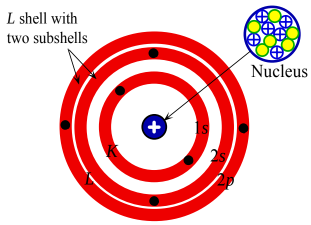
# Elementary Materials Science Concepts

- Atomic Structure:




$1s^2 2s^2 2p^2$ or $[He]2s^2 2p^2$

Fig. 1.1: The shell model of the atom in which the electrons are confined to live within certain shells and in subshells within shells.

From *Principles of Electronic Materials and Devices, Second Edition*, S.O. Kasap (© McGraw-Hill, 2002) http://Materials.Usask.Ca

**Table 1.1**
Maximum possible number of electrons in the shells and subshells of an atom.

| | | Subshell | | | |
|---|---|---|---|---|---|
| | *l* = | 0 | 1 | 2 | 3 |
| | | *s* | *p* | *d* | *f* |
| *n* | **Shell** | | | | |
| 1 | ***K*** | 2 | | | |
| 2 | ***L*** | 2 | 6 | | |
| 3 | ***M*** | 2 | 6 | 10 | |
| 4 | ***N*** | 2 | 6 | 10 | 14 |

From *Principles of Electronic Materials and Devices, Second Edition*, S.O. Kasap (© McGraw-Hill, 2002) http://Materials.Usask.Ca

**Additional Information:**
See: Chapter 2
Materials Science and Engineering – An Introduction, William D. Callister, Jr. 6th Ed or 7th Ed (Wiley, 2003)





# Atomic Structure

- Quantum Mechanics:
  - ✓ Electron orbitals are described by a ***probability distribution.***
  - ✓ The orbitals/probability distribution are characterized by 4 parameters call ***Quantum numbers***.
  - ✓ ***Quantum numbers*** describe the size, shape and spatial orientation of an $e^-$'s probability distribution/density.
  - ✓ The ***Quantum Numbers*** are: $n$, $l$, $m_l$, $m_s$
    - o ***n***: (*principle quantum number*)
      - also called a shell or Bohr orbit.
      - can have integral values: 1, 2, 3, …
      - ***n*** is related the the size & energy of the orbital.
      - As ***n*** increases, the orbital becomes larger & the $e^-$ spends more time further from the nucleus, and the energy is less negative.

## Atomic Structure

- Quantum Mechanics:
  - ✓ The ***Quantum Numbers*** are: ***n***, ***l***, $m_l$, $m_s$
    - o ***l***: (*azimuthal quantum number*)
      - Also called a subshell (of the shell, ***n***)
      - can have integral values from 0 to ***n***-1 for each value of ***n***.
        - » ***l*** = 0, 1, 2, …, (***n***-1) (known as a *selection rule*)
      - This quantum number relates to the shape of atomic orbital.
      - The value of ***l*** for a particular orbital is commonly assigned a letter:
        - » ***l***=0 is called *s*; ***l***=1 is called *p*; ***l***=2 is called *d;* ***l***=3 is called *f*
    - o $m_l$: (*magnetic quantum number*)
      - Can have integral values between *l* & –*l,* including zero.
        - » ***m*** = -***l***, …, -2, -1, 0, +1, +2, …, +***l*** (known as a *selection rule*)
      - The value of $m_l$ relates to the orientation of the orbital in space relative to the other orbitals in the atom.





## Atomic Structure

- Quantum Mechanics:
  - ✓ The ***Quantum Numbers*** are: ***n***, ***l***, $m_l$, $m_s$

**The Azimuthal Quantum Numbers and Corresponding Atomic Orbitals**

| Value of ℓ | 0 | 1 | 2 | 3 | 4 |
|---|---|---|---|---|---|
| Letter used | *s* | *p* | *d* | *f* | *g* |

Table 7.1

**Quantum Numbers for the First Four Levels of Orbitals in the Hydrogen Atom**

| *n* | ℓ | Orbital designation | $m_\ell$ | Number of orbitals |
|---|---|---|---|---|
| 1 | 0 | 1*s* | 0 | 1 |
| 2 | 0 | 2*s* | 0 | 1 |
| | 1 | 2*p* | −1, 0, +1 | 3 |
| 3 | 0 | 3*s* | 0 | 1 |
| | 1 | 3*p* | −1, 0, 1 | 3 |
| | 2 | 3*d* | −2, −1, 0, 1, 2 | 5 |
| 4 | 0 | 4*s* | 0 | 1 |
| | 1 | 4*p* | −1, 0, 1 | 3 |
| | 2 | 4*d* | −2, −1, 0, 1, 2 | 5 |
| | 3 | 4*f* | −3, −2, −1, 0, 1, 2, 3 | 7 |

Table 7.2

S. Zumdahl, Chemistry (Heath, 1986)

## Atomic Structure

- Quantum Mechanics:
  - ✓ The ***Quantum Numbers*** are: ***n***, ***l***, $m_l$, $m_s$
    - o $m_s$: (electron spin magnetic number)
      - Can have the value 1/2 or -1/2
        - » $m_s = \pm\frac{1}{2}$ (*selection rule*)
      - Explains the electron's magnetic moment with two possible orientation
      - Often described as "spin up" (1/2) or spin down (-1/2)
  - ✓ What is the consequence or result of $m_s$?

