Ground State Electronic Configurations for Many Electron Atoms

For a **ONE-ELECTRON ATOM** \( \varepsilon_n = \varepsilon_{K.E.} + \varepsilon_{P.E.} \)

\[
\varepsilon_{P.E.} = \frac{(+Ze)(-e)}{r} = \frac{-Ze^2}{\alpha r}
\]

For **MANY** (i.e. 2 or MORE) **ELECTRON ATOMS**

\[
\varepsilon_{orb} \approx \varepsilon_{P.E.} = \frac{1}{2} \left( \frac{-Ze^2}{\alpha r} \right)
\]

\[
\text{i.e. } \varepsilon_{orb} \approx \frac{-Ze^2}{2\alpha r} ;
\]

where \( Z_{eff} \) is an **EFFECTIVE NUCLEAR CHARGE** and takes account of the fact that for a **MANY-ELECTRON ATOM** an electron in an orbital will be **SCREENED** from the full nuclear charge +Ze by the other electrons in the atom. Thus, for a **MANY-ELECTRON ATOM**, since a 2s electron penetrates to the nucleus more strongly than does a 2p electron

\[
Z_{eff} (2s) > Z_{eff} (2p) \text{ and hence } \varepsilon_{2s} < \varepsilon_{2p}
\]

Similarly, \( \varepsilon_{3s} < \varepsilon_{3p} < \varepsilon_{3d} \). Thus, the orbital energies for a **many-electron atom** depend on BOTH \( n \) AND \( l \)

\[
\text{Energy} \quad 1s \quad 1s \quad 2s \quad 2p \quad 3p \quad 3p \quad 3d
\]
Thus, the electronic configuration for B (Z = 5) is as shown below:

\[
\text{UNPAIRED ELECTRON} \quad \downarrow\quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad 1s^2 2s^2 2p^1
\]

The sixth electron is placed in a VACANT 2p orbital to avoid the ELECTRON REPULSION which will occur when 2 electrons are placed in the SAME SPATIAL ORBITAL -- such REPULSION would RAISE the energy of the atom.

This result is summarised in HUND'S RULE:

Other things being equal, THE STATE OF LOWEST ENERGY corresponds to the MAXIMUM NUMBER OF UNPAIRED, PARALLEL SPINS.

Thus the electron configuration for N (Z = 7) is 1s^2 2s^2 2p^3 where each of the three 2p orbitals are SINGLY OCCUPIED. When we come to the O atom (Z = 8) we must place the eighth electron in a 2p orbital so that it is PAIRED UP with an electron of OPPOSITE SPIN -- this gives the electron configuration 1s^2 2s^2 2p^4.
The electron configuration for the F atom \((Z = 9)\) is \(1s^2\ 2s^2\ 2p^5\) and that for Ne \((Z = 10)\) is \(1s^2\ 2s^2\ 2p^6\). We proceed in a similar way for the next long period (i.e. for the atoms Na through Ar)

**Summary: Construction of Ground State Electronic Configurations**

1. Arrange atomic orbitals (ao's) in order of *increasing energy*

2. Assign electrons to the *LOWEST ENERGY AO'S consistent with*
   
   (i) *the Pauli Exclusion Principle*
   
   (ii) *Hund's Rule*