CBE544 - HW 5 due @ 5pm Friday November 11th, 2023

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In this homework you will learn how to run DFT calculations using Quantum ESPRESSO and the Atomic Simulation Environment (ASE) on the computer cluster Anvil. Please follow the guidelines provided on the course website:
https://upenncbe544.github.io/CBE544-2023.github.io/

Before you start with the homework assignment make sure that you go through the material in the "Getting Started" section including:
- "Logging Into the Computing Clusters"
- "Basic UNIX"
- "Python Tutorial"

Next walk yourself through the ASE Tutorial which consists of three sections:
- "Introduction to ASE"
- "Getting Started with DFT"

If you get stuck on any of the theory, refer back to the Density Functional Theory - A Practical Introduction

Please complete the following tasks once you are familiar with the basics:

1. (30%) Determine the lattice constant a_{DFT} for MgO by using DFT calculations as outlined in the "Getting Started with DFT Calculations" section.

   (a) Plot the DFT calculated total energies as a function of the guessed lattice constants. Obtain the calculated lattice constant, a_{DFT}, which gives rise to the minimum total energy.

   (b) Compare calculated (a_{DFT}) with the experimentally measured lattice constant (a_{EXP}). Provide reference used for comparison.

2. (20%) Check the convergence of the bulk total energy as a function of number of k-points.

   (a) Provide a convergence plot (total energy vs. k-point).
   (b) At what k-point has the total energy converged? Why? Provide the rationale behind your choice.

3. (50%) Construct a (100) surface of MgO.

   (a) Calculate the total energy of the (100) surface of MgO by performing a geometry optimization calculation.
   (b) Adsorb ONE CO_2 molecule onto one of the surface oxygen sites. There are many possible CO_2 orientations (e.g., side on, end on) and bond lengths to start with, but

in this part only choose one orientation and use a bond length of 1.179 Å. Calculate the total energy of the system. You may use the built-in ASE structural relaxation to find the lowest total energy.

(c) Calculate the adsorption energy of CO_2. Is this a physisorption or chemisorption? Provide reference for justification if needed.

$$E_{ads} = E_{MgO+CO_2} - E_{CO_2} - E_{MgO}$$

with E_{CO_2}= -1090.607 eV

(d) Write a script to plot the density of states (DOS).