Unit 6 – Notes – Quantum Mechanics

Breaking down the electron cloud.

Electron hierarchy
❖ Energy levels (shells)
❖ Subshells (sublevels-s,p,d,f)
❖ Orbitals (clouds)

❖ Each atom has a certain number of energy levels (same as period number)
(Principle Quantum # n)
❖ These energy levels contain a certain number of sublevels.
(Angular Momentum Quantum # l - shape of the orbital)
❖ Each sublevel contains a certain number of orbitals. (n^2)

The number of sublevels an energy level contains is equal to the energy level number.
(Principle Quantum # n)
Example: Potassium is in period 4, which means it has 4 energy levels and 4 sublevels:
       (Principle Quantum # 4)
       Its 1st energy level has 1 sublevel(s)
       Its 2nd energy level has 2 sublevels (s,p)
       Its 3rd energy level has 3 sublevels (s,p,d)
       Its 4th energy level has 4 sublevels (s,p,d,f)
So, potassium has a <u>total</u> of 10 sublevels.

n = # of sublevels per level
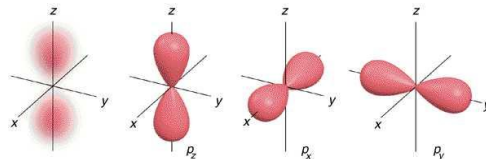**n^2 = # of orbitals per level**
Sublevel sets: s-1, p-3, d-5, f-7

Each sublevel has its own shape. (Quantum # l)
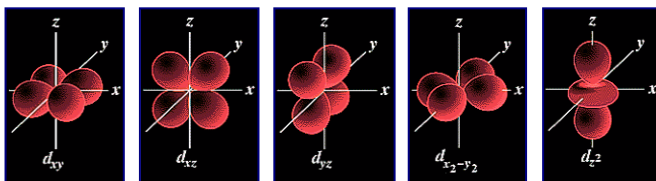The shape is based on calculated probability.
The **first sublevel** (*s - sharp*) contains **1 orbital** and <u>is sphere shaped.</u>

The **second sublevel** (*p - principal*) contains **3 orbitals**, which are each dumbbell shaped and follow the X, Y or Z.

The **third sublevel** (*d - diffuse*) contains **5 orbitals**, which are each cloverleaf shaped except the last one, which is like a dumbbell with a ring.


Magnetic Quantum Number (m_l)
    ❖ Orientation of orbital
    ❖ Specifies the exact orbital
       within each sublevel

The **fourth sublevel** (*f - fundamental*) contains **7 orbitals** and is too complex to draw in 2D.

The Periodic Table breaks down into 4 blocks.
Each block represents one of the shapes or sublevels. That is the shape of the outer sublevel of the valence shell. **Remember "n" represents principle quantum number or energy level or period!**
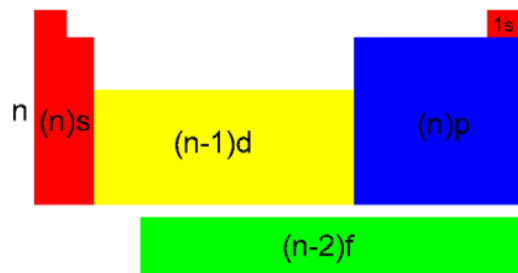
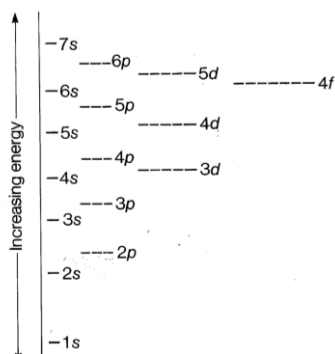Electrons are assigned to energy levels, sublevels and orbitals based on **three principles or rules**.
1.Aufbau Principle
Electrons enter the lowest energy level available first.
Not necessarily in numerical order.
Example: $3s \rightarrow 3p \rightarrow 4s \rightarrow 3d$

Within an energy level, the *s* sublevel has the least energy, then *p*, then *d*, then *f*.

The Aufbau diagram follows the Periodic Table read left to right, top to bottom. Lower energy fills up first. Note: the valence electrons are in the <u>energy level with the highest number</u>.

