CBE5440 - HW 5

In this homework, you will learn how to run density functional theory (DFT) calculations using Quantum ESPRESSO and the Atomic Simulation Environment (ASE) on the national super computer ACCESS on the Anvil cluster. Please follow the guidelines provided on the course website: `https://github.com/UPennCBE544/CBE544-2025`.

Before you start with the homework assignment, make sure that you go through the material in the Github, Cluster.md, section including:

- Logging Into the Computing Clusters
- Basic UNIX
- Python Tutorial

Next, walk yourself through the ASE Tutorial which consists of these 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*.

Tasks

You will study a 2D material known as MXene and how it interacts with a simple atom to learn about bond formation on solids.

1. (50%) Study the convergence and formation of a bare Nb_2C MXene using a 2×2 cell. Specifically, calculate and analyze the total energy of the system 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.
   (c) Once you have found an optimal value for the k-points, calculate the formation energy of the MXene using the following reference values: $E_{Nb_{(s)}}$ = -1613.7 eV, $E_{C_{(s)}}$ = -164.7 eV. Please provide the formula that you use for the formation energy.

2. (50%) Evaluate adsorption of Cl on different bindings sites of the bare MXene and compare the thermodynamic stability of adsorption between the different sites: fcc, hcp, and top.

   (a) Adsorb a single Cl atom on the MXene in 3 different high-symmetry sites. There are many different initial positions to initialize your structure in to start the calculation. For efficiency and to save compute time, please use the following as guidelines:

   - For fcc site, use the Nb atom in the bottom layer as (x,y) reference coordinate. Initiate the Cl atom 4.4 Å above the Nb atomic plane in the +z direction.
   - For hcp site, use C atom in the middle layer as your (x,y) reference coordinate and initiate the Cl atom 3.1 Å above the Nb atomic plane in the +z direction.
   - For top site use Nb atom as reference (x,y) coordinate and initiate the Cl atom 1.5 Å above the Nb atomic plane in the +z direction.

   (b) Calculate the adsorption energy of Cl using the following formula

$$E_{\text{ads}} = E_{Nb_2C+Cl} - E_{Cl} - E_{Nb_2C} \tag{1}$$

   with $E_{Cl} = 477.602$ eV. Is the observed adsorption considered to be physisorption or chemisorption? And compared to bare Nb_2C MXene, is the Cl-terminated Nb_2C MXene more stable? Provide reference for justification if needed.

   (c) Perform a density of states (DOS) calculation for the system. Plot the DOS vs. energy. Note that you will have to correct the energy by the Fermi energy. Using the plot, decide whether the material is a metal, semiconductor, or an insulator and explain your reasoning.