ASE tutorial

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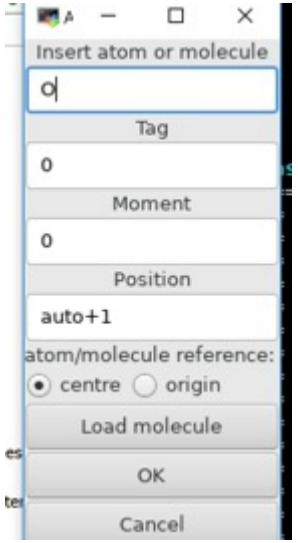
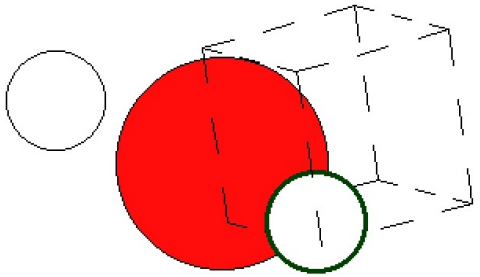
How to make molecules visually

Close your MobaXterm connection and open a new connection to scholar, this will make sure you have the default ase-gui which is faster than the GPAW version

Type “ase-gui” into the command window when you are inside the che697_tutorial folder, you will get a new window
At the top hit “Edit” and then “Add Atoms” the shortcut for this is ctrl+A (super useful to know). In this window type “O” to make an oxygen atom and press “OK”
You should see an oxygen atom. You can move it by clicking it and pressing ctrl+M (move). For now, add 2 more hydrogens using the same method, and move them so it looks like water. It doesn’t have to be perfect, DFT will fix it for us (a very bad guess may give you errors though, if the code thinks your system is O(g) + H2(g) instead of H2O(g)





Here’s mine, its ok I guess.
But the dashed box (our periodic boundary conditions) are too small, let’s fix that

How to make molecules visually

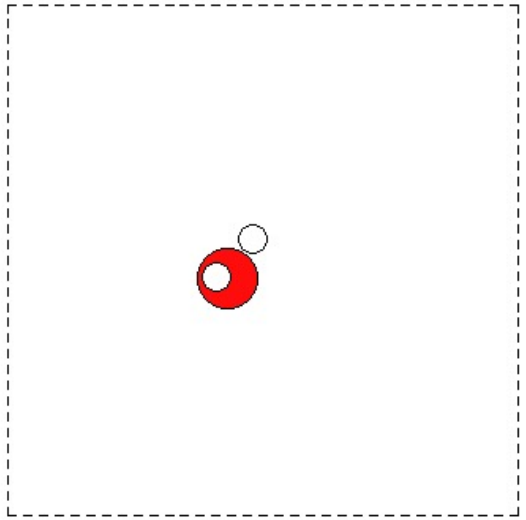
Press ctrl+S to enter the save screen. Name your molecule “H2O.POSCAR” the .POSCAR is the file type we will use and hit save

You can now exit out of ase-gui and go back to the terminal. If you “ls” you should see the H2O.POSCAR file in the folder, open it with nano or vi.

The file format is very straightforward. Line 1 is the types of atoms in our system, line 3-5 is the unit cell (in this case it’s a cube that’s 1 A in each direction) line 6 says there’s 1 oxygen and 2 hydrogens. Line 7 specifies that the coordinates are Cartesian and not in reduced lattice coordinates, and then lines 8-10 are the xyz coordinates of our atoms. Change the unit cell so that it’s 10 A on each side. Make sure to save the file!

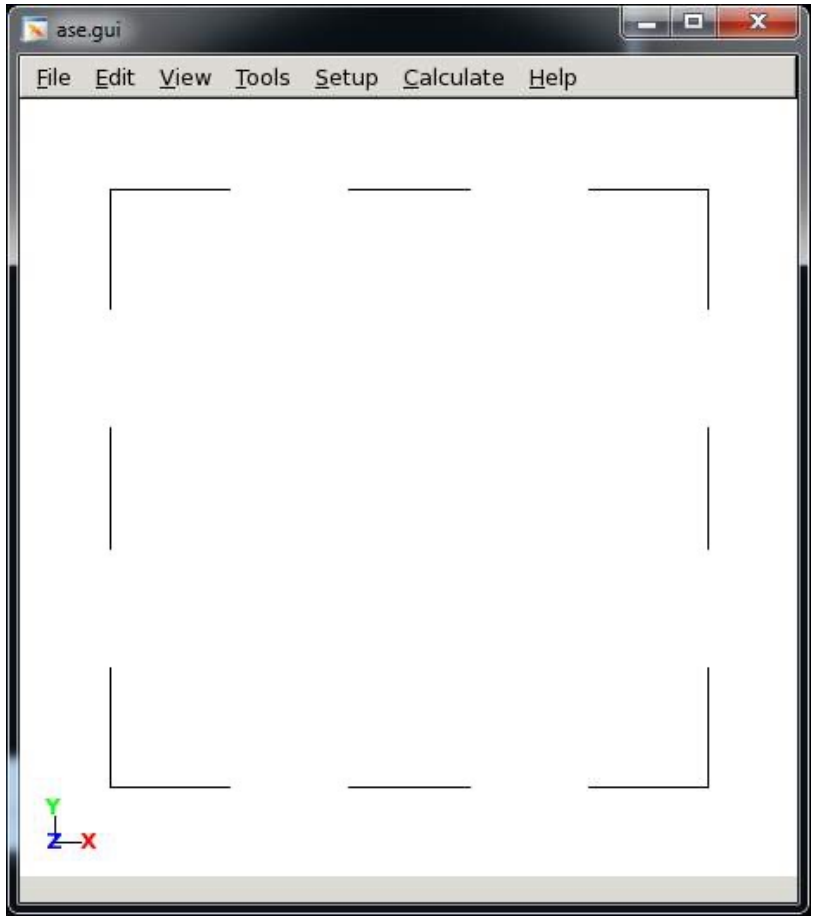
```
O  H
 1.0000000000000000
     1.0000000000000000    0.0000000000000000    0.0000000000000000
     0.0000000000000000    1.0000000000000000    0.0000000000000000
     0.0000000000000000    0.0000000000000000    1.0000000000000000
   1   2
Cartesian
 -0.0589456038420923  0.3143765538244921  0.9474665156052362
 -0.4311766911404283  0.8214392597543443  1.7248540829767469
  0.9207716398387578  0.1144753833073797  0.9613821348974676
```

Open H2O.POSCAR using ase-gui to visualize it by typing “ase-gui H2O.POSCAR” and you should have a bigger box. Select all the atoms, move them to the center of the box (using expert mode), and re-save H2O.POSCAR. (Did we really need to drag the molecule?)