2. Pauli Exclusion Principle
Each orbital can contain only 2 electrons. And if it has 2 they must spin opposite.
Therefore,

sublevel	# of orbitals	total electrons held
s	1	2 e-
p	3	6 e-
d	5	10 e-
f	7	14 e-

Total e- is also equal to the number of elements in one row of that block.
(Formula $2n^2$ will tell the # of electrons for that energy level)

Each e- revolves around the nucleus and rotates on its axis. They can <u>rotate clockwise or counterclockwise</u>. <u>The spins are represented by arrows</u>: Opposite spins will attract, like spins will repel. This is why an orbital cannot contain more than 2 e-.

3. Hund's Rule
When filling a sublevel that has multiple orbitals (*p, d, f*), put one e-, having the same spin, in each orbital first until each has one, then start doubling up.
You must draw all the orbitals for a sublevel, even if they aren't occupied.
The reason is because the sublevels and orbitals represent probability. The orbitals show where the e- is likely to be, not necessarily where it is.

Steps for drawing e⁻ configuration:

Using Aufbau, draw a set of boxes to represent the sublevel ($s = 1$, $p = 3$, $d = 5$, $f = 7$)

2. Using Pauli and Hund, fill the boxes with arrows to represent the electrons.

3. Keep going until all e⁻ are used up.

Example: **Carbon**

↓↑		↓↑		↑	↑	

1s   2s   2p
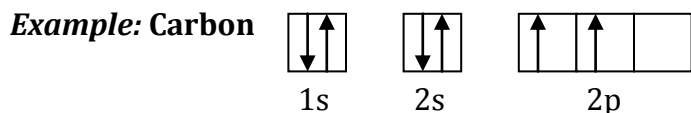
Method of writing e⁻ configuration by skipping the boxes and arrows and numbers and letters.

Example: Carbon $1s^2\ 2s^2\ 2p^2$ Notice the superscripts add up to the atomic number.

Beginning number is energy level. Letter s, p are the orbital shape. Superscripts are the electrons.

We can shorten using noble gas. Start with Noble Gas that precedes the number of your element. Put the Noble Gas is brackets. [He] $2s^2sp^2$

IONS: Can draw e⁻ configurations (boxes and arrows) and write shorthand and quantum numbers for ions just like for neutral (ground state) atoms. Only difference is ions have **gained or lost e⁻**

S : [Ne] $3s^23p^4$ S²⁻ : [Ne] $3s^23p^6$ gained two electrons

Ga: [Ar] $4s^23d^{10}4p^1$ Ga³⁺ : [Ar] $3d^{10}$ lost three electrons

Ions always **lose and gain electrons** from the highest **numbered energy level**.

The highest numbered energy level contains the bonding electrons or valence electrons.

The third representation of electrons is called the Lewis Dot Diagram.

A **Lewis symbol (Lewis dot diagram)** is a symbol in which the electrons in the valence shell (outer energy level) of an atom or simple ion are represented by dots placed around the letter symbol of the element. Each dot represents one electron. **Negative ions gain electrons and positive ions lose electron.**

Lewis Dot Diagrams

- A Lewis dot structure is like a simplified electron energy level model.

- The Lewis structure contains the element symbol with dots representing electrons.

- The only electrons shown are those on the outer energy level or valence electrons.

- The electrons are placed around the element symbol, one at a time, clockwise or counterclockwise, and then grouped in pairs as more electrons are added.

PERIODIC TABLE
ELEMENTS 1–20

HYDROGEN 1							HELIUM 2
H·							He·
LITHIUM 3	BERRYLLIUM 4	BORON 5	CARBON 6	NITROGEN 7	OXYGEN 8	FLOURINE 9	NEON 10
Li·	Be·	·B·	·C·	·N·	·O·	:F·	:Ne:
SODIUM 11	MAGNESIUM 12	ALUMINUM 13	SILICON 14	PHOSPHORUS 15	SULFUR 16	CHLORINE 17	ARGON 18
Na·	Mg·	·Al·	·Si·	·P:	·S:	:Cl:	:Ar:
POTASSIUM 19	CALCIUM 20						
K·	Ca·						

Oxygen: $1s^2\ 2s^2\ 2p^4$ ·Ö·

Chlorine: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^5$:Cl·   Chloride ion Cl⁻ : $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6$:Cl: