**VASP\_HW1**

1. Perform a calculation to find the minimum energy configuration (volume and ions positions) of Si in both FCC and Diamond structures (relax both the ions and the volume). Report the energy and the lattice parameter of each structure and compare their energies.

The lattice parameter for the diamond structure was 5.5(Å) and for FCC was 4.3(Å). The energy for FCC was E0=-.55160130E+01(eV) and for diamond E0= -.11861234E+02(eV). Diamond has a more negative energy, meaning it is a more stable structure than FCC.

1. Starting from the structures obtained in problem1 calculate the energy vs. volume and the bulk modulus of both structures.
2. Starting from the diamond structure obtained in problem1 perform convergence test with respect to K-points and cutoff energy.
3. Start Ex4 and Ex5 (under Lab7) from the GitHub and include the outputs in your HW folder on the GitHub.