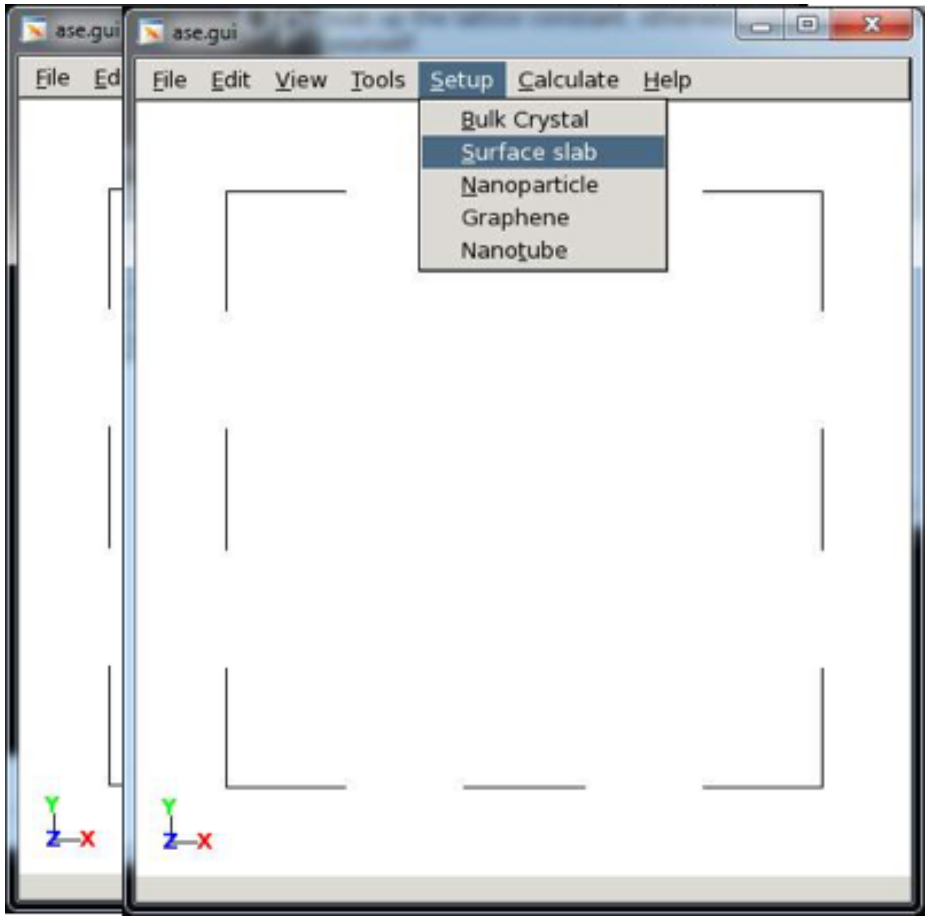


It should look like this now.

