Homework 3 due @ 5pm Friday Apr 12nd 2019

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://ccml-uconn.github.io/CHEG-5395-4995/

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. Determine the total energy of a (2x2) Pt(111) surface.
2. Provide a plot of the total energies as a function of relaxing steps.
3. Calculate the total energy of CO adsorbing on the four high symmetry sites (fcc, hcp, ontop, and bridge).
   a. Provide each E_{ads}.
   b. Which is the most stable adsorption site?
4. Calculate the most stable adsorption site for O on Pt(111), and report the E_{ads}

Things to remember

1. **Run your calculations in `scratch` partition**
2. **One directory for one calculation**
3. **Change the `posin=read("init.traj")` in `qe-opt.py`**