Ch5 Modern Atomic Theory

Mrs. Medina

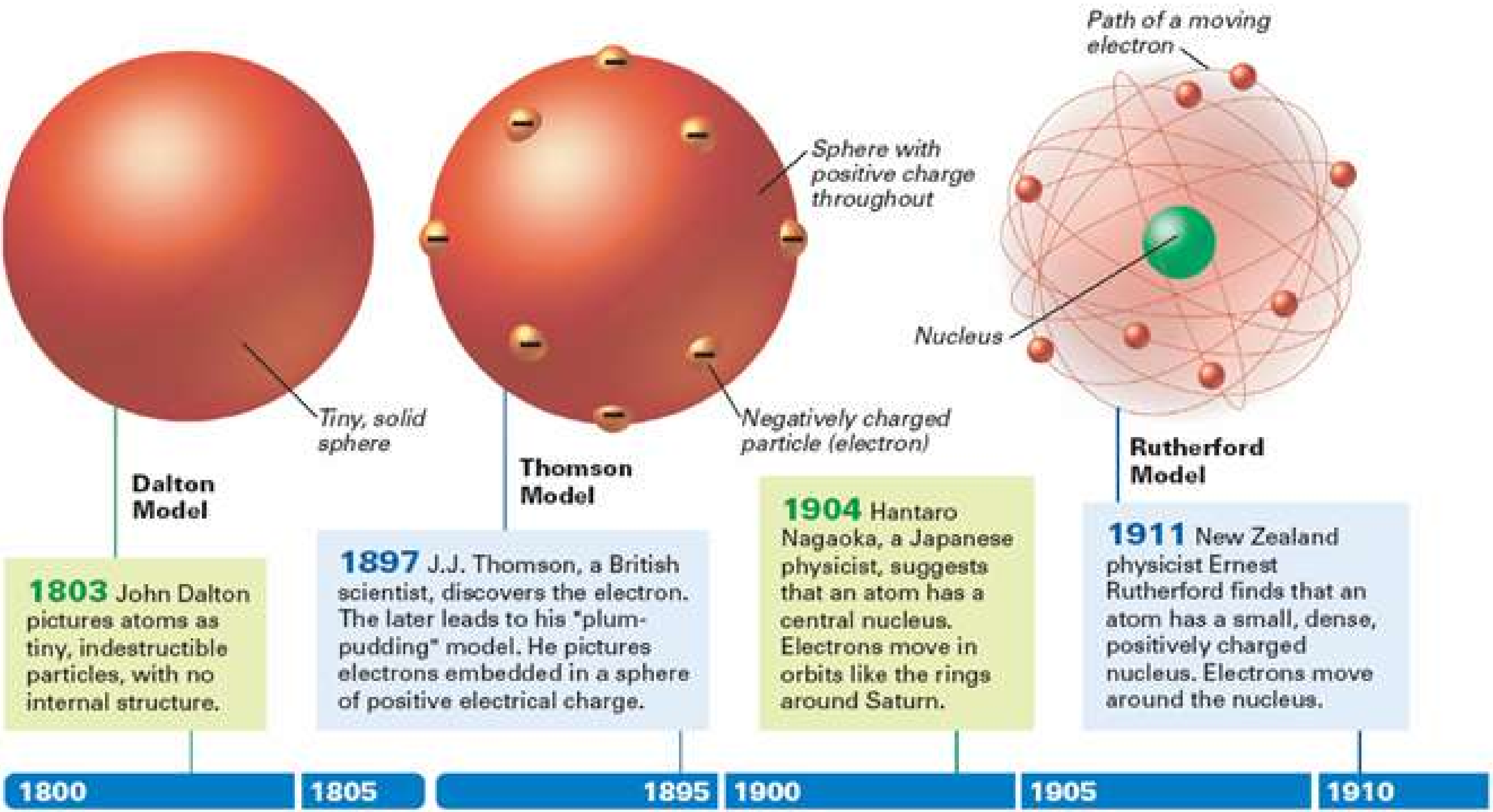
Why do metals glow when heated?

Models of the Atom

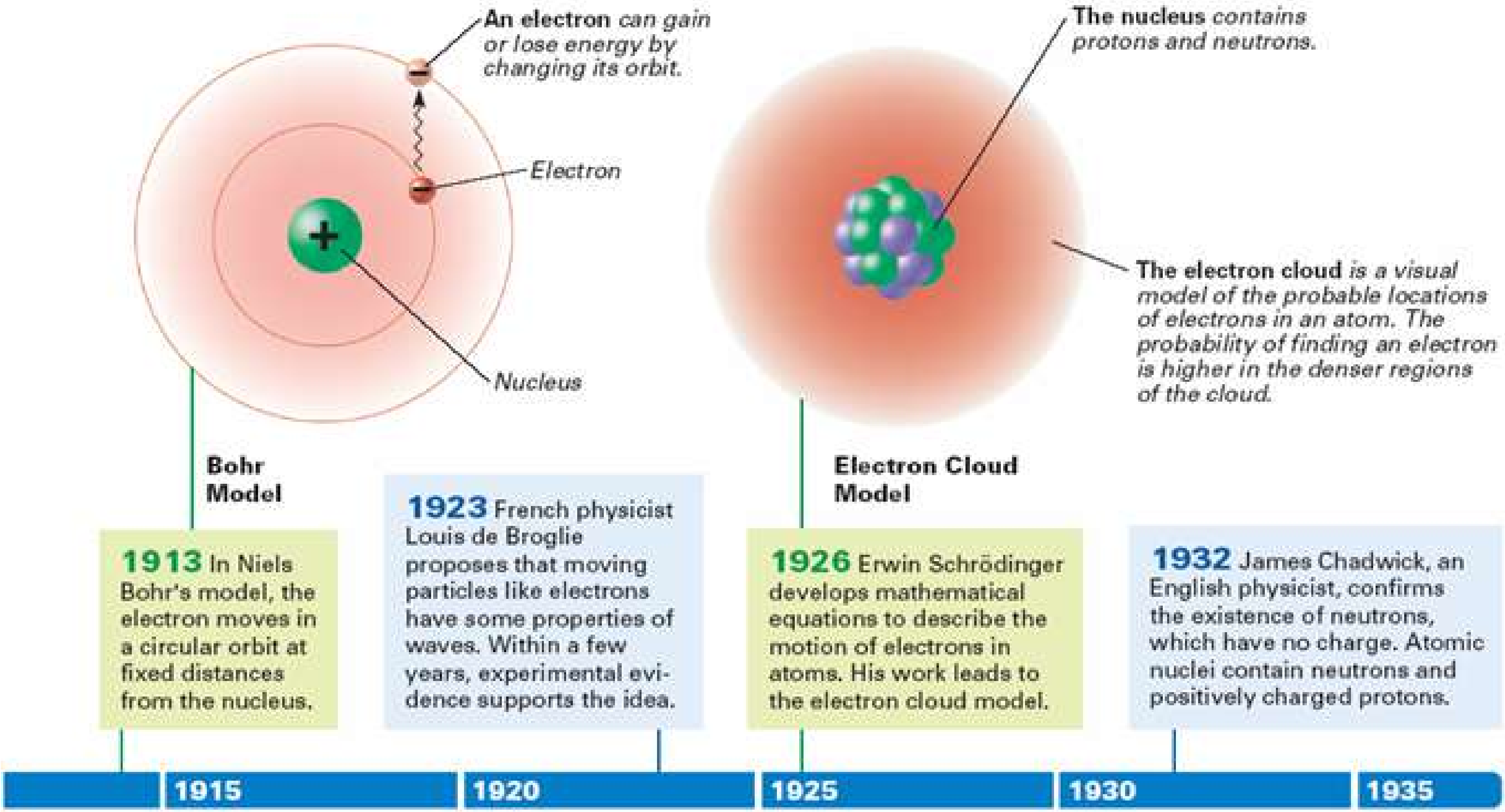
- A model should explain not just what the material is made of (composition) but also how it is going to behave (changes).