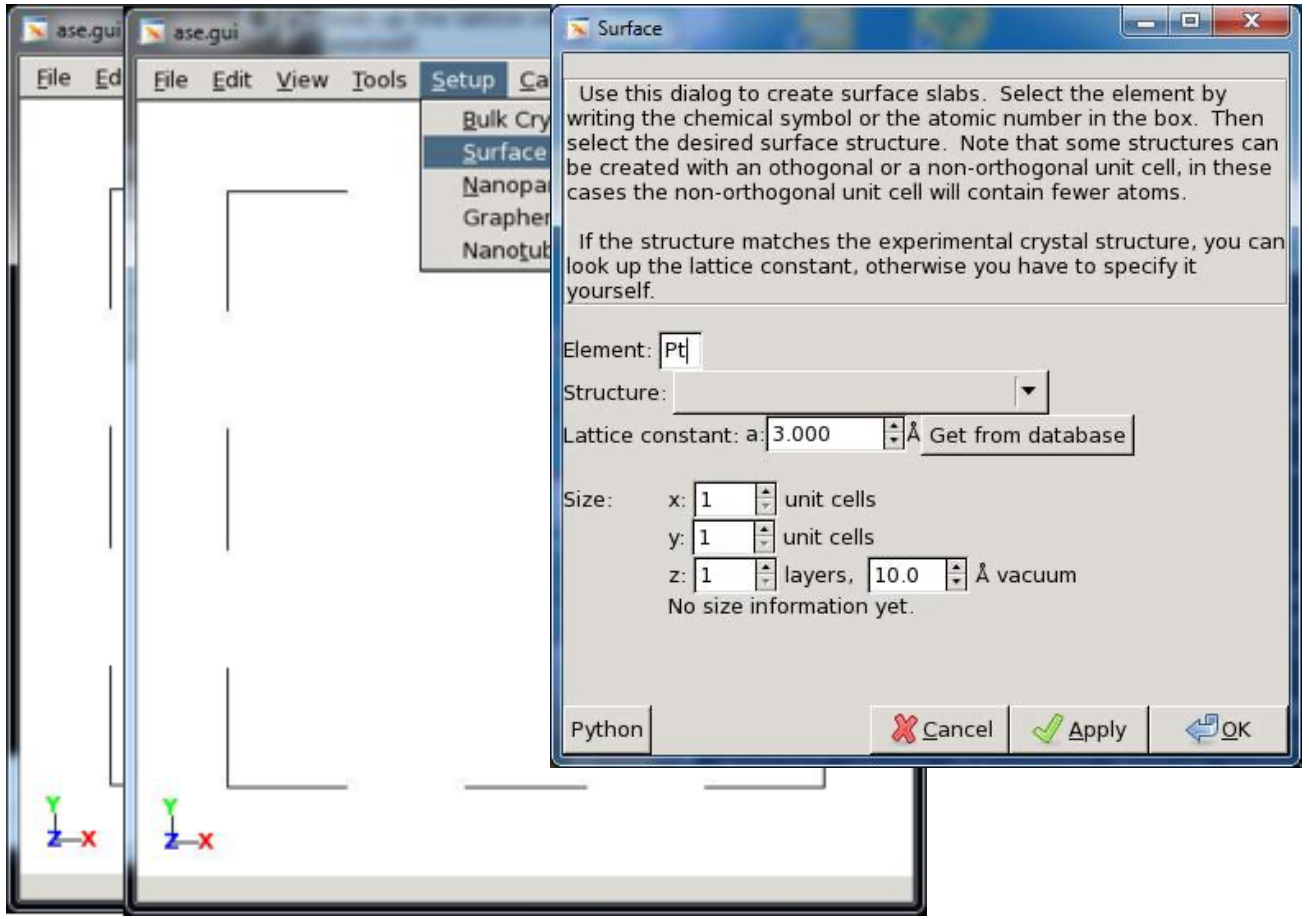
Building atomic model



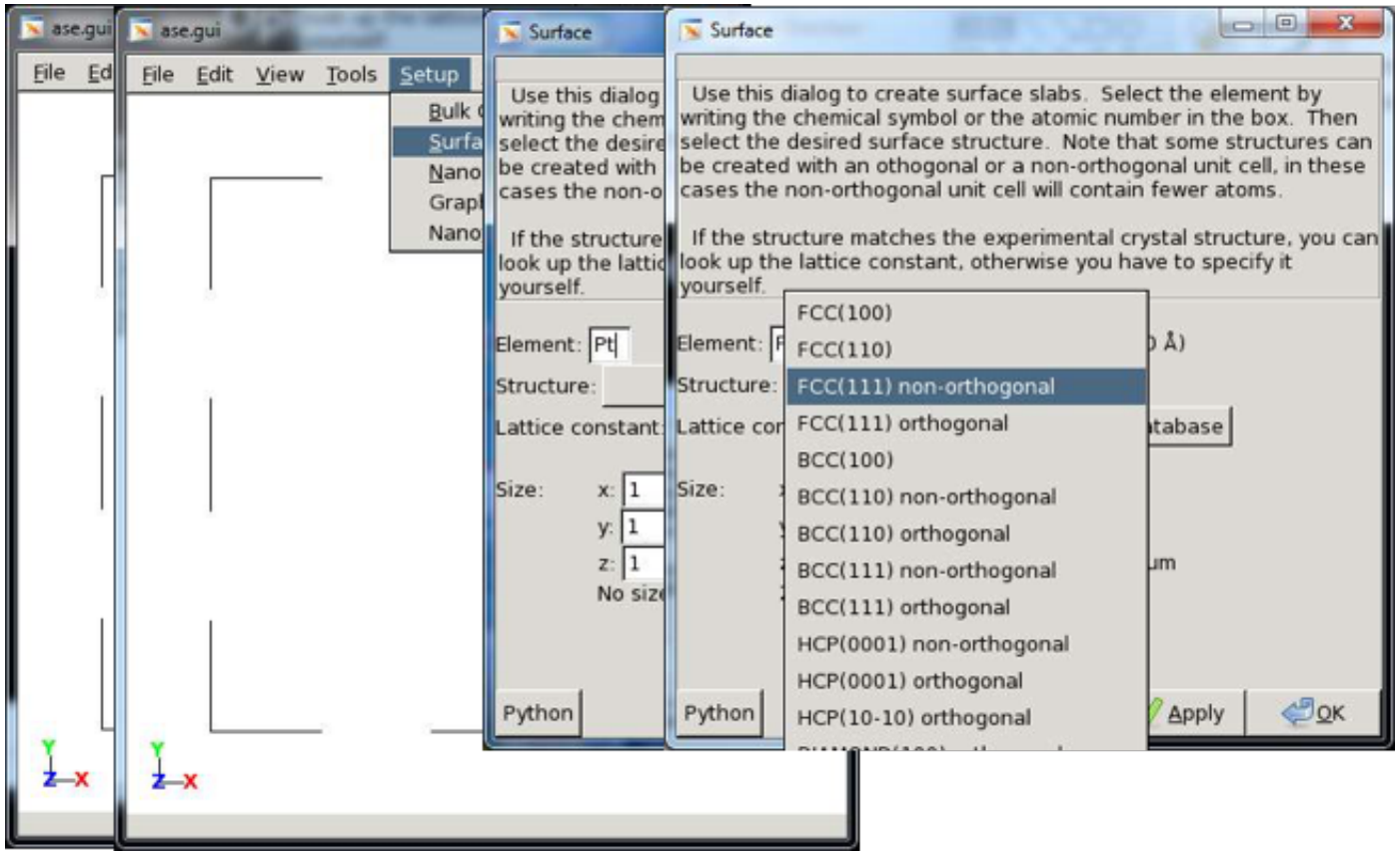
Building atomic model



