

Preliminary Activity for Investigating Atoms and Ions with Computers!

Part I: The Aufbau Principle

The primary objective of this Preliminary Activity is to introduce and familiarize one with the Open-Source Pseudopotential Interface/Unification Module (OPIUM) and Xmgrace. You will use OPIUM to run all-electron calculations and Xmgrace to plot the resulting wavefunctions.

You will use the directions provided in the Hydrogen and Carbon lessons, and will work through them in your groups along with the instructor. The instructor will also assist in working through obtaining data from the created plots and generating new plots in Xmgrace.

The following data must be obtained from the output files: Total energy for each configuration, the orbitals, their filling, and the atomic orbital energies.

For your assigned elements, you will run calculations for to determine the correct electron configuration for the neutral atom. You should have desired test configurations written out prior to getting started. To run multiple configurations using one input file for the same element, you will add the [Configs] keyblock at the bottom of your input file. For example, to do so for carbon, add the following at the end of the input file:

```
[Configs]
2
#
200 2.00 -
210 2.00 -
#
200 1.00 -
210 3.00 -
```

In [Configs], the number 2 tells one how many test configurations are being examined. The # separates the different configurations, and the only orbitals included in the test configurations should be the valence orbitals. In this case, one would be examining how changing the electron configuration affects the valence orbital and total energies. One can test as many test configurations as one desires.

After completing the Preliminary Activity, you will investigate the assigned researchable questions below. Use reference sources to find out more about quantum numbers, wavefunctions and nodes before planning and conducting your investigation.

Questions

1. How are quantum numbers and radial nodes related?
2. Within a particular quantum number, what is the relationship between radial nodes and type of orbital?
3. How can the correct electron configuration be identified?
4. Is the Aufbau Principle obeyed in all circumstances? (Focus on transition metals)

Note:

The plan you submit for instructor approval must include the electron configurations you plan to test for the assigned elements, how you plan on identifying different configurations in your lab notebook and files, the commands you will need to use to operate the software, and a plan to tabulate, plot, and share data with the class.