# equation of state: birch 3rd order.  chisq = 0.1586D-11
# a0 = 10.2037 a.u., k0 =  968 kbar, dk0 =  4.23 d2k0 = -0.006 emin =  -89.28929
# a0 =  5.39957 Ang, k0 =  96.9 GPa,  V0 = 265.592 (a.u.)^3,  V0 = 39.357 A^3

#############################################################################
# Lat.Par       E_calc         E_fit       E_diff    Pressure      Enthalpy
# a.u.            Ry             Ry           Ry         GPa           Ry
#############################################################################
  9.50000     -89.24235     -89.24235     0.00000      32.32      -88.77149
 10.00000     -89.28594     -89.28594     0.00000       6.66      -89.17284
 10.05000     -89.28742     -89.28741    -0.00000       4.85      -89.20367
 10.10000     -89.28845     -89.28845    -0.00000       3.17      -89.23300
 10.15000     -89.28907     -89.28907     0.00000       1.59      -89.26088
 10.16000     -89.28914     -89.28914     0.00000       1.28      -89.26629
 10.17000     -89.28920     -89.28920     0.00000       0.98      -89.27164
 10.18000     -89.28924     -89.28925     0.00000       0.69      -89.27694
 10.19000     -89.28927     -89.28928     0.00000       0.39      -89.28218
 10.20000     -89.28929     -89.28929     0.00000       0.11      -89.28737
 10.21000     -89.28929     -89.28929    -0.00000      -0.18      -89.29251
 10.22000     -89.28927     -89.28927    -0.00000      -0.46      -89.29759
 10.23000     -89.28924     -89.28924    -0.00000      -0.74      -89.30262
 10.24000     -89.28919     -89.28919    -0.00000      -1.01      -89.30759
 10.25000     -89.28913     -89.28913     0.00000      -1.28      -89.31252
 10.26000     -89.28905     -89.28905     0.00000      -1.54      -89.31738
 10.28000     -89.28886     -89.28886    -0.00000      -2.06      -89.32697
 10.30000     -89.28861     -89.28861    -0.00000      -2.57      -89.33635
 10.32000     -89.28831     -89.28830    -0.00000      -3.06      -89.34553
 10.34000     -89.28794     -89.28794    -0.00000      -3.54      -89.35451
 10.37000     -89.28731     -89.28731     0.00000      -4.24      -89.36761
 10.40000     -89.28655     -89.28655     0.00000      -4.90      -89.38027
 10.44000     -89.28537     -89.28537     0.00000      -5.75      -89.39651
 10.48000     -89.28400     -89.28400     0.00000      -6.54      -89.41201
 10.50000     -89.28324     -89.28324    -0.00000      -6.93      -89.41949
```