- Rutheford's atomic model could not explain the chemical properties of elements.
    - Basically, it couldn't explain why things change color when heated.

Atomic Model Timeline



Atomic Model Timeline

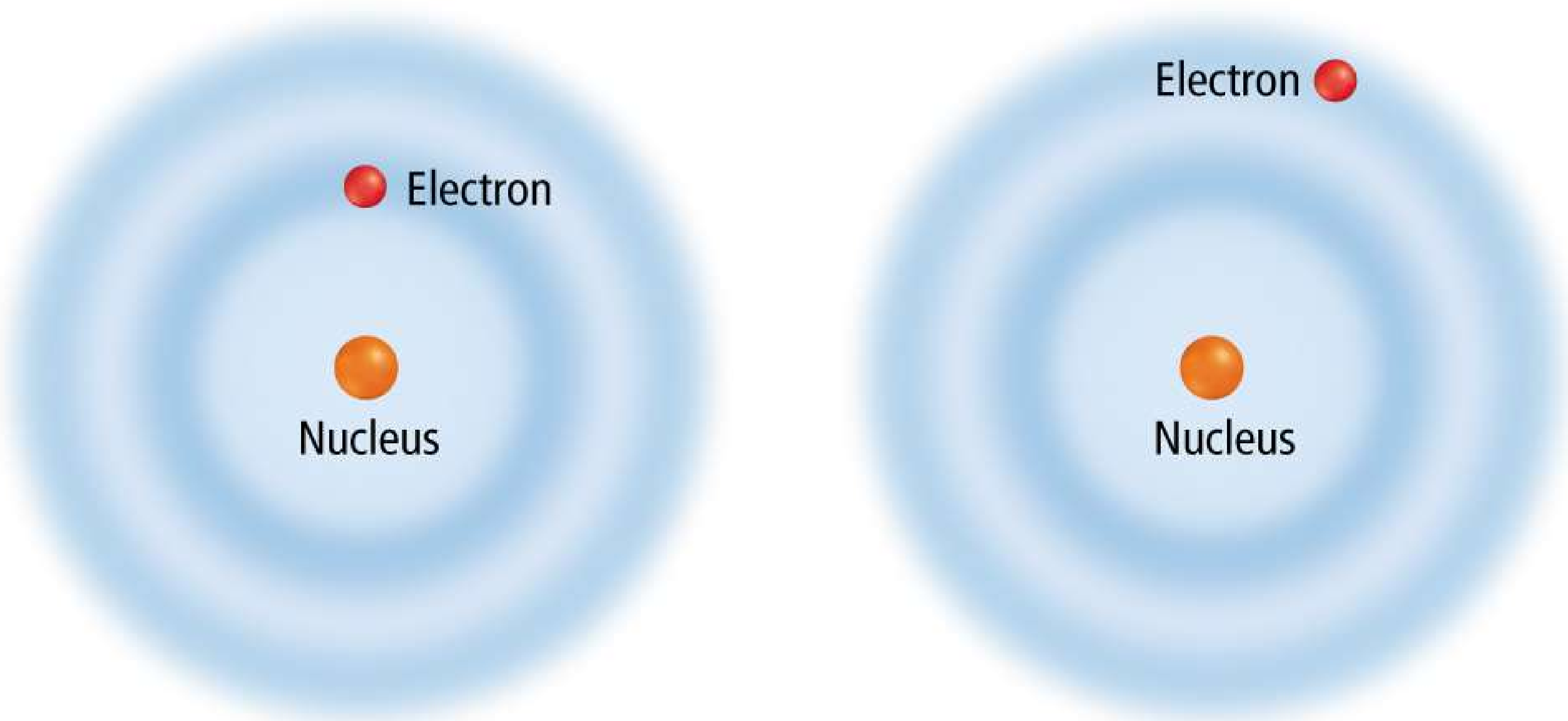


The Bohr Model

- Niels Bohr (1885-1962) was a Danish physicist and a student of Rutherford's.