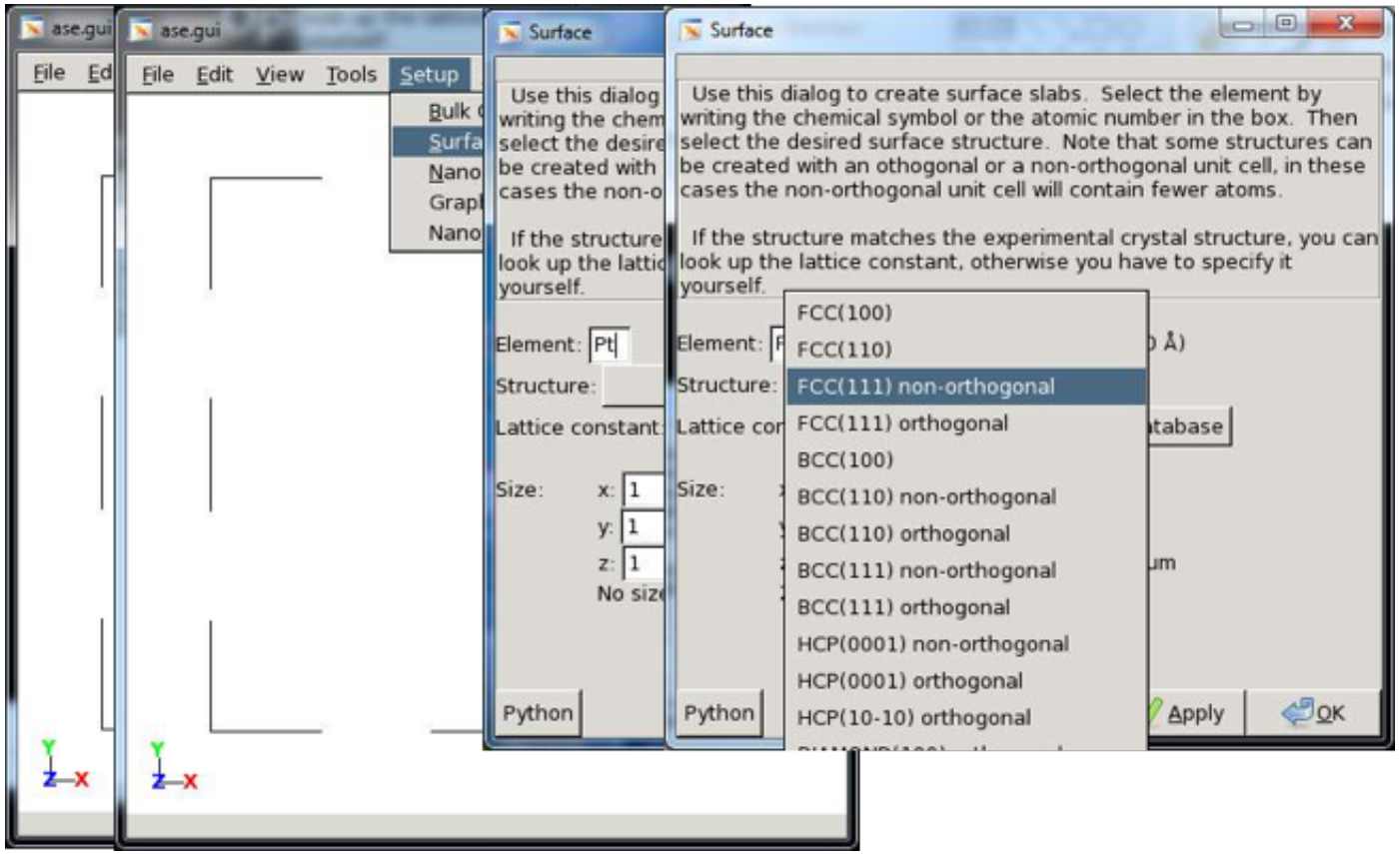
Building atomic model



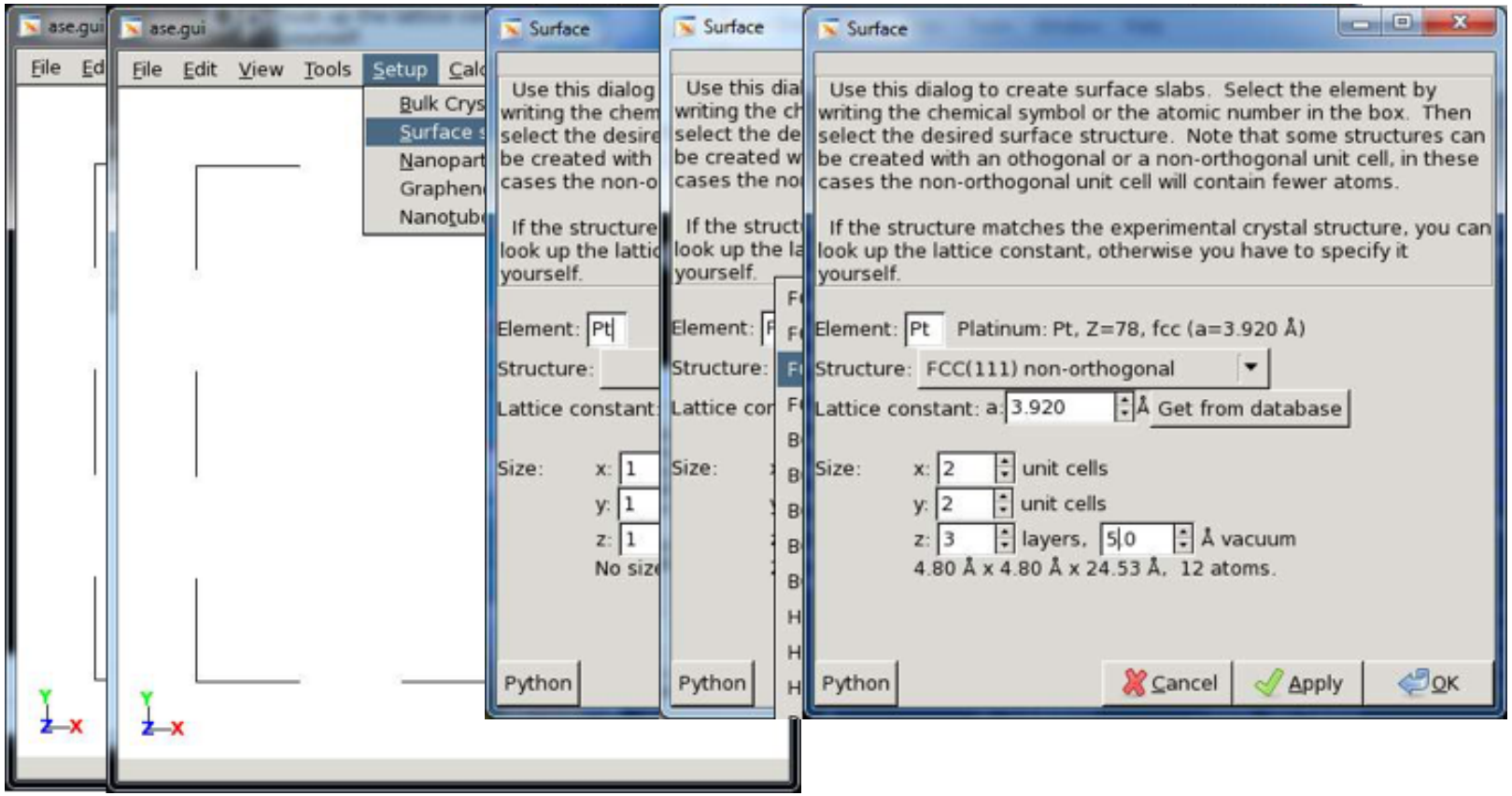
Building atomic model



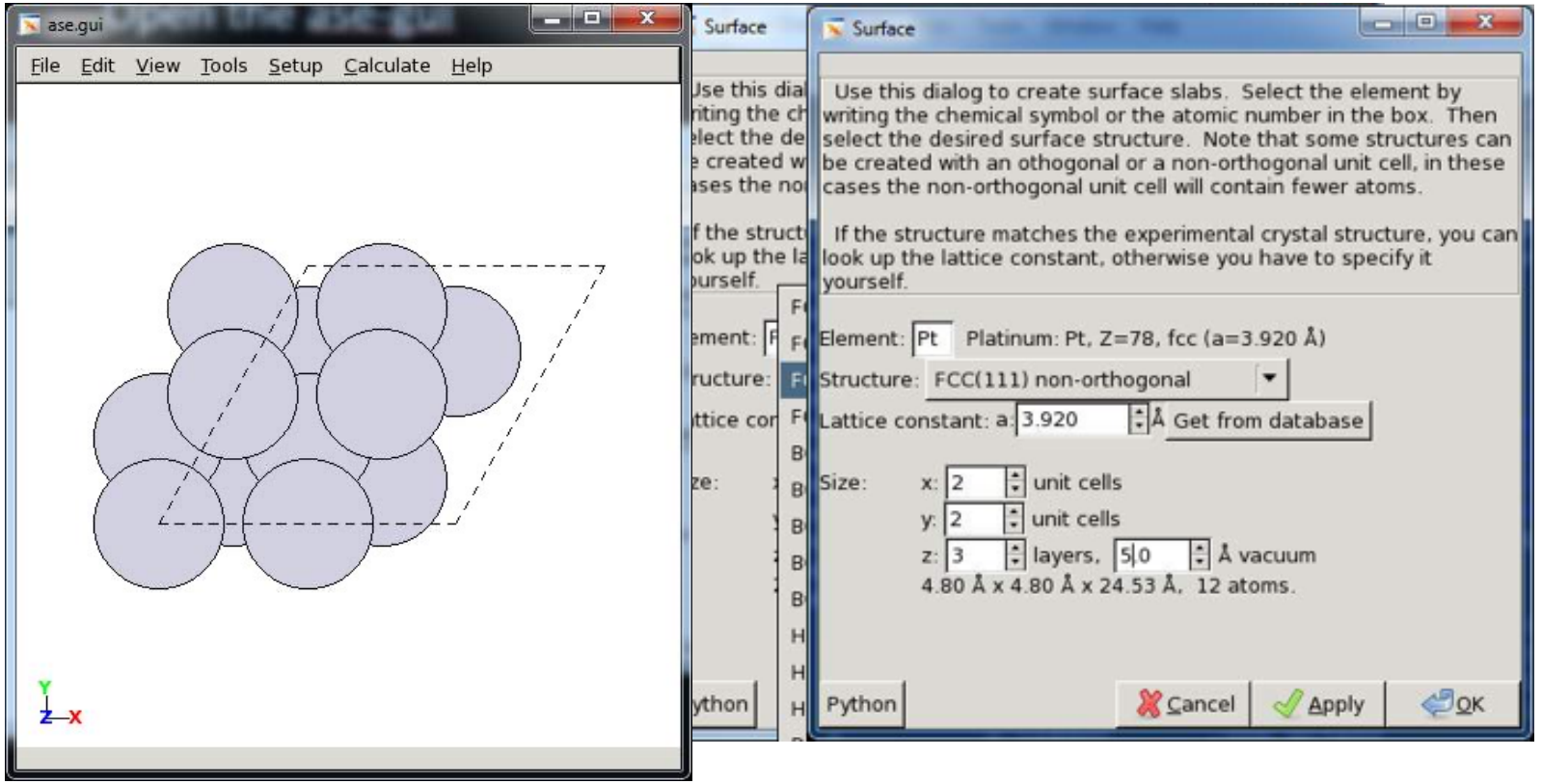
