Nanoparticle Simulation Help Sheet

How to rotate and examine nanoparticles in the GUI

If the size.py had been specified through the terminal to be the size of 500 atoms, then Figure 1 is the default view that would be seen.

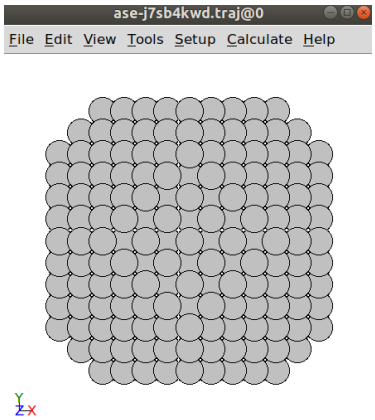

Figure 1: An example nanoparticle for the size.py script when set to 500 atoms in size.

1. Right click and drag the structure for a range of different views, such as Figure 2.

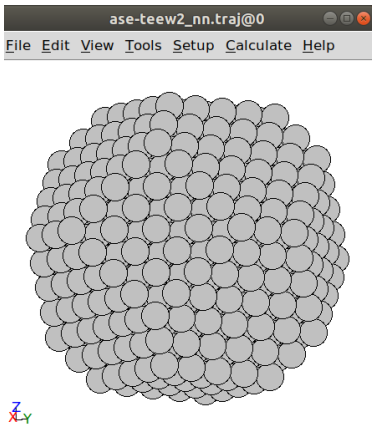

Figure 2: An example nanoparticle for the size.py script if the size was set to 500 atoms and rotated.

2. To view the nanoparticle from one of the axes, one of the keys X, Y or Z can be pushed to give the viewpoint from that axis.
3. After you are finished viewing this nanoparticle it can simply be exited.

To be noted is the X, Y and Z axes in the bottom left hand corner. These can be helpful if an orientation is reached that is confusing and want to reorient the structure with an axis.

How to measure a distance between atoms (diameter)

1. An outermost atom can be left clicked and an opposite atom can be selected by holding down 'ctrl' and left clicking.
2. An estimate of a nanoparticles size can be taken as shown in Figure 3 in the units of **Å** which is equivalent to $\mathbf{10^{-10}}$ **m**.

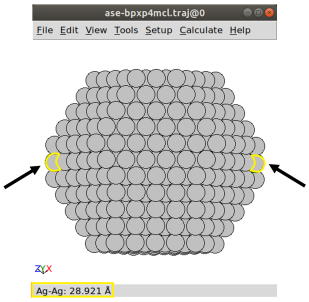

Figure 3: An example nanoparticle for the size.py script if the size was set to 500 atoms and rotated.

Note: This atom distance will change depending on what two atoms are selected on the outside of the nanoparticle.

How to measure the number of atoms in a nanoparticle

In order to find the amount of atoms in a nanoparticle, by clicking edit and select all. This will count the amount of atoms within the nanoparticle as shown in Figure 4. Alternatively one could drag a box over the whole structure - similar to how one might take a screenshot, which will also allow all atoms to be selected. Below is the size.py script when it has been specified to be 500 atoms in size. However, the script builds a model which is 711 atoms in size. This is because the script is programmed to make full shells around the atom and will be rounded up (in this script) accordingly.

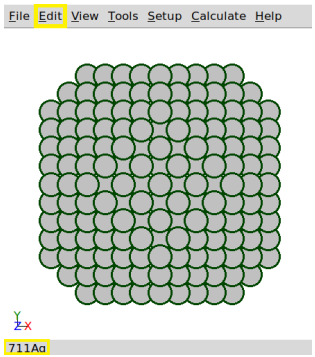

Figure 4: An example atom count for the size.py nanoparticle that was specified to 500 atoms.

The yellow box indicates the amount of a certain element (Ag - silver in this case) in the nanoparticle.

How to edit scripts

The python scripts can be modified by a text editor, in this case an editor called Sublime will be used. Sublime is an external editor which can be navigated via a mouse and keyboard.
To use Sublime, subl will preface the name of the script to edit, which includes comments to guide students use of the scripts. A complete example of this is shown in Figure 5.

1. Type "subl" followed by the name of the script to be edited.
2. Once the text editor has opened, a script should be seen. Any changes made must be followed by pressing 'ctrl s' and exited by the 'x' indicated by the yellow circle. If the script was not correctly saved you will be prompted to do so.