- In 1913, Bohr introduced his atomic model based on the simplest atom, hydrogen (only 1 electron)
  - **Bohr proposed that an electron is found only in specific circular paths, or orbits, around the nucleus.**

Bohr Model

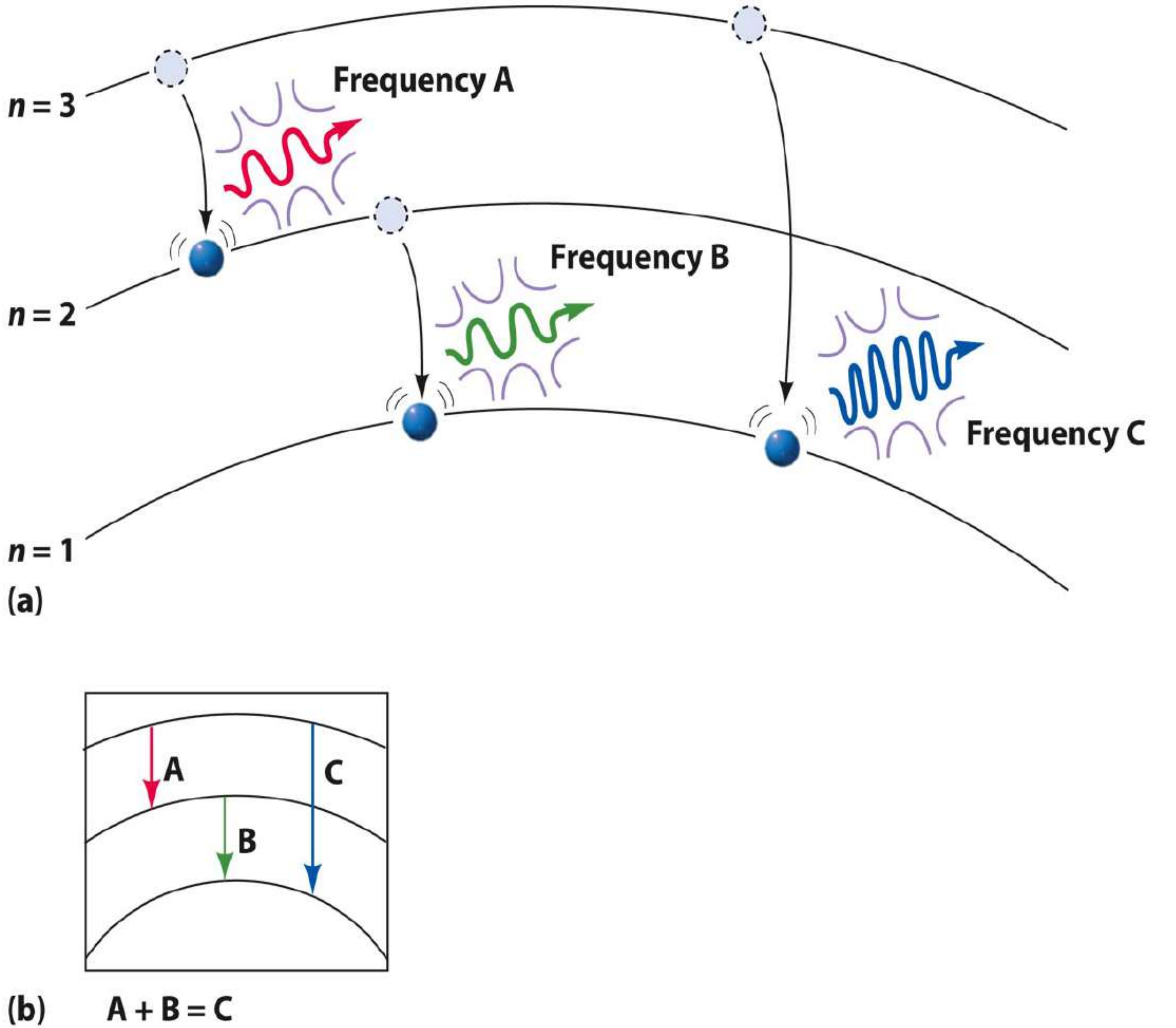


Ground state **Excited state**

The Bohr Model

- Each electron has a **fixed energy = an energy level**.
  - Electrons can jump from one energy level to another.
  - Electrons can not be or exist between energy levels.
- A **quantum** of energy is the amount of energy needed to move an electron from one energy level to another energy level.

The degree to which they move from level to level determines the frequency of light they give off.

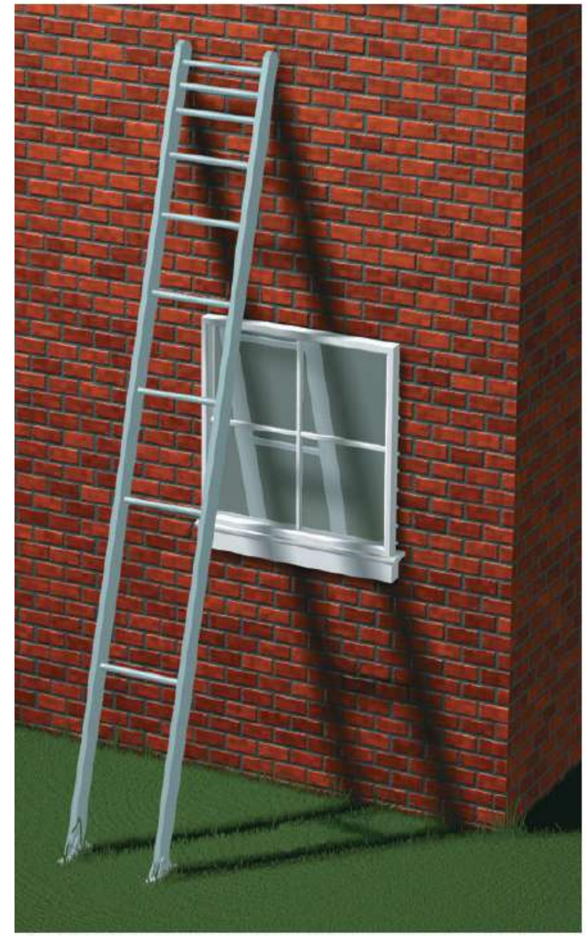


Bohr Model

- To move from one level to another, the electron must gain or lose the right amount of energy.
- The higher the energy level, the farther it is from the nucleus.
  - Gain energy to move to higher energy levels (away from nucleus)
  - Lose energy to move to lower energy levels (closer to nucleus)

The Bohr Model

- The amount of energy required to go from one energy level to another is the not same for the electrons.
- Higher energy levels are closer together. This means it takes less energy to change levels in the higher energy levels.



