Lab 05 – Structure Optimization

1. **Equilibrium lattice constant of Diamond Carbon.**
   1. Calculate the equilibrium lattice constant of diamond using Quantum Espresso. The experimental value is 6.74 bohr. Use the cutoff and *k* point grid criteria you obtained from the force convergence calculations (if you haven’t completed these, use a cutoff of 90 Ryd and a 9 x 9 x 9 *k*point grid). Make sure to record all the relevant parameters (*k* points, cutoffs, etc.). You’ll want to make a plot of energy vs lattice constant and fit a 2nd degree polynomial.
   2. From your 2nd degree polynomial fit, what is the effective spring constant?
   3. How does the experimental value compare with the calculated value (use percent error)?
   4. Deliverables:
      1. Table of DFT results (highlight or bold the equilibrium lattice constant)
      2. Plot of total energy vs lattice constant
      3. Answer to part (b) and (c)
2. **Equilibrium lattice constant of BaTiO3.**
   1. Calculate the equilibrium lattice constant of BaTiO3 using Quantum Espresso. The experimental value is 7.56 bohr. Use the cutoff and *k* point grid criteria you obtained from the force convergence calculations (if you haven’t completed these, use a cutoff of 90 Ryd and a 4 x 4 x 4 *k*point grid). Make sure to record all the relevant parameters (*k* points, cutoffs, etc.). You’ll want to make a plot of energy vs lattice constant and fit a 2nd degree polynomial.
   2. From your 2nd degree polynomial fit, what is the effective spring constant?
   3. How does the experimental value compare with the calculated value (use percent error)?
   4. Deliverables:
      1. Table of DFT results (highlight or bold the equilibrium lattice constant)
      2. Plot of total energy vs lattice constant
      3. Answer to part (b) and (c)