Quantum Mechanical Model of the Atom

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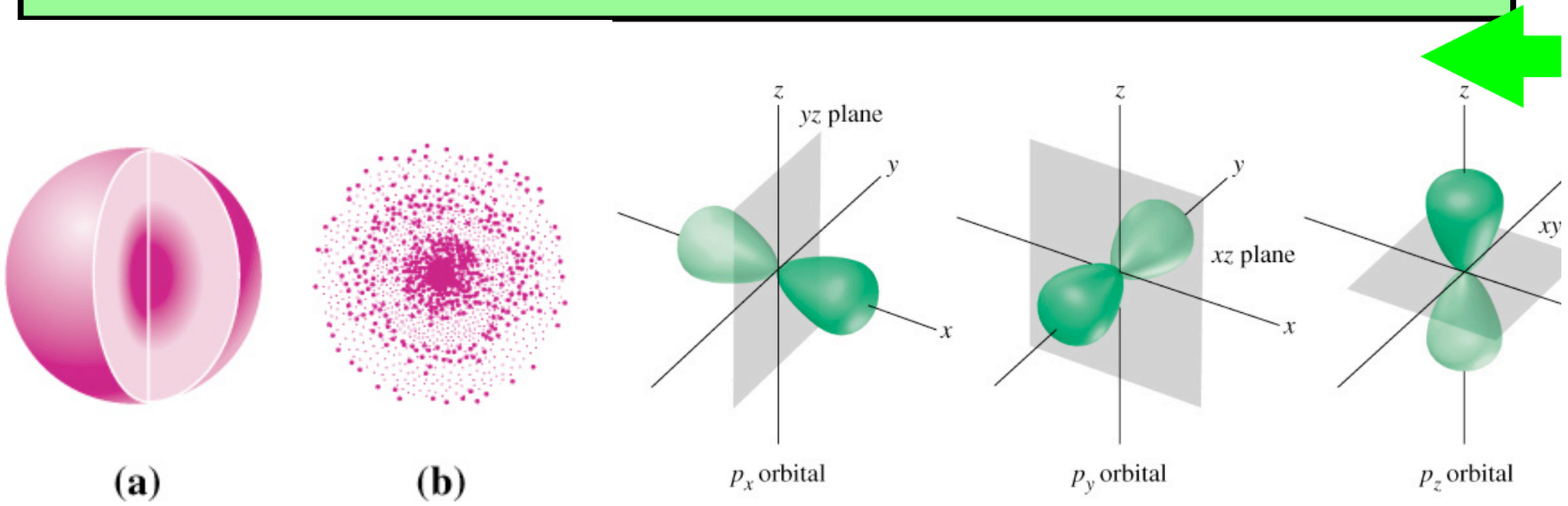
Updates to Bohr Model:

-Electrons are NOT in circular orbits around nucleus.

-Electrons are in a 3-D region around the nucleus called **atomic orbitals.**

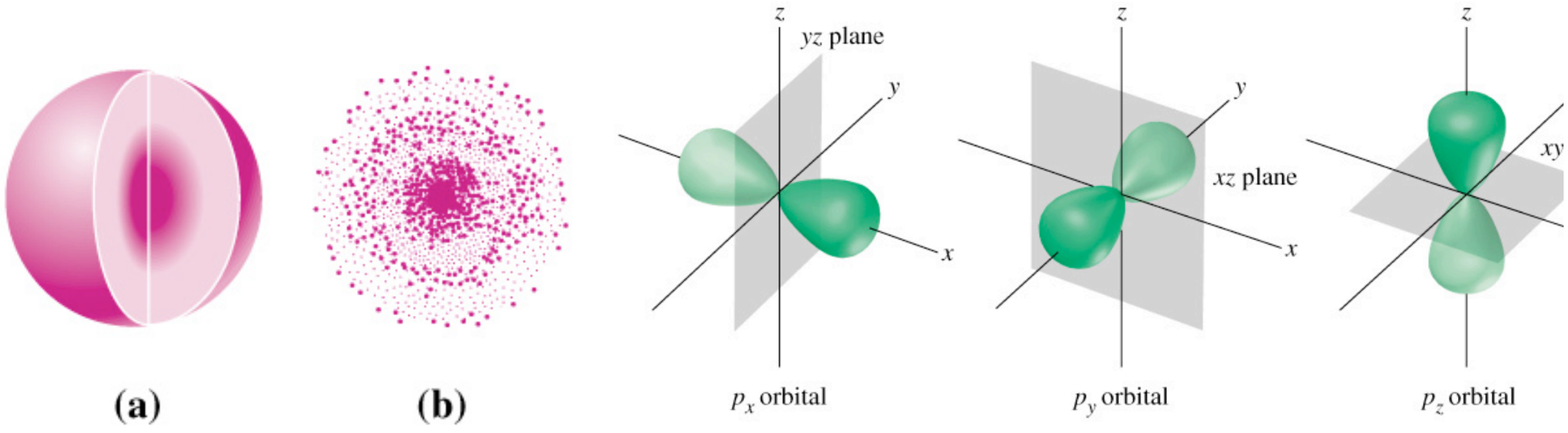
-The atomic orbital describes the probable location of the electrion