Building atomic model



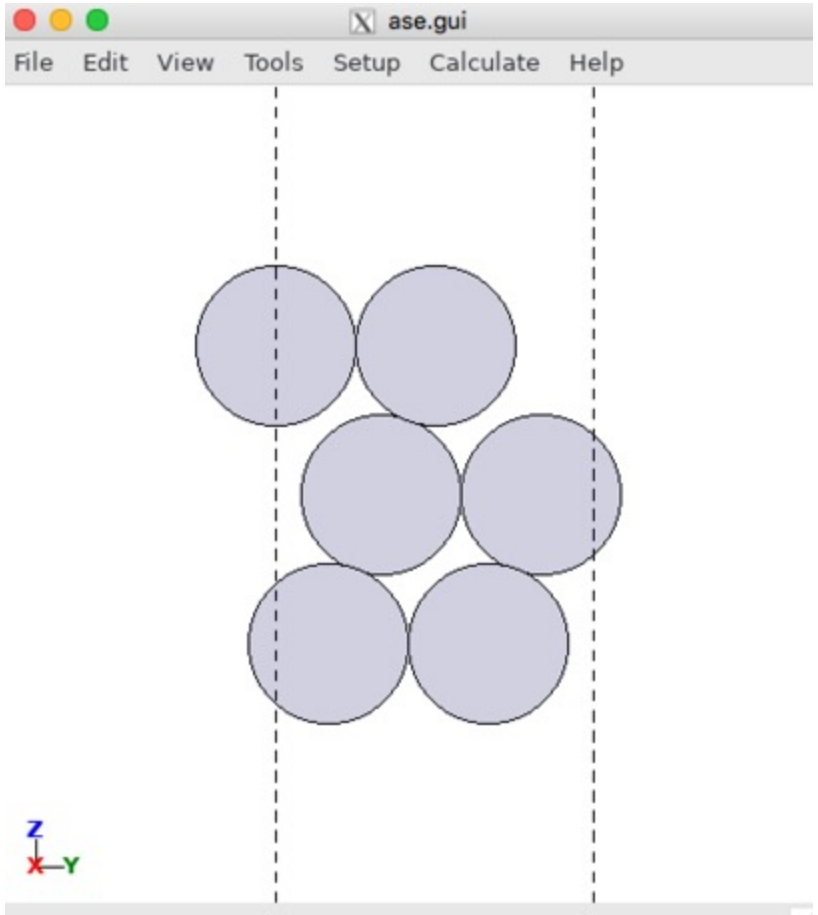
Building atomic model

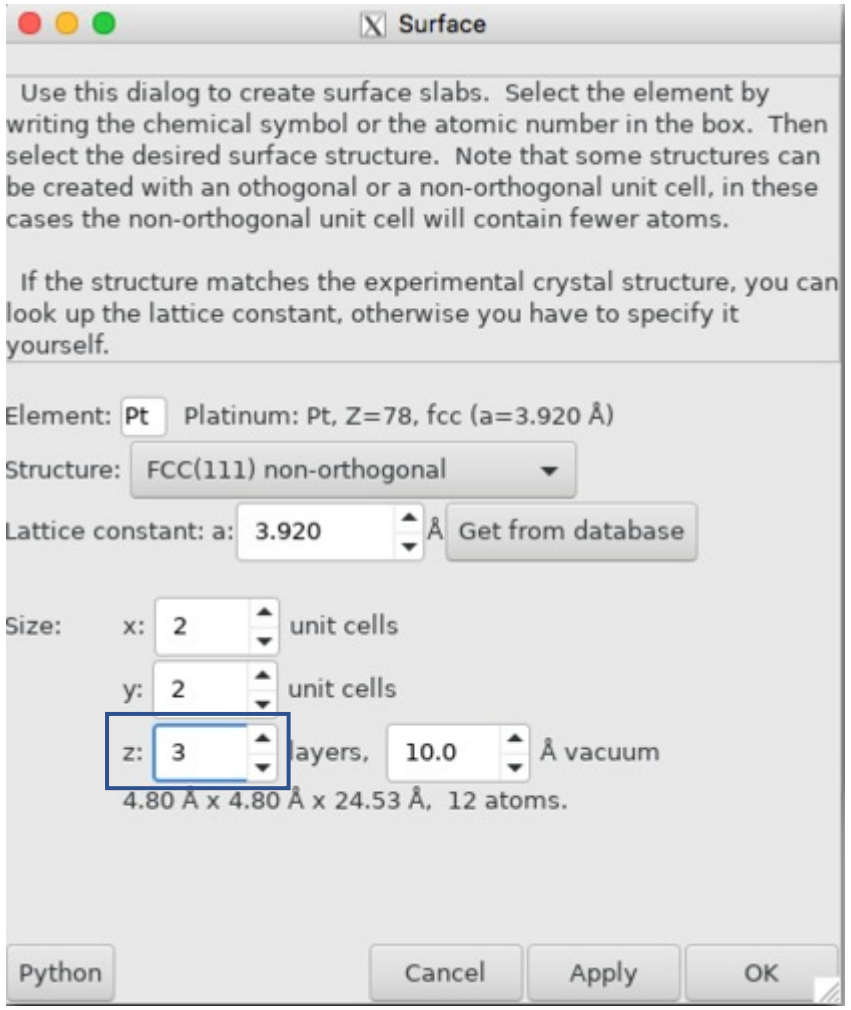