- **The Bohr model was tested with the hydrogen element but failed to explain the energies absorbed and emitted by atoms with more than one electron.**

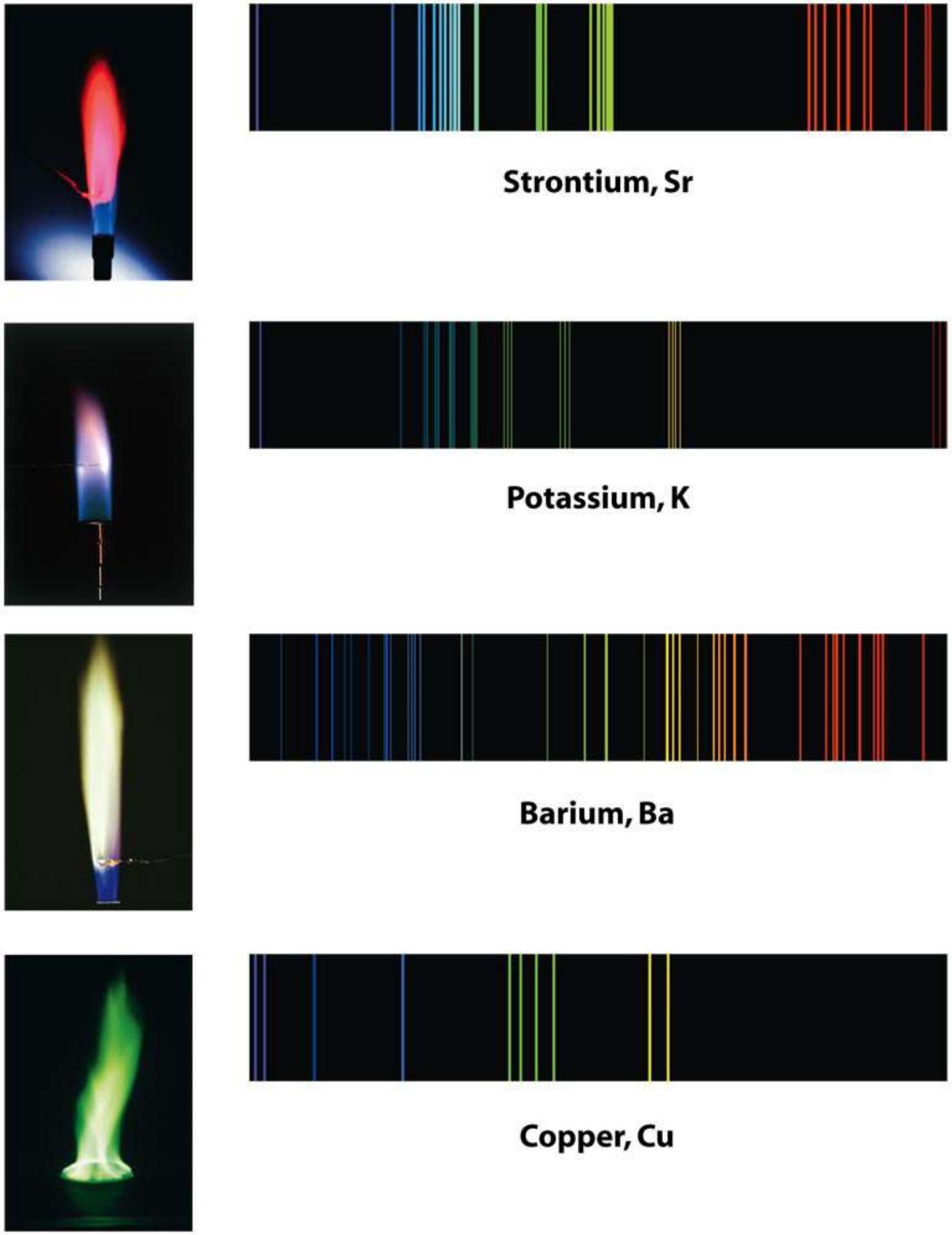
Did you know that an element can be identified by its emission spectra?

– When atoms absorb energy, electrons move into higher energy levels. These electrons then lose energy by emitting light when they return to lower energy levels.

Mercury

Nitrogen

Fingerprints of certain atoms



Atomic Spectra

– When atoms absorb energy, electrons move into higher energy levels. These electrons then lose energy by emitting light when they return to lower energy levels.

An Explanation of Atomic Spectra

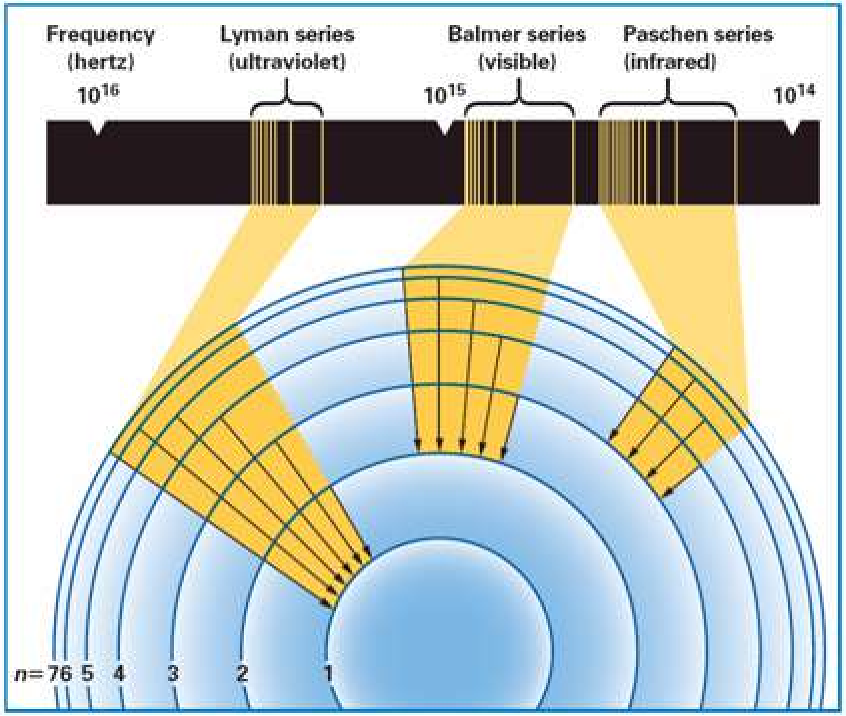
- In the Bohr model, the lone electron in the hydrogen atom can have only certain specific energies.
  - When the electron has its lowest possible energy, the atom is in its **ground state.**
  - Excitation of the electron by absorbing energy raises the atom from the ground state to an excited state.
  - A quantum of energy in the form of light is emitted when the electron drops back to a lower energy level.