Quantum Mechanical Model of the Atom

There are different kinds of atomic orbitals that differ in the amount of energy and shapes (where the electron probably is).

The atomic orbitals get filled by electrons in a certain order.



Where does this model come from? A quick history.

1. Louis de Broglie: Electrons behave with **wave** and **particle** properties at the same time.

$$\lambda = \frac{h}{m \cdot v}$$

2. Werner Heisenberg: It is impossible to know both the position and velocity of an electron simultaneously. ***Heisenberg's Uncertainty Principle**

3. Erwin Shrodinger: Refined the wave-particle theory proposed by de Broglie.

Developed an equation that treated an electron like a wave and predicted the **probable** location of an electron around the nucleus called the **atomic orbital.**

For a single particle in three dimensions:

$$i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + V(x,y,z)\psi$$

where

- ψ is the wavefunction, which is the amplitude for the particle
- m is the mass of the particle.
- $V(x,y,z)$ is the potential energy the particle has at each position.

***The quantum mechanical model of the atom treats an electron like a wave.**

The quantum mechanical model describes the probable location of electrons in atoms by describing:

-Principal energy level

-Energy sublevel

-Orbital (in each sublevel)

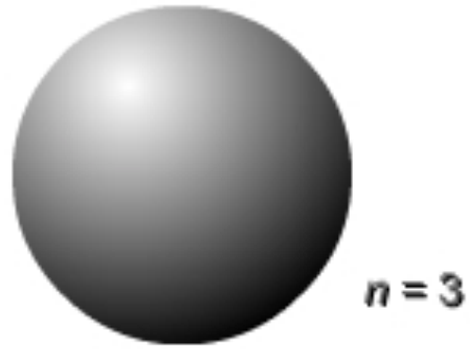
-Spin

Principal Energy Level (n)
-"shells"

Indicates the relative size and energy of atomic orbitals.

n=integers: n= 1, 2, 3, etc.

- As n increases:
  - > orbital becomes larger
  - > electron spends more time farther away from nucleus
  - > atom's energy level increases



As the principle quantum number *n* increases, the size and energy of the orbital both increase, but the shape remains essentially the same.

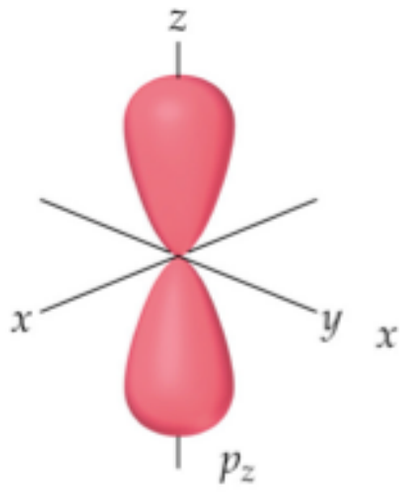
http://www.chem.ox.ac.uk/vrchemistry/Machinery/html/page02.htm

