CBE544 - Homework 5 due Friday, November 12, 2021

Send a digital .pdf copy to csl1191@seas.upenn.edu and alevoj@seas.upenn.edu

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 Stampede2. Please follow the guidelines provided on the course website
https://upenncbe544.github.io/CBE544-2021.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 two sections:
- "Introduction to ASE", and
- "Getting Started with DFT".

1. (50%) Determine the lattice constant a_{DFT} for cubic $SrTiO_3$ by using DFT calculations as outlined in the "Getting Started with DFT Calculations" section.
   a) Write a Python script to perform an Equation of State fit to determine a_{DFT}. Provide a plot of the fit and the Python script used.
   b) How well does a_{DFT} compare with the experimentally measured a_{EXP} for $SrTiO_3$?
2. (25%) Determine the convergence of the total energy as a function of k-points.
   a) Provide a convergence plot. Provide the Python plot script used.
   b) At what k-point has the total energy converged? Why? Provide the rationale behind your choice.
3. (25%) Construct a BO_2-terminated (001) surface of $SrTiO_3$. Calculate the total energy of the BO_2-terminated (001) surface of $SrTiO_3$ by performing a geometry optimization calculation.