**MSE 551**

**HW#2 Due:09/12/2017**

1. Calculate the Energy vs. distance of two atoms using the LJ potentials we used in the class.
   1. If I perform the test for few data points I get a shape that was expected, however upon using more points, the energy minimum is not nearly as negative as expected (based off the graph uploaded in LEC2). I am unsure as to what the error might be.
2. Calculate minimum Energy and lattice parameter for Al using the eam potential for the following structures:
3. SC
   1. Lattice constant (Angstroms): 2.68705318650982
   2. Minimum Energy (eV): -3.06265447774
4. BCC
   1. Lattice constant (Angstroms): 3.21911196315487
   2. Minimum Energy (eV): -6.60323678084
5. FCC
   1. Lattice constant (Angstroms): 4.04976352616037
   2. Minimum Energy (eV): -13.2732688882

Compare and comment on the result.

1. Calculate Energy vs. Volume curve for Al FCC structure using the eam potential. Then estimate the bulk modulus.
   1. For some reason the graph did not come out as a parabola, but assuming it should be, I put a line of best fit for it on there. I will set V0 as the original lattice parameter, 64(A3).
2. Brief summary of your class project.

Find a method of using molecular dynamics to simulate an amorphous structure, specifically chalcogenide glasses with copper in them. Use VASP to calculate the electronic band structure of copper atoms within a crystalline version of the chalcogenide glass.

Note: Use MATLAB, python or shell script to produce E vs. d and E vs.V