CBE544 - Homework 5 due April 10^{th} 2019

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Perform Density Functional Theory (DFT) calculations

In this homework you will learn how to run DFT calculations using VASP and the Atomic Simulation Environment (ASE) on the computer cluster Chestnut. Please follow the guidelines provided on the course website https://cbe544.github.io/CBE544-2019.github.io/

Before you start with the homework assignment make sure that you have made yourself acquainted with, that you understand and master the material in the "Getting Started" section including: "Logging Into the Computing Clusters", "Basic UNIX", and "Python Tutorial".

Next walk yourself through the ASE Tutorial which consists of two sections: "Introduction to ASE", and "Getting Started with DFT".

1. (50%) Determine the lattice constants a_{DFT} and c_{DFT} for $LiCoO_2$ by using DFT calculations as outlined in the "Getting Started with DFT Calculations" section.
   a. Write a Python script to perform an Equation of State fit to determine a_{DFT}. Provide a plot of the fit and the Python script used. Repeat this for c_{DFT}.
   b. How well does a_{DFT} compare with the experimentally measured a_{EXP} for $LiCoO_2$?

2. (25%) Determine the convergence of the total energy as a function of k-points.
   a. Provide a convergence plot.
   b. At what k-point has the total energy converged? Why? Provide the rationale behind your choice

3. (25%) Construct a $LiCoO_2$ (104) surface using ASE. Then perform an appropriate geometry relaxation optimization calculation and report the final energy. Comment on the changes to the structure that you see after the relaxation.