CBE544 - HW 5 due @ 5pm Friday November 11th 2022

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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 Stampede. Please follow the guidelines provided on the course website `https://upenncbe544.github.io/CBE544-2022.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

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. Note: Keep the same calculator (EMT())
   (a) Plot the DFT calculated total energies as a function of the guessed lattice constants (use 5 points - from 3 to 4). Determine the Equation of State using a quadratic fit to obtain the calculated lattice constant a_{DFT} .
   (b) Compare calculated (a_{DFT}) with the experimentally measured lattice constant (a_{EXP}). Provide reference used for comparison
2. (10%) Calculate the bulk modulus B of Ti_2C.
3. (20%) Check the convergence of the bulk total energy as a function of number of k-points.
   (a) Provide a convergence plot.
   (b) At what number of k-points has the total energy converged? Provide the rationale behind your choice of k-point numbers
4. (40%) Determine the reactivity of Ti_2C towards O.
   (a) Calculate the total energy of Ti_2C.

(b) Calculate the total energy of a system with one O atom binding to a high symmetry site (fcc, hcp, ontop, and bridge) on the basal plane of Ti_2C. Use the built in ASE structural relaxation to find the lowest total energy.

(c) Calculate the adsorption energy E_{ads} for each site using the following equation:

$$E_{Ads} = E_{Ti_2C+O_{Ads}} - E_{Ti_2C} - \frac{1}{2}E_{O_2}$$

with E_{O_2} = -926.9862 eV

(d) Which is the most stable adsorption site? Are there any unstable adsorption sites?

(e) Based on the most stable E_{ads}, do you expect the bare Ti_2C basal plane to get oxidized or not?