An Explanation of Atomic Spectra

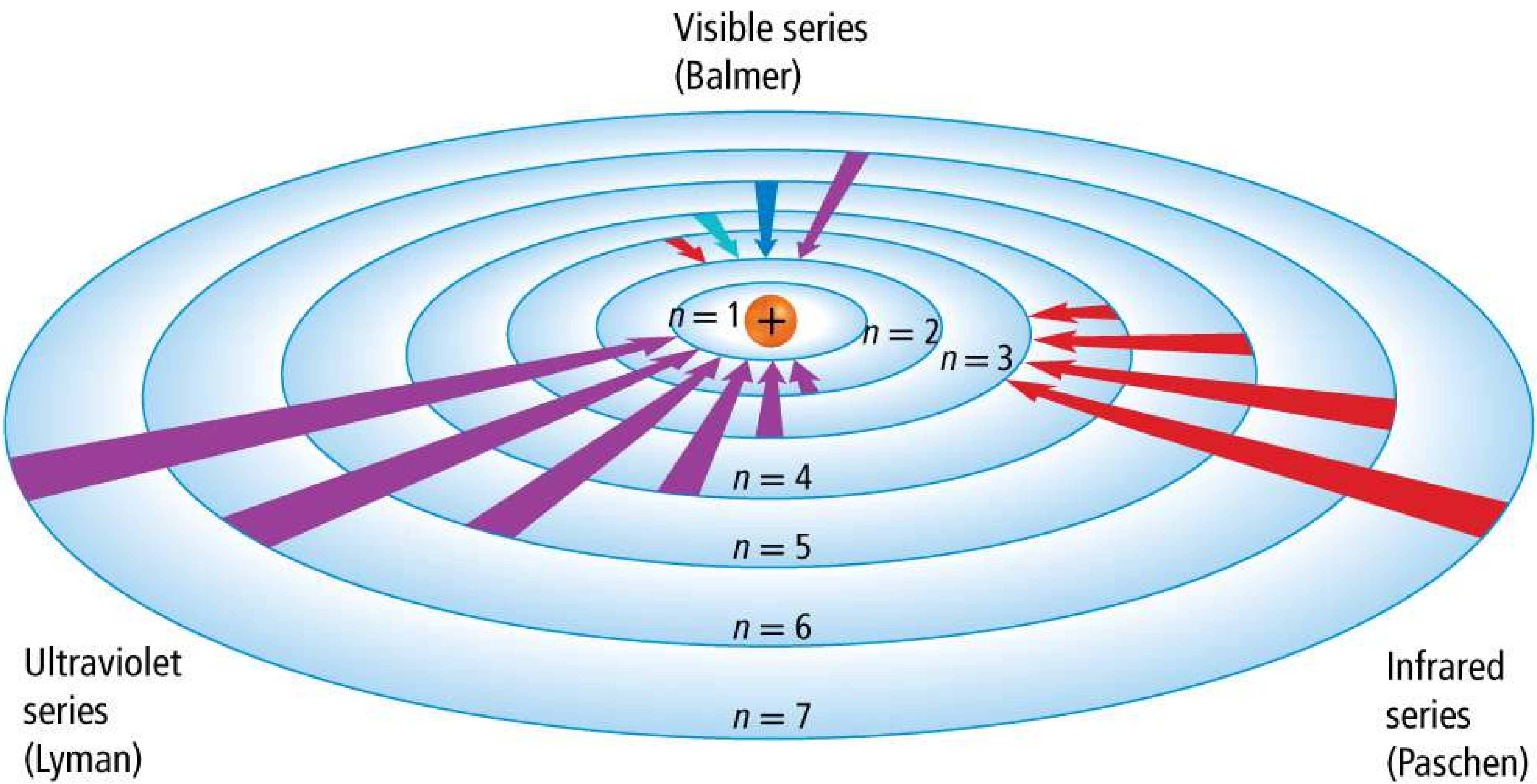
– The light emitted by an electron moving from a higher to a lower energy level has a frequency directly proportional to the energy change of the electron.

An Explanation of Atomic Spectra

- The three groups of lines in the hydrogen spectrum correspond to the transition of electrons from higher energy levels to lower energy levels.



Bohr's Model


Visible series
(Balmer)
n = 1
n = 2
n = 3
n = 4
n = 5
n = 6
n = 7
Ultraviolet
series
(Lyman)
Infrared
series
(Paschen)

The Quantum Mechanical Model

- Rutherford's and Bohr's model focused on describing the path of the electron around the nucleus like a particle (like a small baseball).

- Austrian physicist **Erwin Schrödinger (1887–1961)** treated the electron as a wave.

  - The modern description of the electrons in atoms, the **quantum mechanical model**, comes from the mathematical solutions to the Schrödinger equation.

Schrodinger Equation

$$\hat{H}\,\psi = E\,\psi$$

Electrons as Waves

EVIDENCE: DIFFRACTION PATTERNS

VISIBLE LIGHT

ELECTRONS

The Quantum Mechanical Model

- The propeller blade has the same probability of being anywhere in the blurry region, but you cannot tell its location at any instant. The electron cloud of an atom can be compared to a spinning airplane propeller.
  - **The quantum model determines the allowed energies an electron can have and how likely it is to find the electron in various locations around the nucleus.**

