CBE544 - Homework 5 due @ 5pm Friday March 24^{rd} 2017

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Perform Density Functional Theory (DFT) calculations

In this homework you will learn how to run DFT calculations using Quantum ESPRESSO and the Atomic Simulation Environment (ASE) on the computer cluster Stampede. Please follow the guidelines provided on the course website https://cbe544.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 three sections: "Introduction to ASE", "Getting Started with DFT", and "Adsorption".

1. (30%) Determine the lattice constant a_{DFT} for Ti_2C by using DFT calculations as outlined in the "Getting Started with DFT Calculations" section.
   a. Provide a plot of the total energies as a function of the lattice parameter ($\sim$ 5 points) and the quadratic fit you used with the equation of state to determine a_{DFT}.
   b. How well does a_{DFT} compare with the experimentally measured a_{EXP} for Ti_2C?

2. (10%) Calculate and report the two-dimensional bulk modulus B of Ti_2C.

3. (20%) 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

4. (40%) Calculate the adsorption energy of N E_{ads} on the four high symmetry adsorption sites (fcc, hcp, ontop, and bridge).
   a. Provide each E_{ads}.
   b. Which is the most stable adsorption site?