1. **Familiarizing yourself with Quantum Espresso (QE)**

Units in QE:

1 bohr = 0.529177249 Å

1 Rydberg (R) = 13.6056981 eV

1 eV = 1.60217733 x 10-19 Joules

We will use QE to perform DFT simulations and review concepts from Weeks 1 and 2.

Open terminal and do

conda activate qe

Create a directory anywhere you prefer and name it mae6260\_lab2. Within this directory, create another directory named simple\_scf. From Canvas, download simple\_scf.in into this directory.

In this first exercise, we will determine the energy of a primitive Si system of two atoms in a face-centered cubic lattice (this will be explained subsequently). We will execute a self-consistent field (scf) calculation without geometry optimization, i.e., all atoms are fixed in their initial positions.

1. Let’s analyze the input script, simple\_scf.in, what do you observe?
2. Where do we obtain the pseudopotential in the &control name list? (<https://www.quantum-espresso.org/pseudopotentials>)
3. What is going on in the &system name list? We can look at this in Ubuntu using the software XCrySDen:

xcrysden –-pwi simple\_scf.in

Display > Primitive cell mode

1. Run QE:

cd wherever\_your\_directory\_is/mae6260\_lab2/simple\_scf/

pw.x -in simple\_scf.in > simple\_scf.out

1. Let’s analyze the output, simple\_scf.out:

awk '/total energy/' simple\_scf.out

What do you observe?

Can you extract the values into a text file? I tried the following:

cat simple\_scf.out | grep -oP '(?<=total energy).\*?(?=Ry)' | awk '{print $2}'

Can you write a Python script to plot these values?

1. **Energy convergence test**

In this second exercise, we run convergence tests to determine the ground-state energy of our system of interest. Ideally, convergence tests must be performed prior to starting any studies of new systems due to the variational nature of DFT calculations.

Create a directory in mae6260\_lab2 named energy\_convergence. From Canvas, download batch.sh into this directory.

1. To execute the script, do:

cd /content/mae6260\_lab2/energy\_convergence/

chmod +x batch.sh

./batch.sh

Did you run into any errors?

1. While that is running, let’s analyze the script, batch.sh, what can you infer?
2. Can you create scripts for extracting all final energies and plot this data?
3. **Vacancy formation energy**

In the third exercise, we will synthesize everything that we have touched on so far to calculate the vacancy formation energy in silicon.

* 1. So far, we have been using the minimal number of atoms required to minimize computational costs, using two Si atoms in a primitive cell. To introduce a single vacancy defect in a bigger cell (supercell), we need to use a conventional, cubic simulation box.

Create a directory in mae6260\_lab2 named vacancy. Copy the simple\_scf.in script into this directory, rename it as perfect\_crystal.in and open it using xcrysden. Go to Display > Unit of Repetition > Translational asymmetric unit. Then, save it using File > Save XSF Structure.

Open the saved .xsf file, what can you observe?

Copy and paste the conventional cell coordinates into perfect\_crystal.in and change the atomic number 14 to Si. Change the ATOMIC\_POSITIONS card to angstroms.

As we are now using conventional coordinates, we need to include a card called CELL\_PARAMETERS. Where can we get this information and what units should we specify?

What other parameters do we need to modify?

Run the simulation and extract the total energy for this system.

* 1. Now that we have the total energy of a perfect Si crystal, let’s introduce single vacancy defect. Copy perfect\_crystal.in and rename it as single\_vacancy.in.

How can we introduce a single vacancy? What parameters need to be changed?

Visualize your new input file, does everything make sense?

Run the simulation and extract the total energy for this system.

* 1. To get an accurate ground-state energy, we will need to “relax” the system. Copy single\_vacancy.in and rename it as single\_vacancy\_relax.in. Change the following name lists:

&control

calculation = 'relax'.

…

&electrons

conv\_thr = 1.0d-8

…

&ions

ion\_dynamics = 'bfgs'

Run the simulation and extract the total energy for this system.

Visualize the output. What can you observe?

1. Let’s calculate the vacancy formation energy using a simple approximation:

Compare your values with literature values (<https://doi.org/10.1103/PhysRevLett.108.066404>). What can you observe and how do you explain these observations?

**REMEMBER TO BACKUP EVERYTHING YOU NEED!**