**Pauli Exclusion Principle:**

- In a given atom, no two $e^-$'s can have the same set of four quantum numbers.
- An orbital defined by ***n***, ***l***, $m_j$, can hold only two $e^-$'s, and they must have opposite spins.





## Atomic Structure

- Quantum Mechanics:

**Table 2–1** Quantum numbers to **n** = 3 and allowable states for the electron in a hydrogen atom: The first four columns show the various combinations of quantum numbers allowed by the selection rules of Eq. (2–46); the last two columns indicate the number of allowed states (combinations of **n**, ***l***, **m**, and **s**) for each ***l*** (subshell) and **n** (shell, or Bohr orbit).

| n | $l$ | $m_l$ | $m_s$ | Allowable states in subshell | Allowable states in complete shell |
|---|---|---|---|---|---|
| 1 | 0 | 0 | $\pm\frac{1}{2}$ | 2 | 2 |
| 2 | 0 | 0 | $\pm\frac{1}{2}$ | 2 | 8 |
| | 1 | −1 | $\pm\frac{1}{2}$ | 6 | |
| | | 0 | $\pm\frac{1}{2}$ | | |
| | | 1 | $\pm\frac{1}{2}$ | | |
| 3 | 0 | 0 | $\pm\frac{1}{2}$ | 2 | 18 |
| | 1 | −1 | $\pm\frac{1}{2}$ | 6 | |
| | | 0 | $\pm\frac{1}{2}$ | | |
| | | 1 | $\pm\frac{1}{2}$ | | |
| | 2 | −2 | $\pm\frac{1}{2}$ | 10 | |
| | | −1 | $\pm\frac{1}{2}$ | | |
| | | 0 | $\pm\frac{1}{2}$ | | |
| | | 1 | $\pm\frac{1}{2}$ | | |
| | | 2 | $\pm\frac{1}{2}$ | | |

$m_l = m$

$m_s = s/h$

Eqn. 2-46 refers to ***selection rules***

Streetman & Banerjee, Solid State Electronic Devices (Prentice Hall, 2000)

## Atomic Structure

- Quantum Mechanics:
  - ✓ From the 1st 2 ***Quantum Numbers***, *n* and *l*, we can determine the ***electronic configuration*** of atoms which is logically followed by the periodic table – how $e^-$'s fill sub-orbitals.
  - ✓ 1s, 2s, 2p, 3s, 3p, 3d, 4s, 4p, 4d, …
  - ✓ $1s^2$, $2s^2$, $2p^6$, $3s^2$, $3p^6$, $3d^{10}$, $4s^2$, $4p^6$, $4d^{10}$, …
  - ✓ H: $1s^1$
    - o He: $1s^2$
    - o Li: $1s^2$, $2s^1$
    - o Be: $1s^2$, $2s^2$
    - o B: $1s^2$, $2s^2$, $2p^1$
    - o C: $1s^2$, $2s^2$, $2p^2$
    - o N: $1s^2$, $2s^2$, $2p^3$
    - o O: $1s^2$, $2s^2$, $2p^4$
    - o Cl: $1s^2$, $2s^2$, $2p^5$
    - o Ne: $1s^2$, $2s^2$, $2p^6$