Building atomic model

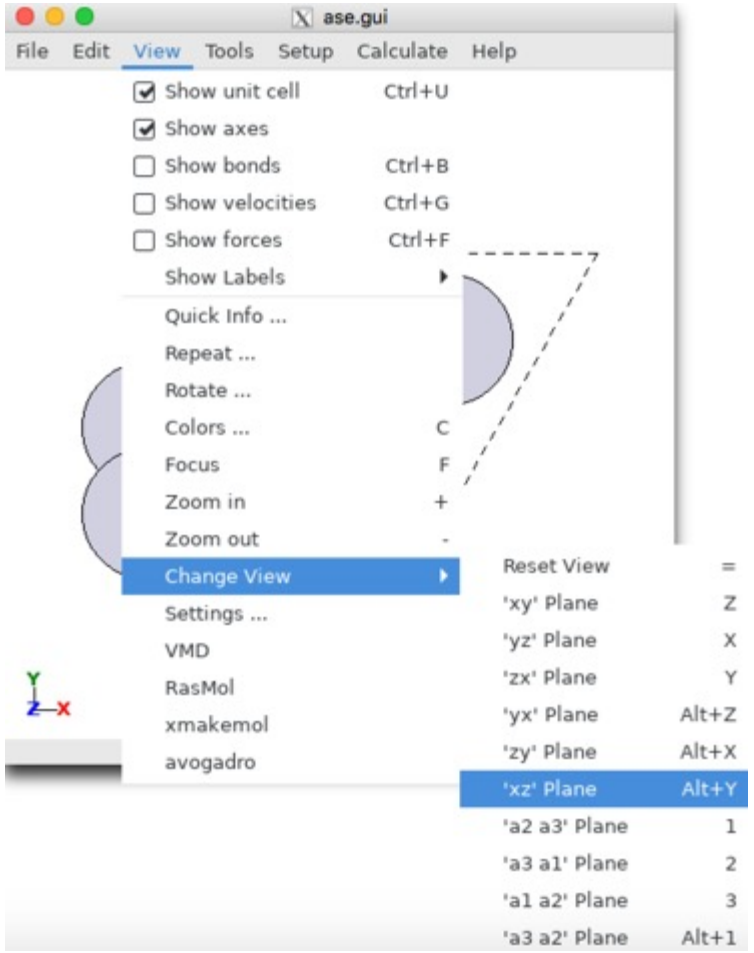


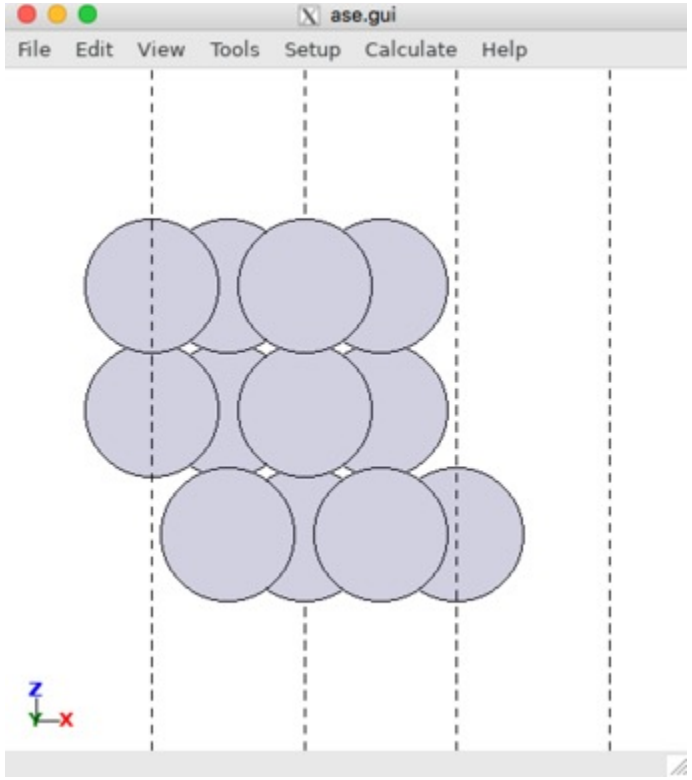
Building atomic model: Pt(111)