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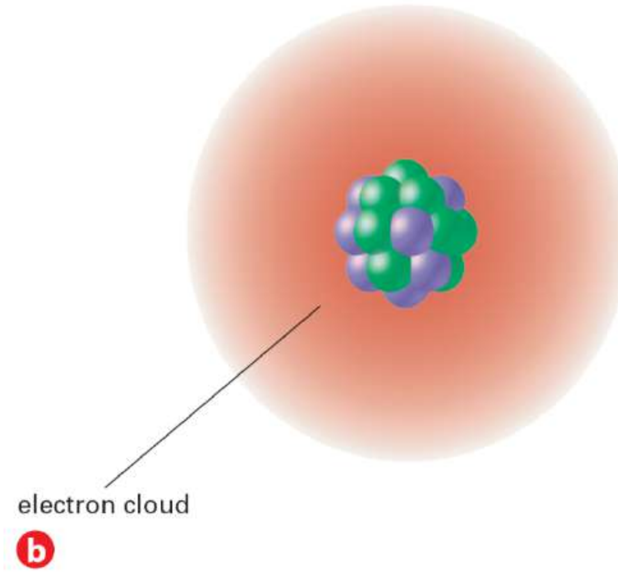
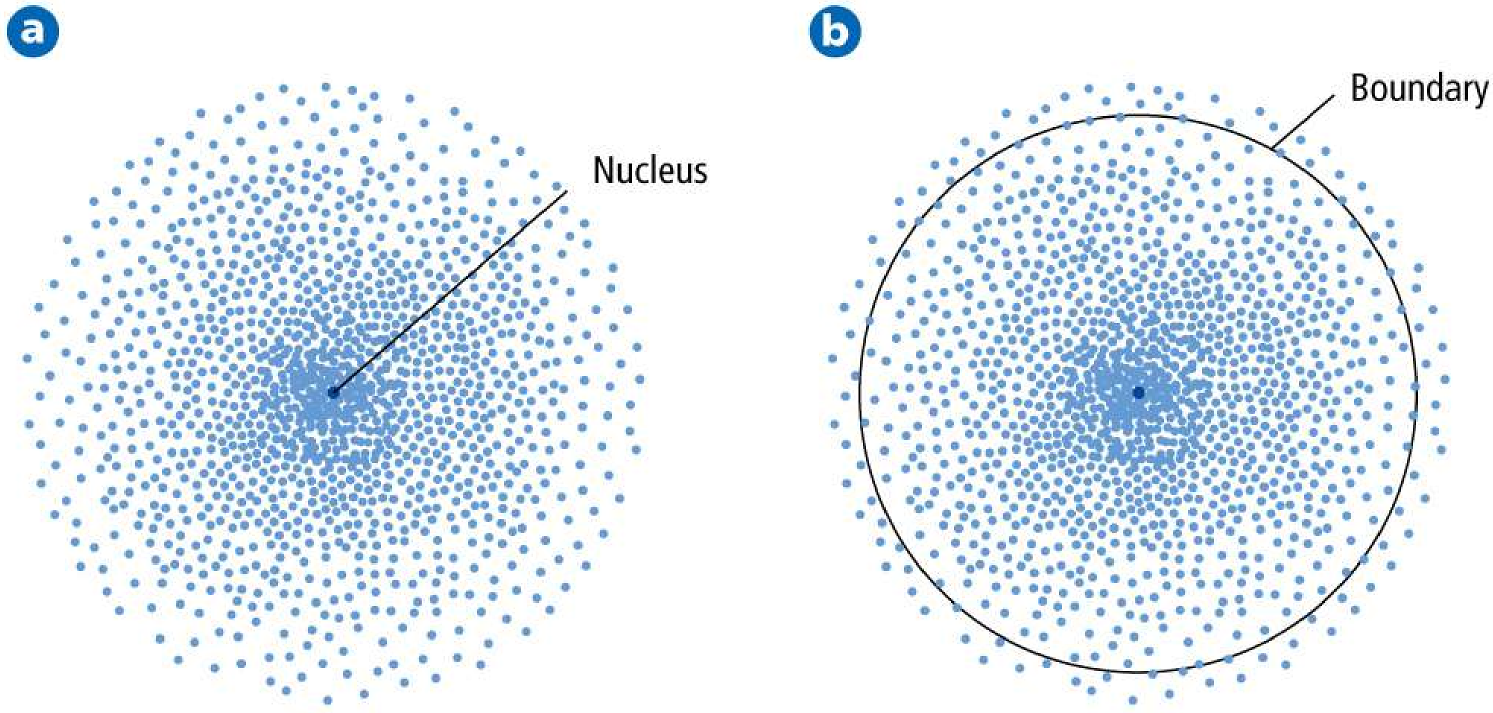
The Quantum Mechanical Model

- The probability of finding an electron within a certain volume of space surrounding the nucleus can be represented as a fuzzy cloud.
  - The cloud is more dense where the probability of finding the electron is high.



Atomic Orbitals

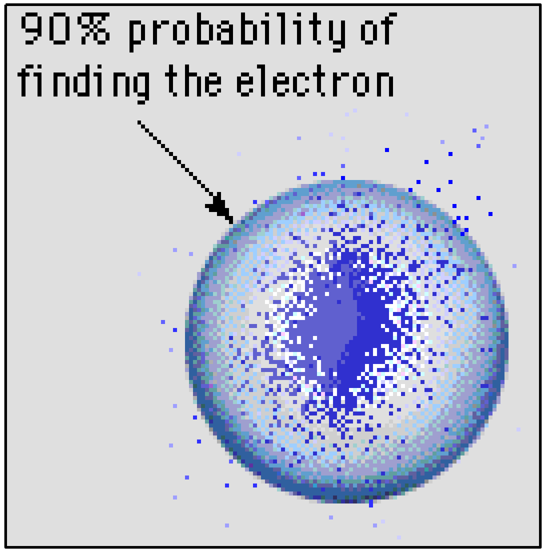
- (fuzzy cloud) = An **atomic orbital** is often thought of as a region of space in which there is a high probability of finding an electron.



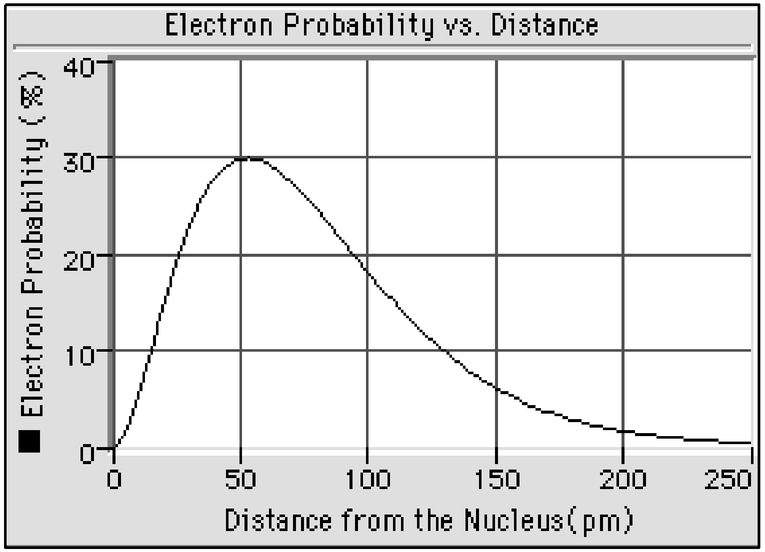
Density Maps

Quantum Mechanics

- **Orbital** ("electron cloud")
  - Region in space where there is 90% probability of finding an e^-