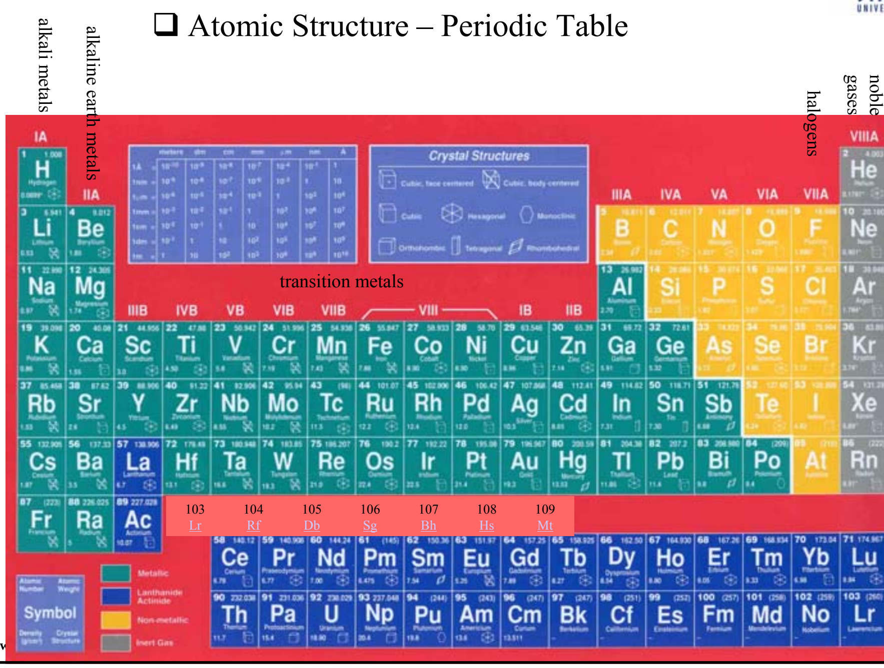
| Sub-Orbital | Value of *l* quantum number | Number of states |
|---|---|---|
| s | 0 | 2 |
| p | 1 | 6 |
| d | 2 | 10 |





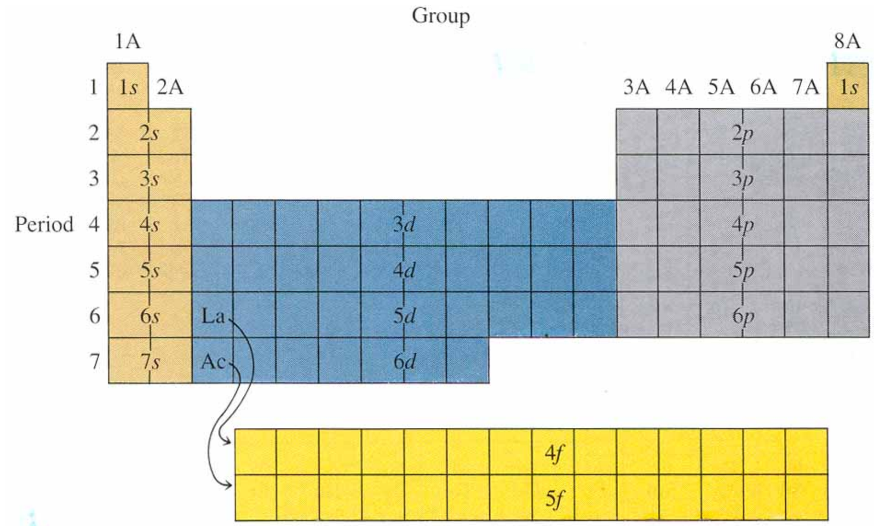
## Atomic Structure

- Atomic Structure – Periodic Table



# Atomic Structure

- ❑ Atomic Structure – Periodic Table
  - ✓ Electronic configuration






S. Zumdahl, Chemistry (Heath, 1986)



MSE 310
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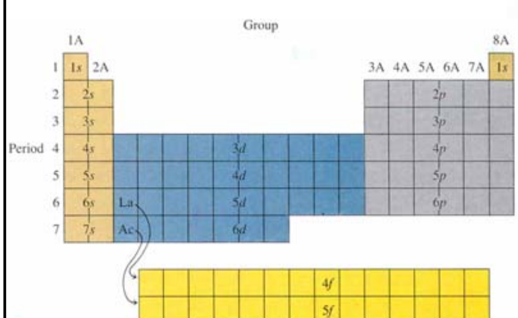
# Atomic Structure

- ❑ Atomic Structure – Periodic Table
  - ✓ Electronic configuration



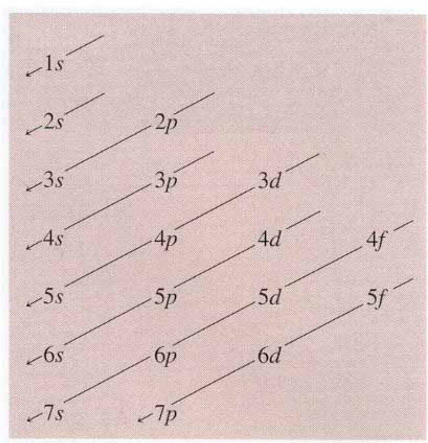




**Figure 7.29** A diagram that summarizes the order in which the orbitals fill in polyelectronic atoms.



S. Zumdahl, Chemistry (Heath, 1986)

## Atomic Structure

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- Atomic Structure – Periodic Table
  - ✓ Electronic configuration

**Sample Exercise 7.7** **Electron Configurations**

Give the electron configurations for sulfur (S), cadmium (Cd), hafnium (Hf), and radium (Ra) using the periodic table inside the front cover of this book.

