NANO266 Lab 4 - Al surfaces

Author

May 11, 2015

1 Introduction

In this lab, we will look surface calculations with PWSCF.

2 Initial setup

By this stage, you should already have everything set up. Make sure you are in the lab4 folder by doing:

cd <path/to/repo>/labs/lab4

3 Running calculations

You will still be running the calculations using the queues on Comet. However, it is important to note that surface calculations can take much longer than bulk calculations. It is therefore imperative that you perform these calculations prudently. It is very easy to burn through all the allocated CPU time if you are not careful.

4 Q1 (20 points): The (100) surface of Al

We will first start by calculating the energy of the (100) surface in Al. You need to perform a convergence with respect to both slab and vaAlum size. Use an energy cutoff of 50 Ry with a k-point grid of $8 \times 8 \times 1$.

1. Start by first finding the equilibrium structure of fcc Al. You have already done this in lab 3, but we are going to do this again using the SCF method, i.e., by plotting the equation of state of energy versus the lattice parameter. Converge your lattice parameter to within 0.001 angstroms. For reference, the experimental lattice parameter is 4.05 angstroms. A template file `Al.fcc.pw.in.template` has already been provided. Please use the `scf.py` script to perform these calculations. As usual, please scan with a fairly coarse grid (e.g., 0.01 increments) before performing scans with a more dense grid near the minimum energy.

2. Using the lattice parameter you obtained in part 1, perform a calculation of the Al (100) surface. A sample `Al100.pw.in.template` file has been provided to you, as well as a `fcc_surface_generator.py`. Let's see what the input file does by typing:

   ```
   python fcc_surface_generator.py --a 6.92 --nslab 3 --nvac 3
   ```

The output should be something like the following:

```
 &CONTROL
  calculation = 'relax' ,
  outdir = './tmp' ,
  prefix = 'Al_100',
  pseudo_dir = './' ,
  tprnfor = .True.,
  tstress = .True.,
 /
 &SYSTEM
  ibrav = 6,
  celldm(1) = 6.92,
  celldm(3) = 6,
  nat = 12,
  ntyp = 1,
  ecutwfc = 50,
  ecutrho = 250,
  occupations = 'smearing',
  smearing = 'cold',
  degauss = 0.025,
 /
 &ELECTRONS
  diagonalization = 'david',
  conv_thr = 1.D-6,
  mixing_beta = 0.7,
 /
 &IONS
  ion_dynamics = 'bfgs',
 /
ATOMIC_SPECIES
  Al   26.98  Al.pbe-n-kjpaw_psl.0.1.UPF
ATOMIC_POSITIONS crystal
  Al 0.0 0.0 0.0
  Al 0.5 0.5 0.0
  Al 0.5 0.0 0.0833333333333
  Al 0.0 0.5 0.0833333333333
  Al 0.0 0.0 0.166666666667 0 0 0
  Al 0.5 0.5 0.166666666667 0 0 0
```

```
  Al 0.5 0.0 0.25 0 0 0
  Al 0.0 0.5 0.25 0 0 0
  Al 0.0 0.0 0.333333333333
  Al 0.5 0.5 0.333333333333
  Al 0.5 0.0 0.416666666667
  Al 0.0 0.5 0.416666666667
K_POINTS automatic
  8 8 1   0 0 0
```

There are several important things to note about this input file:

- The `calculation` parameter has been set to `relax`. This allows the atoms to move, but fixes the cell shape.
- The `ibrav` tag has been set to 6, which is a tetragonal cell. To perform a surface calculation, we are extending the cell in the c-direction and removing atoms. So we are breaking symmetry in that direction.
- The `celldm(3)` parameter is set to 6. This means that we have constructed a supercell where the c lattice parameter is 6 $\times$ that in the a and b directions.
- In the ATOMIC_POSITIONS section, note the c fractional coordinate of each atom. The conventional fcc cell has four atoms. Look at how each group of four atoms are related to each other by a translation in the c direction. It is absolutely critical that you understand that the c fractional coordinate depends on **both your slab size as well as your vacuum size**! Also, we have fixed all atoms except for the top and bottom two atomic layers (denoted by the `0 0 0` after the coordinates.

5 Q2: The (111) surface of Al

6 Q3: Adsorption of H on Al