ECE 695 (Numerical Simulations) – Homework 6

Due March 8, 2017 at 4:30 pm
Email to pbermel@purdue.edu
Please provide the Quantum Espresso inputs for pw.x
(as discussed in lecture).

1. Consider crystalline germanium as shown in the figure below. Your analysis can be performed using Quantum ESPRESSO (QE), available via `https://nanohub.org/tools/dftqe`.

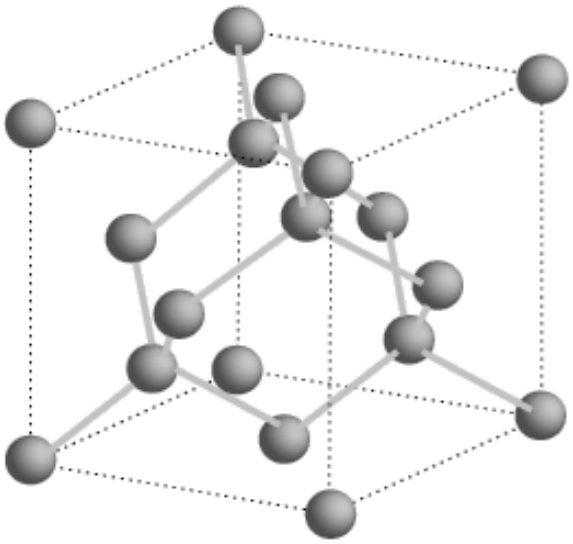

Figure 1: Diamond lattice structure for crystalline germanium. While the geometry is similar to crystalline silicon, the lattice constant is different.

1a. Using the QE GUI, use the 'cell relax' simulation to determine the lattice constant of the germanium lattice (in angstroms). Please note the most important assumptions made in performing your calculation. Please provide the resulting input file to pw.x for SCF calculations, as generated by the tool.

1b. How close is this result to the literature value of the germanium lattice constant? How close is this value to the literature value of the silicon lattice constant, and what does this imply about the growth of germanium on silicon?

2. In this problem, we will consider two different structures of molybdenum disulfide (MoS_2),as depicted below.

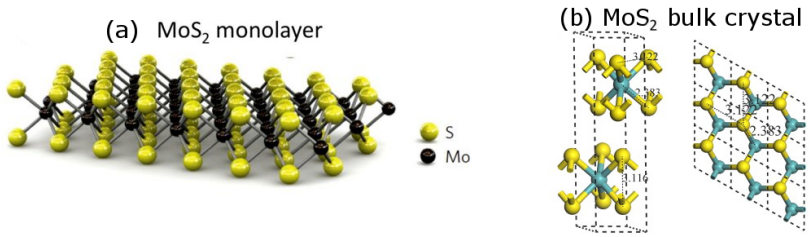

Figure 2: (a) Structure of MoS_2 monolayer; (b) Structure of MoS_2 bulk crystal.

2a. Using the QE GUI, plot the band structure and density of states for a monolayer of MoS_2, as depicted in Fig. 2(a). Please provide the resulting input files to pw.x for SCF calculations, as generated by the tool.

2b. Plot the band structure and density of states for bulk MoS_2, as depicted in Fig. 2(b). **Hint:** the bulk crystal has 6 atoms in the unit cell, and the Mo and S atoms are swapped in their lateral positions between adjacent layers. Please provide the resulting input files to pw.x for SCF calculations, as generated by the tool.

2c. What is the change in both the band gap value and band gap type in going from a bulk to a monolayer structure? How could this be observed in an experiment?