**Solution**

*Sulfur* is element 16 and resides in Period 3, where the 3*p* orbitals are being filled (see Fig. 7.30). Since sulfur is the fourth among the "3*p* elements," it must have four 3*p* electrons. Its configuration is

$$\text{S:}\quad 1s^2 2s^2 2p^6 3s^2 3p^4 \quad \text{or} \quad [\text{Ne}]3s^2 3p^4$$

*Cadmium* is element 48 and is located in Period 5 at the end of the 4*d* transition metals, as shown in Fig. 7.30. It is the tenth element in the series and thus has 10 electrons in the 4*d* orbitals, in addition to the 2 electrons in the 5*s* orbital. The configuration is

$$\text{Cd:}\quad 1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} \quad \text{or} \quad [\text{Kr}]5s^2 4d^{10}$$

*Hafnium* is element 72 and is found in Period 6, as shown in Fig. 7.30. Note that it occurs just after the lanthanide series. Thus the 4*f* orbitals are already filled. Hafnium is the second member of the 5*d* transition series and has two 5*d* electrons. The configuration is

$$\text{Hf:}\quad 1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6 6s^2 4f^{14} 5d^2 \quad \text{or} \quad [\text{Xe}]6s^2 4f^{14} 5d^2$$

*Radium* is element 88 and is in Period 7 (and Group 2A), as shown in Fig. 7.30. Thus radium has two electrons in the 7*s* orbital, and the configuration is

$$\text{Ra:}\quad 1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6 6s^2 4f^{14} 5d^{10} 6p^6 7s^2 \quad \text{or} \quad [\text{Rn}]7s^2$$

S. Zumdahl, Chemistry (Heath, 1986)





## Atomic Structure

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- Atomic Structure – Periodic Table
  - ✓ Electronic configuration:
    - o **<u>Aufbau Principle:</u>** Just as protons are added one by one to the nucleus to build up the elements, electrons are similarly added to these hydrogen like orbitals.

| Element | Elec. Conf. | 1s | 2s | | 2p | |
|---|---|---|---|---|---|---|
| H: | $1s^1$ | ↑ | | | | |
| He: | $1s^2$ | ↑↓ | | | | |
| Li: | $1s^2 2s^1$ | ↑↓ | ↑ | | | |
| Be: | $1s^2 2s^2$ | ↑↓ | ↑↓ | | | |
| B: | $1s^2 2s^2 2p^1$ | ↑↓ | ↑↓ | ↑ | | |
| C: | $1s^2 2s^1 2p^2$ | ↑↓ | ↑↓ | ↑ | ↑ | |
| N: | $1s^2 2s^1 2p^3$ | ↑↓ | ↑↓ | ↑ | ↑ | ↑ |
| O: | $1s^2 2s^1 2p^4$ | ↑↓ | ↑↓ | ↑↓ | ↑ | ↑ |
| F: | $1s^2 2s^1 2p^5$ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑ |

    - o **<u>Hund's Rule:</u>** the lowest energy configuration for an atom is the one having the maximum number of unpaired electrons allowed by the *Pauli Exclusion Principle* in a particualr set of *degenerate* orbitals.
    - o *<u>Degenerate orbitals:</u>* orbitals that have the same energy (same $\boldsymbol{n}$, $\boldsymbol{l}$, $\boldsymbol{m_l}$).

# Atomic Structure



- ❑ Atomic Structure – Periodic Table & Periodic Trends
  - ✓ Atomic Radius

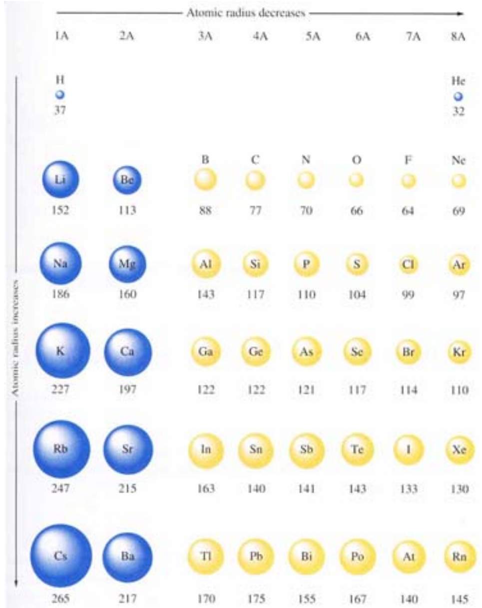


**Figure 7.35**
Atomic radii (in picometers) for selected atoms. Note that atomic radius decreases going across a period and increases going down a group. The values for the noble gases are estimated, because data from bonded atoms are lacking.

S. Zumdahl, Chemistry (Heath, 1986)