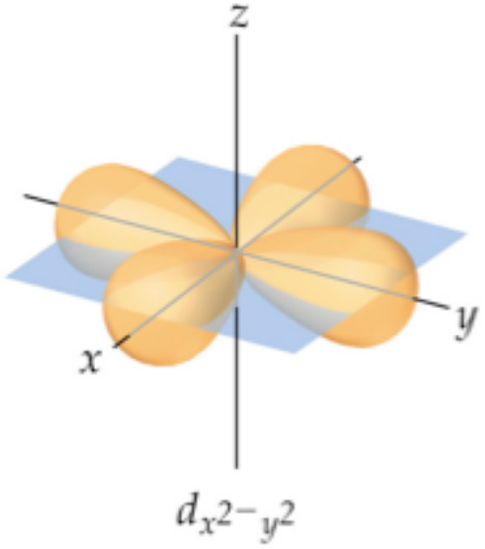
Energy sublevel

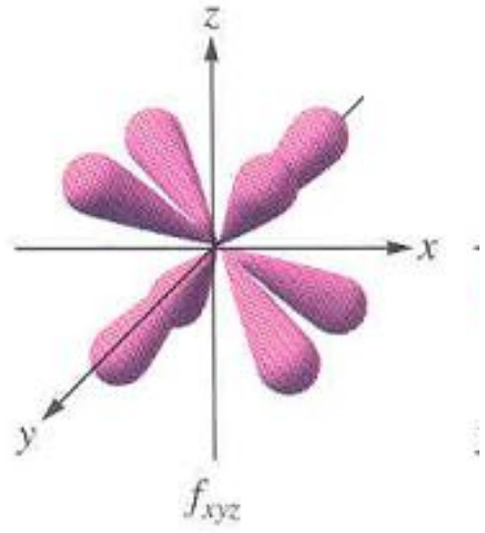
Principal energy levels are broken down into sublevels.

- Sublevels define the orbital shape (s, p, d, f)
  - n=1, 1 sublevel (s)
  - n=2, 2 sublevels (s, p)
  - n=3, 3 sublevels (s, p, d)
  - n=4, 4 sublevels (s, p, d, f)