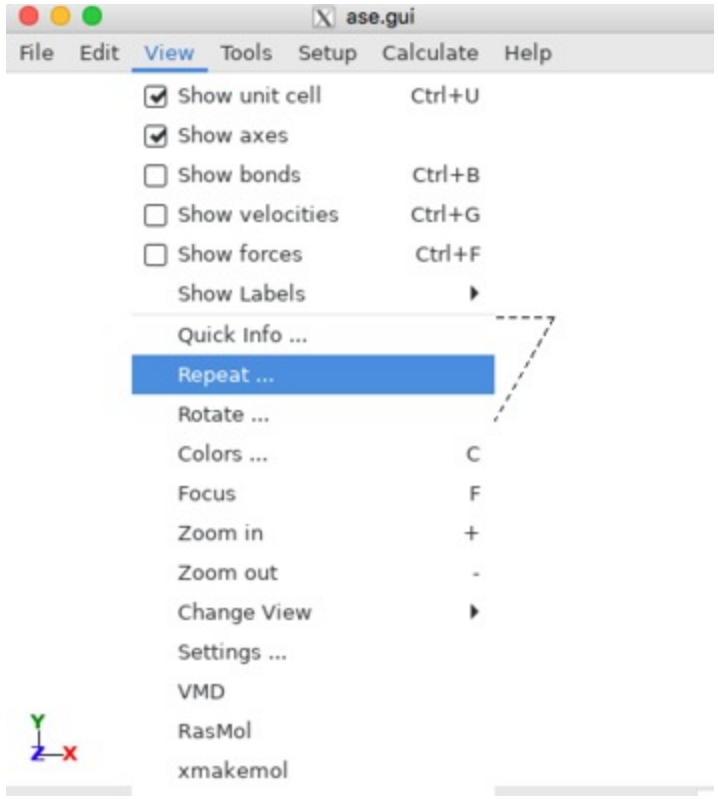
Changing the views

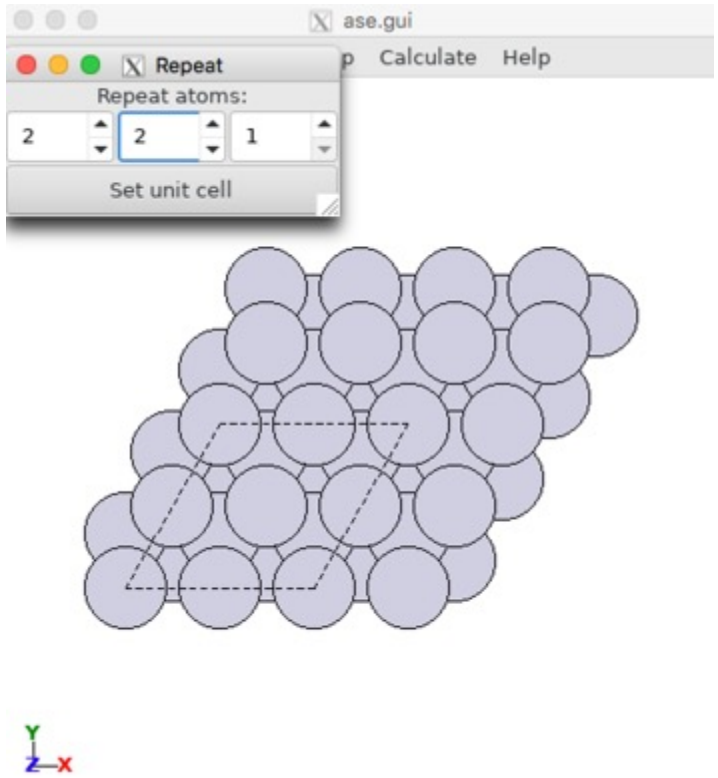




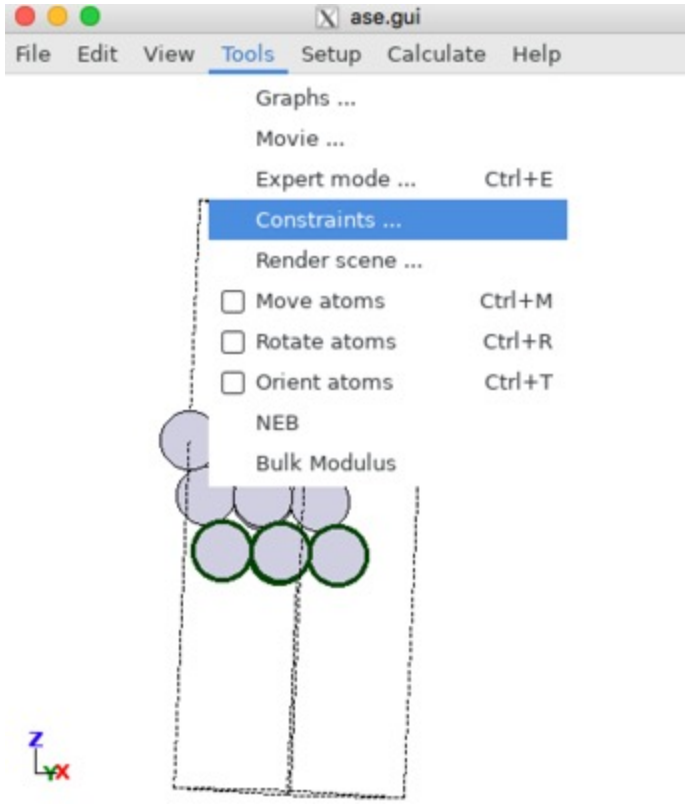
Periodic Boundary Conditions (Repeat)

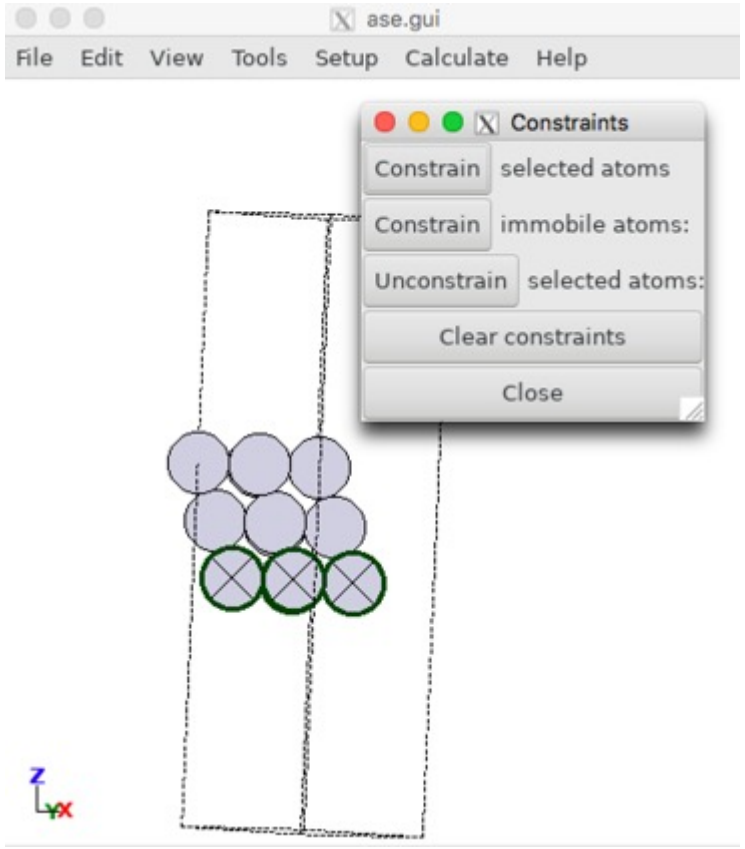
Repeat in x and y directions (“F” recenter)



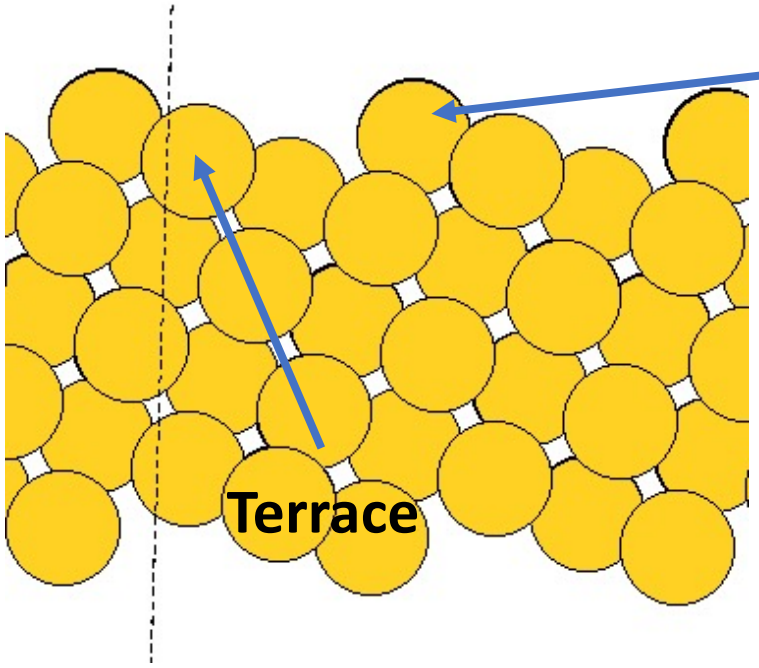


Constraining the bottom layers

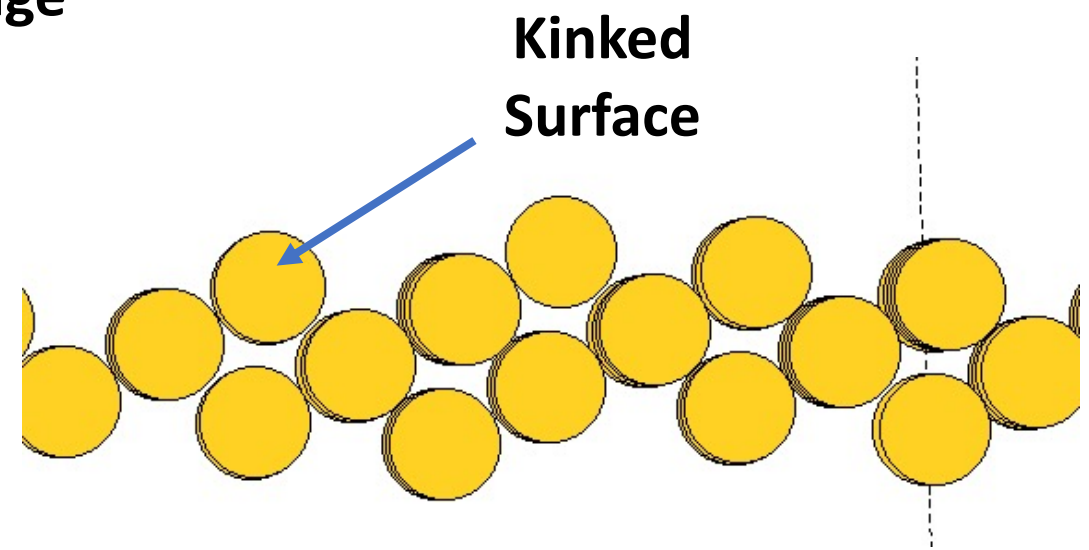




Modelling steps and kinks on a nanoparticle



Au (310) surface



Au (551) surface

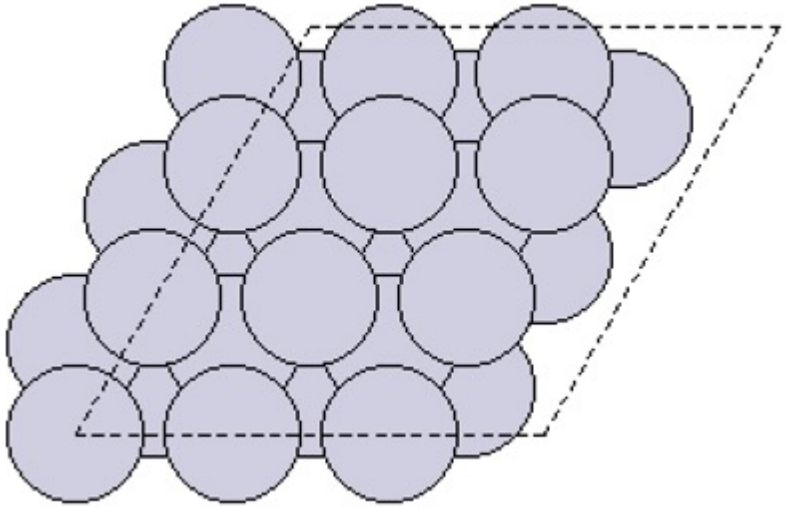
Making surfaces from converged bulk

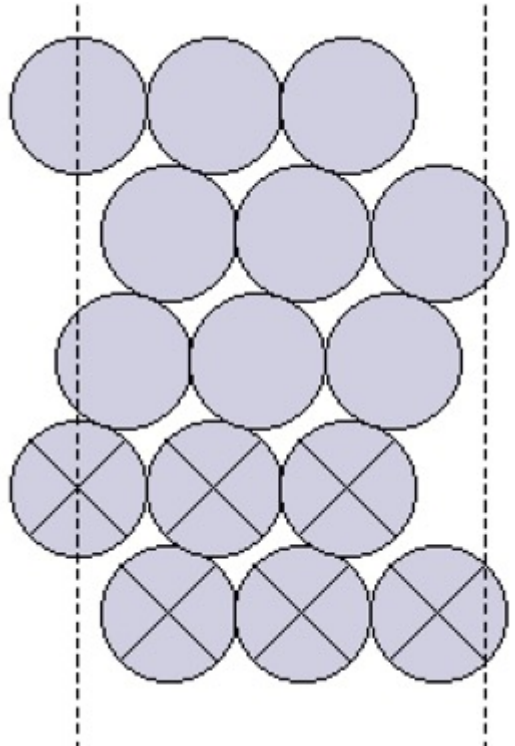
cp /depot/jgreeley/data/class_GPAW/2020/tutorial_4/make_surface.py .
python make_surface.py

```
from ase.build import bulk
from ase.parallel import paropen as open
from gpaw import GPAW, PW, FermiDirac
from ase.io import read, write
from ase.build import *
from ase.optimize import QuasiNewton
from ase.visualize import view
##### choose your input. Make sure only one is selected ###
bulk=read("POSCAR_bulk",format="vasp") #reading the bulk POSCAR file
input_atoms=surface(bulk,(1,0,1),5) #(a,b,c): Miller indices of the surface; l: number of layers
input_atoms.center(vacuum=10, axis=2) #centering the unit cell

view(input_atoms)

write("POSCAR_surface",input_atoms,format='vasp')
~
```

Adsorption on metal surfaces

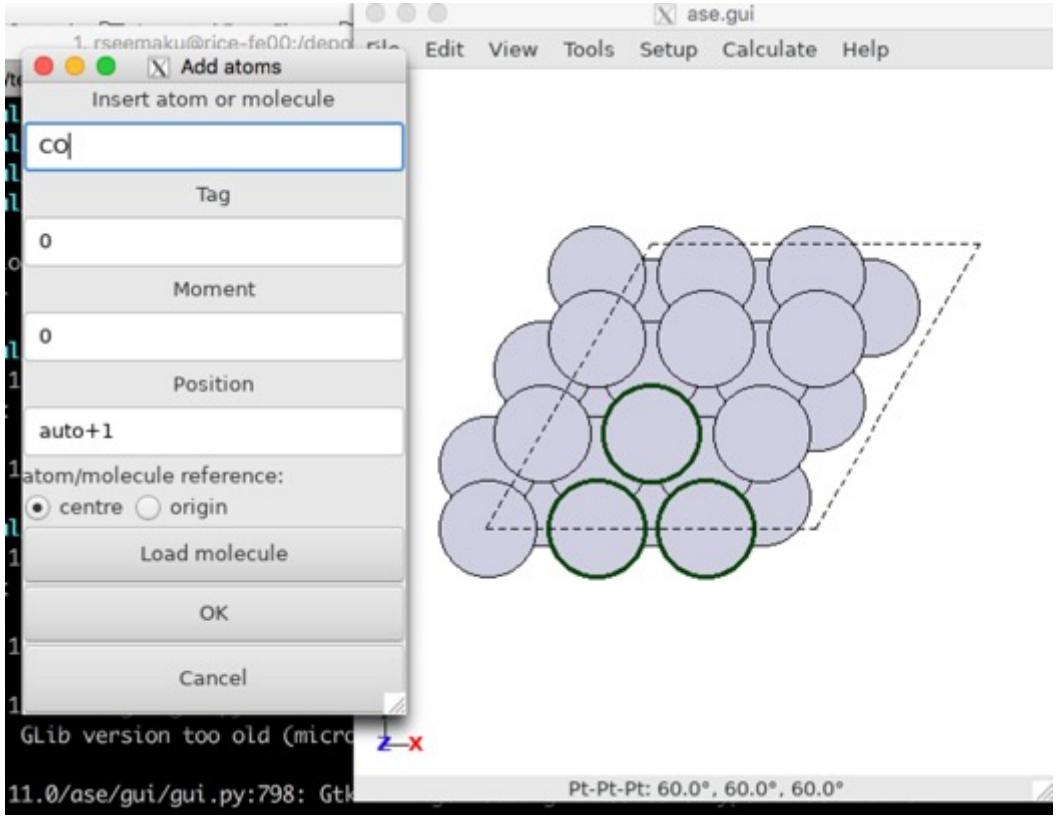
- Make a Pt(111) 3*3*5 surface
- Constrain the bottom layers
- Identify the unique sites (how many are there?)
- Need to do adsorption calculations on all the sites to find the most stable site





Adding adsorbate

- Select the atoms on which to add adsorbate on
- Use add atoms from edit menu
- Type the adsorbate formula
- Does CO bind through C or O on Pt?



Adding adsorbate

- Need chemical intuition to generate initial adsorbate configurations
  - Which atom bonds to the surface
  - How close can the adsorbate be to the surface