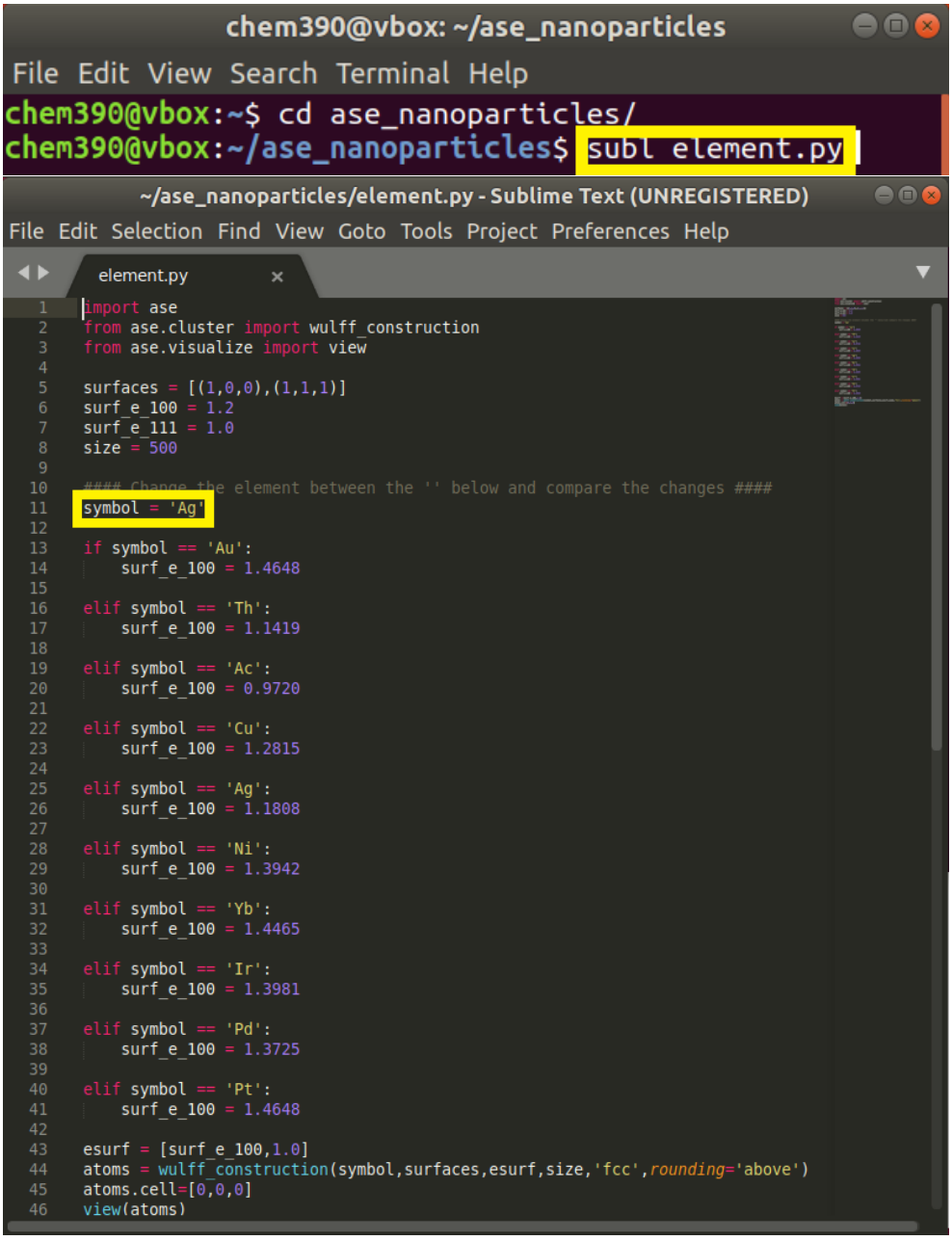

Figure 5: Visual instructions in order to view and edit python scripts.

After the python scripts have been examined and edited they are ready to be run. This is done by typing "python" followed by the script name. This is demonstrated in Figure 6.

1. Type "python" followed by the name of the desired script to be run.

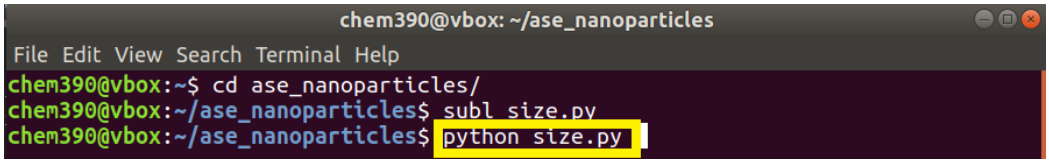

Figure 6: Visual example instructions to run a python script.

What to do when a 'mini movie' is run

When a script such as octa_multiple_colour.py is executed a mini movie is produced and the first appearance is that shown in Figure 7.

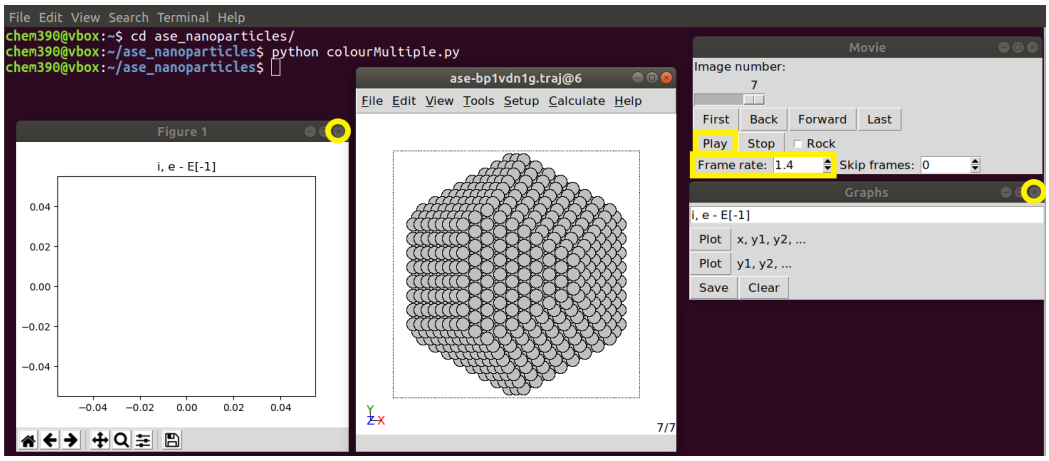

Figure 7: The outputs of a typical 'mini movie'.

As shown by the yellow circles, there are pop ups that can be ignored which appear. The 'Figure 1' and the graphs tabs can be exited, and focus is brought to the nanoparticle and the movie tab. If the play button is pushed, there will be a 'mini movie' played which shows a nanoparticle altering in some way, such as growth. The play rate can also be altered by increasing or decreasing the frame rate, also highlighted with yellow.