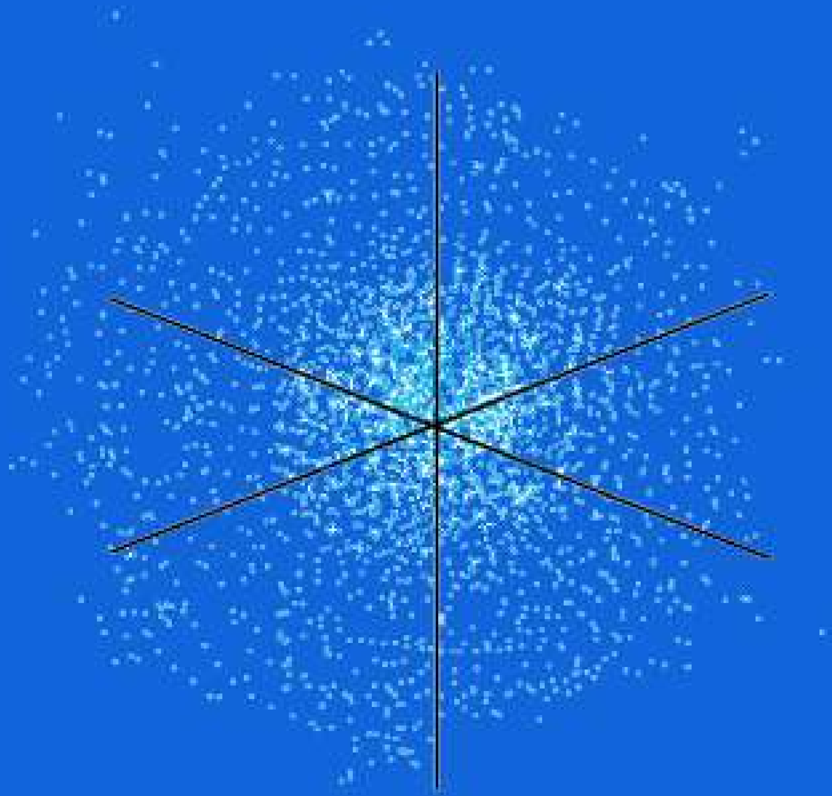


Orbital

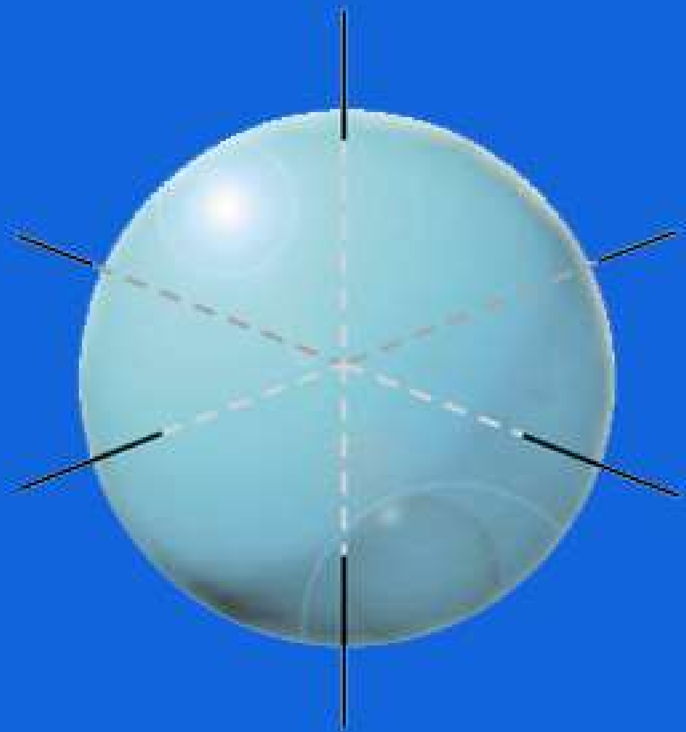


Radial Distribution Curve

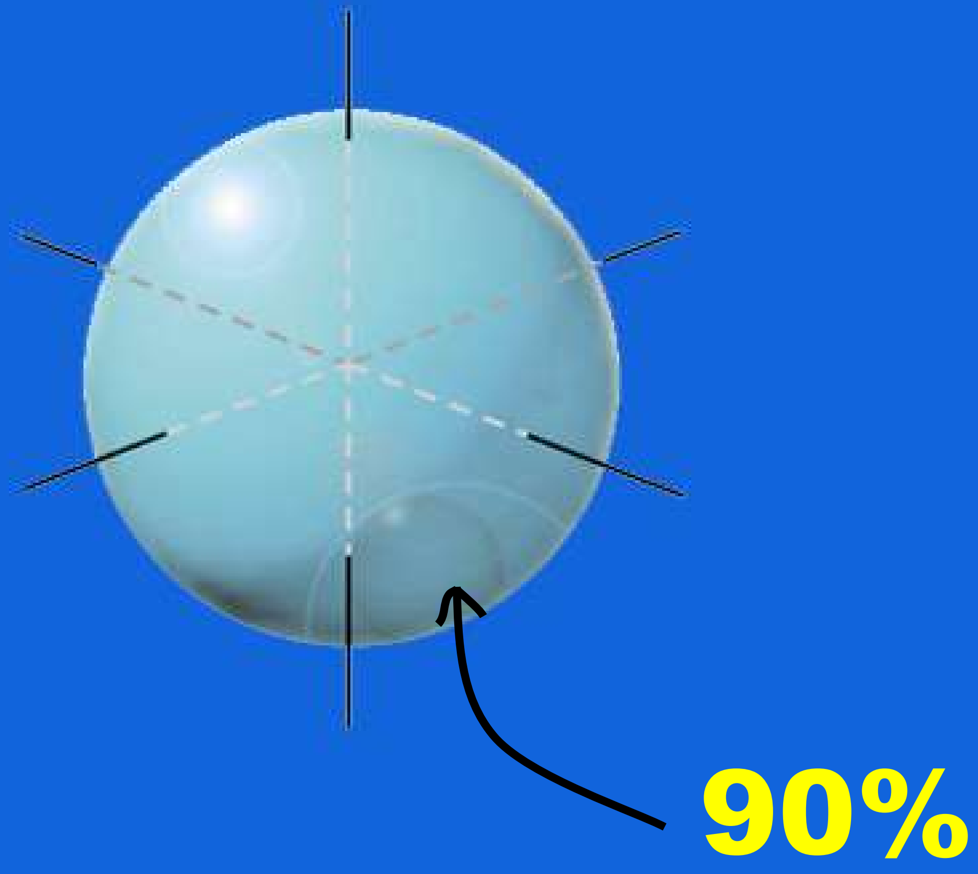
Probability cloud



Atomic orbital



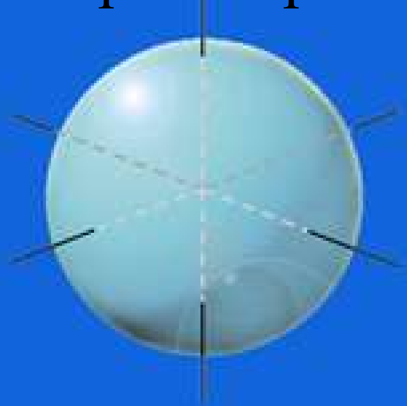
