

1 Morning class week 3 day 4: The Aufbau principle and the different types of atomic electron energies

- Some facts from Chapter 5 of your textbook are presented below. Please spend half an hour examining Chapter 5 of your textbook. It is particularly good to look at the pictures in the textbook. Listed below are some of the facts contained in your book. Please note that even though there are no problems on this page, it is a good idea to read through the page carefully.
 - The energies of the atomic orbitals, for elements H, Li, Na, and K, are shown in the Figure 8-36. In truth, the number of atomic orbitals does not stop with the orbitals shown but actually continues to higher and higher principal quantum numbers of the s , p , d and f type orbitals, eg., $4s$, $5s$, $4p$,... . All atomic orbitals, in a neutral atom, have a negative total energy.

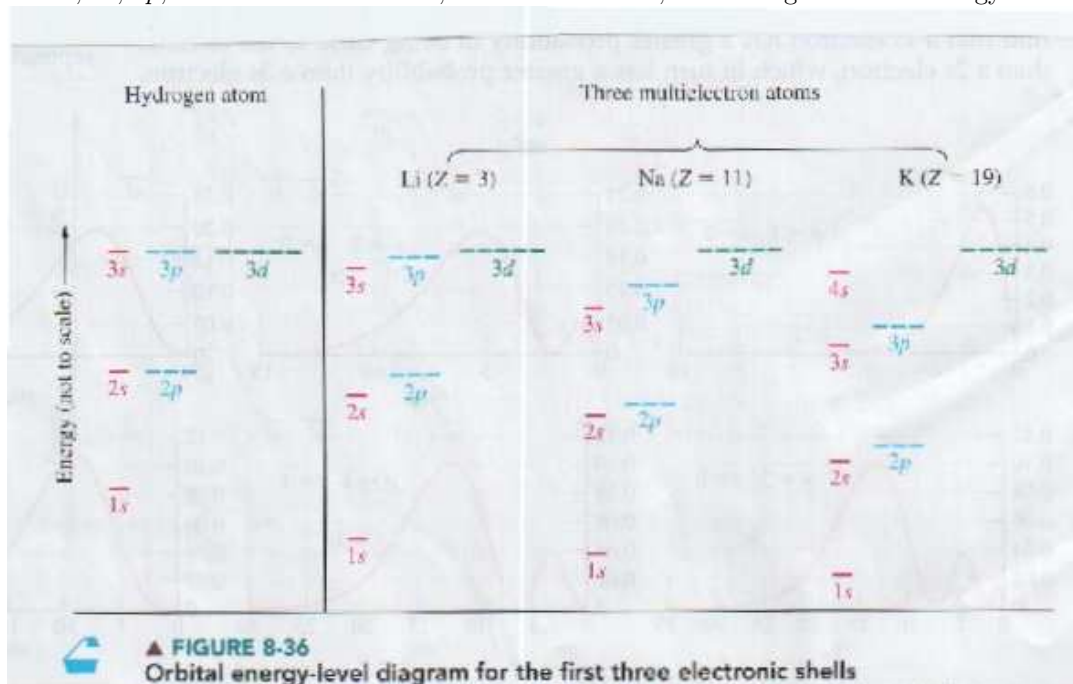


Figure 1: Atomic orbital energies for the first column in the periodic table

- An atomic orbital diagram is a picture like those shown in Figure 8-36 where we represent electrons as \uparrow and \downarrow placed onto the horizontal lines of this diagram. The *Pauli exclusion principle* tells us that at most one \uparrow and \downarrow can be placed onto each horizontal line. The *Aufbau principle* tells us that the most stable arrangement for the electrons is one in which electrons occupy the lowest energy orbitals possible (subject to the restrictions of the Pauli exclusion principle). In this arrangement, the electrons achieve the lowest total energy possible. The lowest possible energy arrangement is the *lowest energy electron configuration*. It is called the *ground state*.
- Hund's rule* tells us that while obeying both the Aufbau principle and the Pauli exclusion principle, in the ground state one places as many electrons with a parallel spin arrangement with one another as is possible. I will elaborate on the meaning of the above sentences in class.
- The information contained in an atomic orbital diagram can also be expressed as an *electron configuration*. In the electron configuration, one states the types of atomic orbitals filled with electrons and appends to each orbital type a superscript which indicates how many electrons fill each orbital group. For example, ground state atomic oxygen, with two $1s$ electrons, two $2s$ electrons and four $2p$ electrons is written: $(1s)^2(2s)^2(2p)^4$.