1s



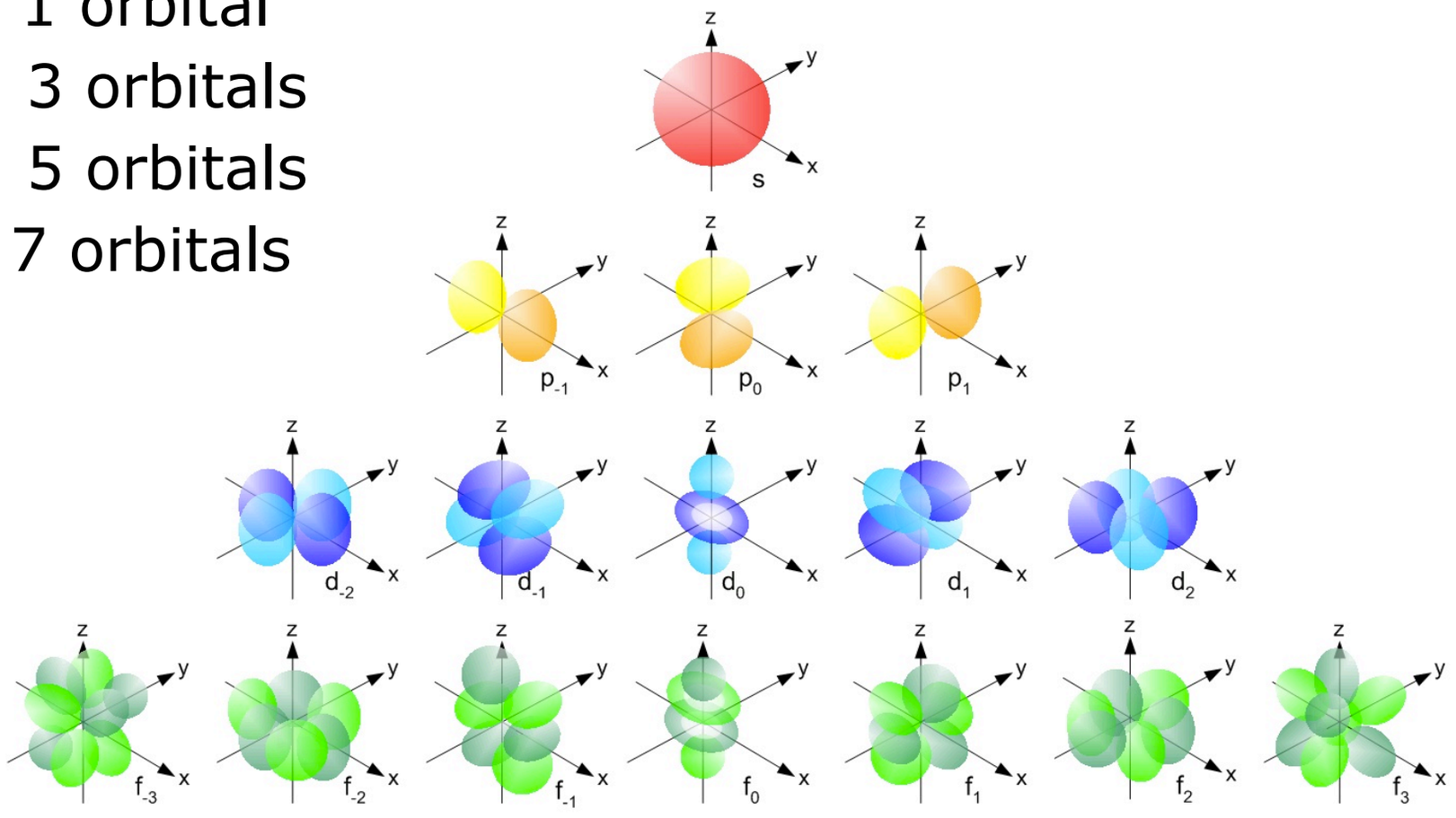




Orbitals (in each sublevel)

Each sublevel has a different number of orbitals.

- s: 1 orbital
- p: 3 orbitals
- d: 5 orbitals
- f: 7 orbitals

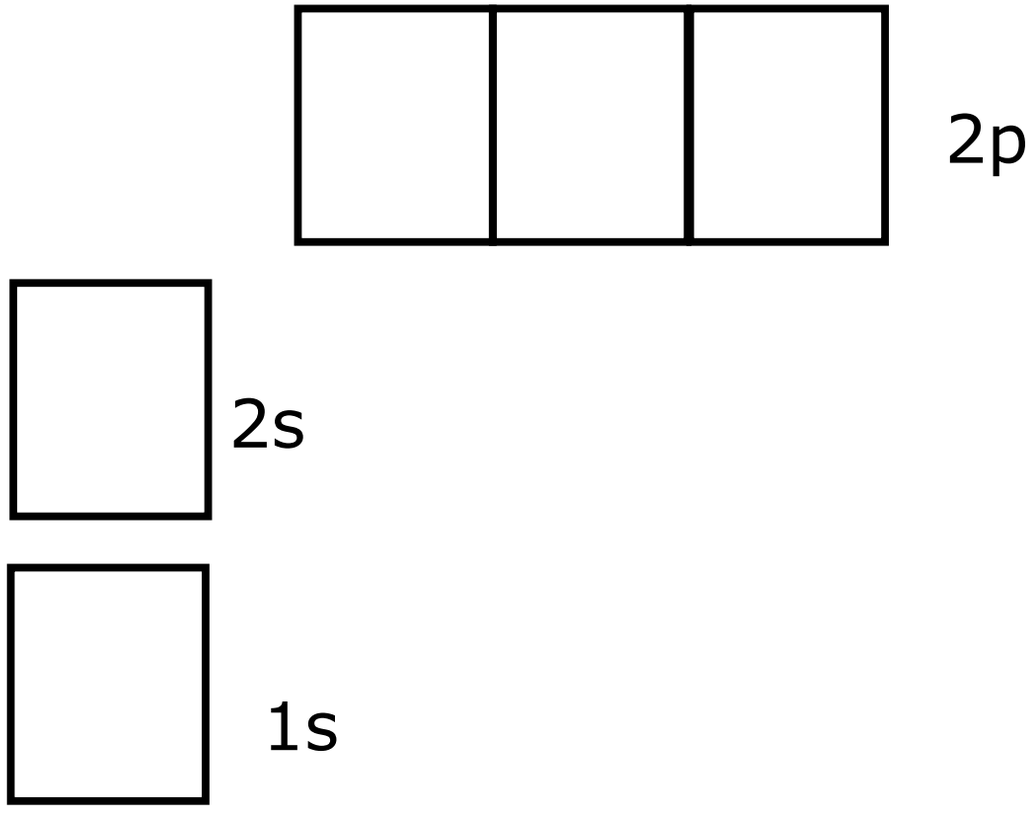


http://edtech2.boisestate.edu/lindabennett1/502/Periodic%20Table%20e%20config/electron%20configuration.html

Spin

Electrons act like they are spinning on an axis

- Generates a magnetic field
- No two electrons in the same orbital can have the same spin



Summary:

TABLE 5.1 Sublevels of the first four energy levels

Principal energy level	*Sublevel*	*Number of orbitals in sublevel*	*Total possible occupying electrons*	
1	*s*	1	2	
2	*s*	1	2	8
	p	3	6	
3	*s*	1	2	18
	p	3	6	
	d	5	10	
4	*s*	1	2	32
	p	3	6	
	d	5	10	
	f	7	14	

In each principal energy level, there are n^2 orbitals.

