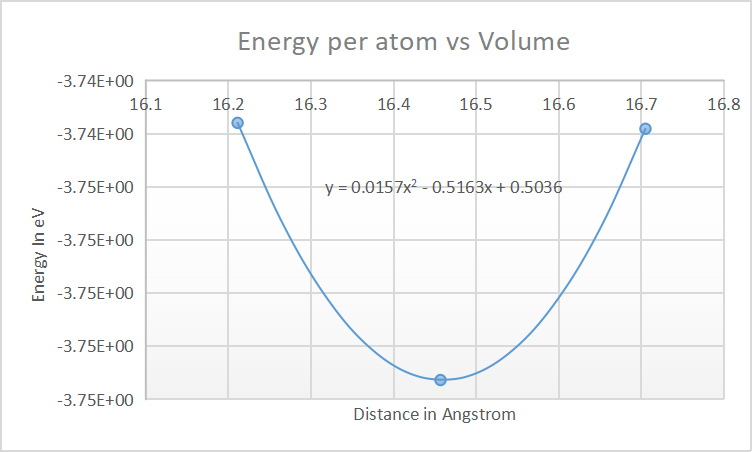
**Hands On assignment 5**

**MM19B027 - Bhuvanesh P**

1. **We try to plot Energy per atom for 0.5% compression and extension of the lattice parameter. The plot is given by**



1. **Bulk Modulus is given by**

E(V) is given by 0.0157V2 - 0.5163V + 0.5036

Here Vo is the equilibrium volume which obtained by differentiating the energy equation and equating it to 0

= 0 = 0.0314V - 0.5163

Which gives Vo as 16.44267 A3

The we double differentiate the energy equation y = 0.0157V2 - 0.5163V + 0.5036 to get = 0.0314

We get B = 0.0314 X 16.44267 = 0.5163 which is in eV/A3

To convert it into SI units, we do

We get 0.82608 X 10 11 Pa or 82.6 GPa . Experimental value is 76 Gpa. The deviation from the actual value is about 8.7 %.