2. **Kinetic vs. potential energy** We have discussed two types of energy: kinetic, the energy of electron motion; and potential, the electrostatic energy. The following statements are always true for electrons in stable molecules and atoms. As expected from the virial theorem,

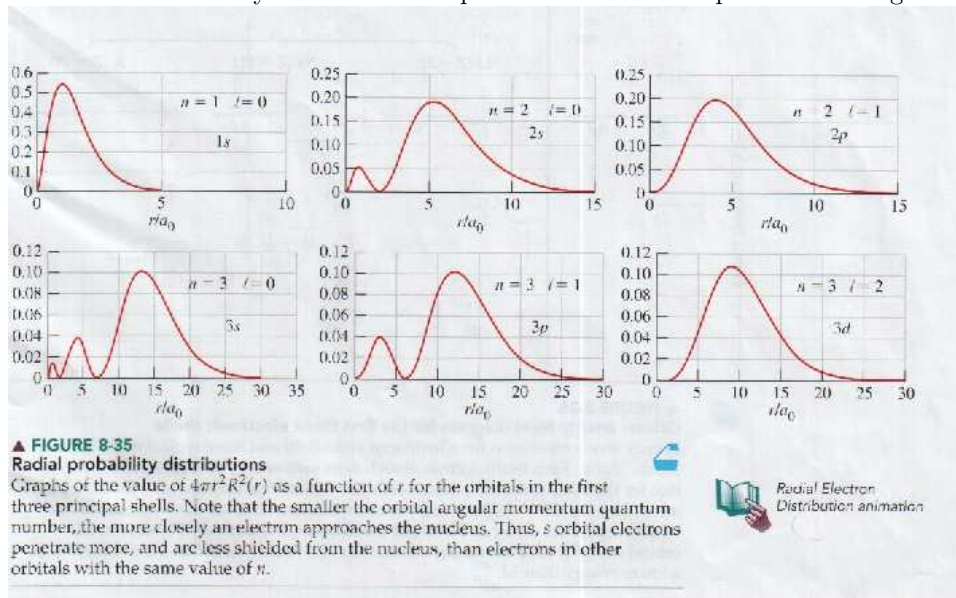
$$E_{\text{potential}} = -2 \times E_{\text{kinetic}},$$

$$E_{\text{total}} = E_{\text{kinetic}} + E_{\text{potential}},$$

$$E_{\text{total}} = \frac{1}{2}E_{\text{potential}},$$

$$E_{\text{total}} = -E_{\text{kinetic}}.$$

- In the H atom, the total energy of an electron in a 1s orbital is -13.6 eV. (An eV is a unit of energy. 1eV/atom or 1 eV/molecule = 96.5 kJ/mole.) What is the average kinetic and potential energy of an electron in a H 1s orbital.
- Examine Figure 8-36, where the total energy of the 1s orbital of H, Li, Na, and K are given. For which of these atoms are the 1s electrons moving the fastest?
- For which is the electrostatic energy the most negative?
- For the Na atom, rank the electrons in 3s, 3p, and 3d orbital from fastest to slowest moving.
- For these same three orbitals, rank the electrostatic energy for electrons in these orbitals from least to most negative.
- Examine the radial distribution functions of the 1s, 2s, and 3s orbitals given in Figure 8-35. For electrons, in which of these orbitals, is the electron on the average closer to the nucleus?
- Based on the data presented in Figure 8-35, electrons in which of these orbitals have the most negative electrostatic energy?
- Based on Figure 8-35, what would one expect the ranking of the total energies of the 1s, 2s, and 3s orbitals to be. Are your answers compatible with the data presented in Figure 8-36?



- All 3p radial distribution functions have similar shapes, but the distance units for the horizontal axes can be and are different. The energies of the H, Li, Na, and K 3p orbitals are as shown in Figure 8-36. Please draw on the same graph qualitatively correct sketches of the H, Li, Na, and K 3p radial distribution functions.
- Review what you have just learned.