In each principal energy level, there are a maximum of $2n^2$ electrons.

Electron Configuration

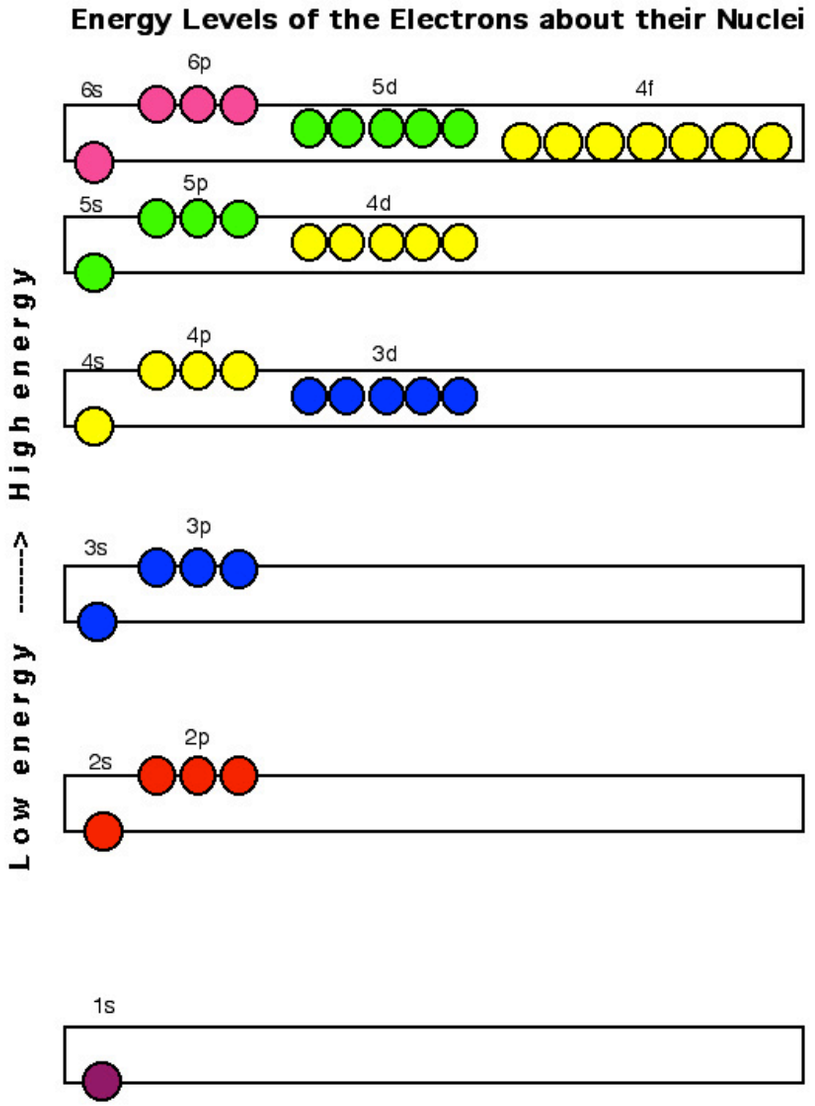
Describes the electron arrangement in atoms.

3 rules for electron configuration at ground state:

1. **Aufbau principle**: Each electron occupies the lowest energy orbital available.

2. **Pauli exclusion principle**: A maximum of 2 electrons may occupy a single atomic orbital, but only if they have opposite spins.

3. **Hund's rule**: a single electron with the same spin must occupy each orbital in a sublevel before they pair up with an electron with an opposite spin.



Electron configuration notation:

List all sublevels in order of filling.

Example:

Na:

Noble-gas notation:

Like a short cut! Put noble gas of previous period (row) in brackets, and then write electron configuration for for the energy level being filled.

Example:

Next Class:

Exceptions to predicted electron configuration.

Valence electrons

Electron-dot diagrams

HW: Quantum Mechanical Model of the Atom Practice

1. How many electrons are in a hydrogen atom?

2. If the electron of hydrogen is in its ground state, which orbital is it in?

3. How many orbitals are possible at the 3rd energy level (n=3)?

4. Draw the shape of an s and a p orbital.

5. What is the difference between the 2s and 1s orbital? How are they similar?

6. How many orbitals are possible at n = 3?

7. How many electrons are possible in n =3?

8. Write the electron configuration notation for Aluminum.

9. Write the noble gas notation for Aluminum