Atomic orbital

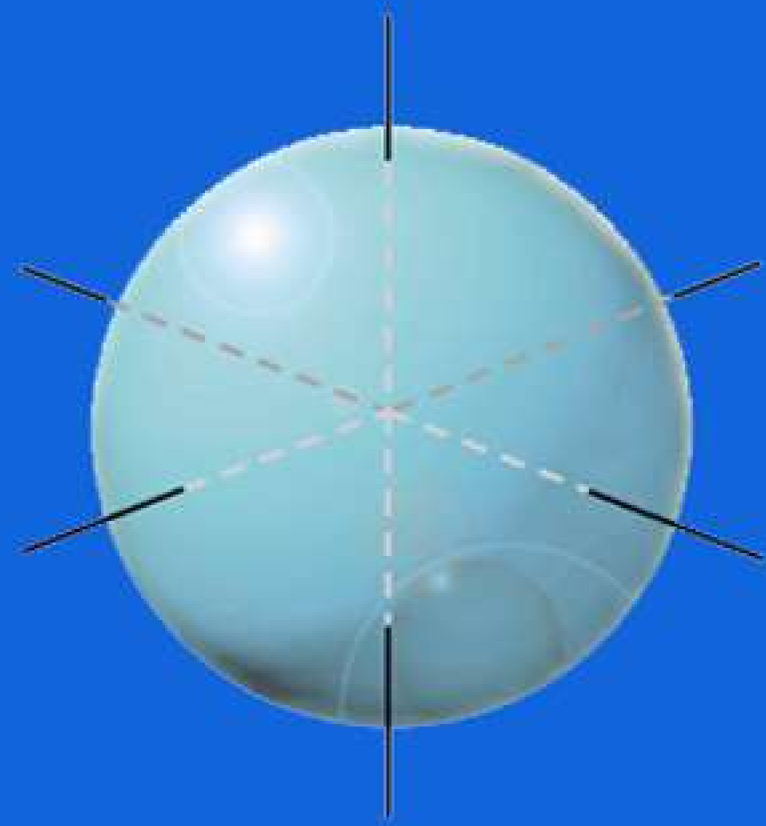


s-orbitals are
spherically shaped.

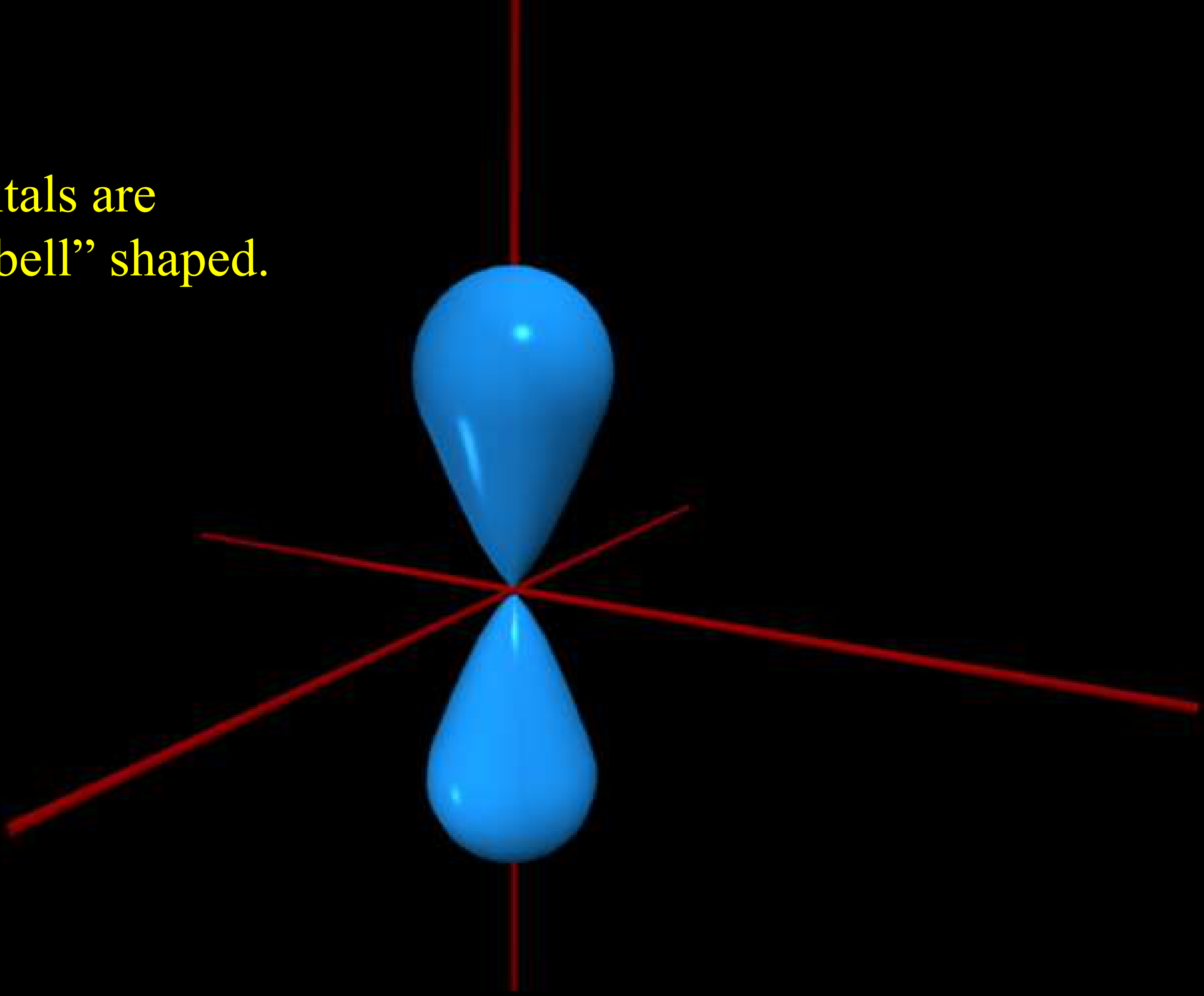
Larger atom—
More electrons
take up more space.

Smaller atom—
Fewer electrons
take up less space.

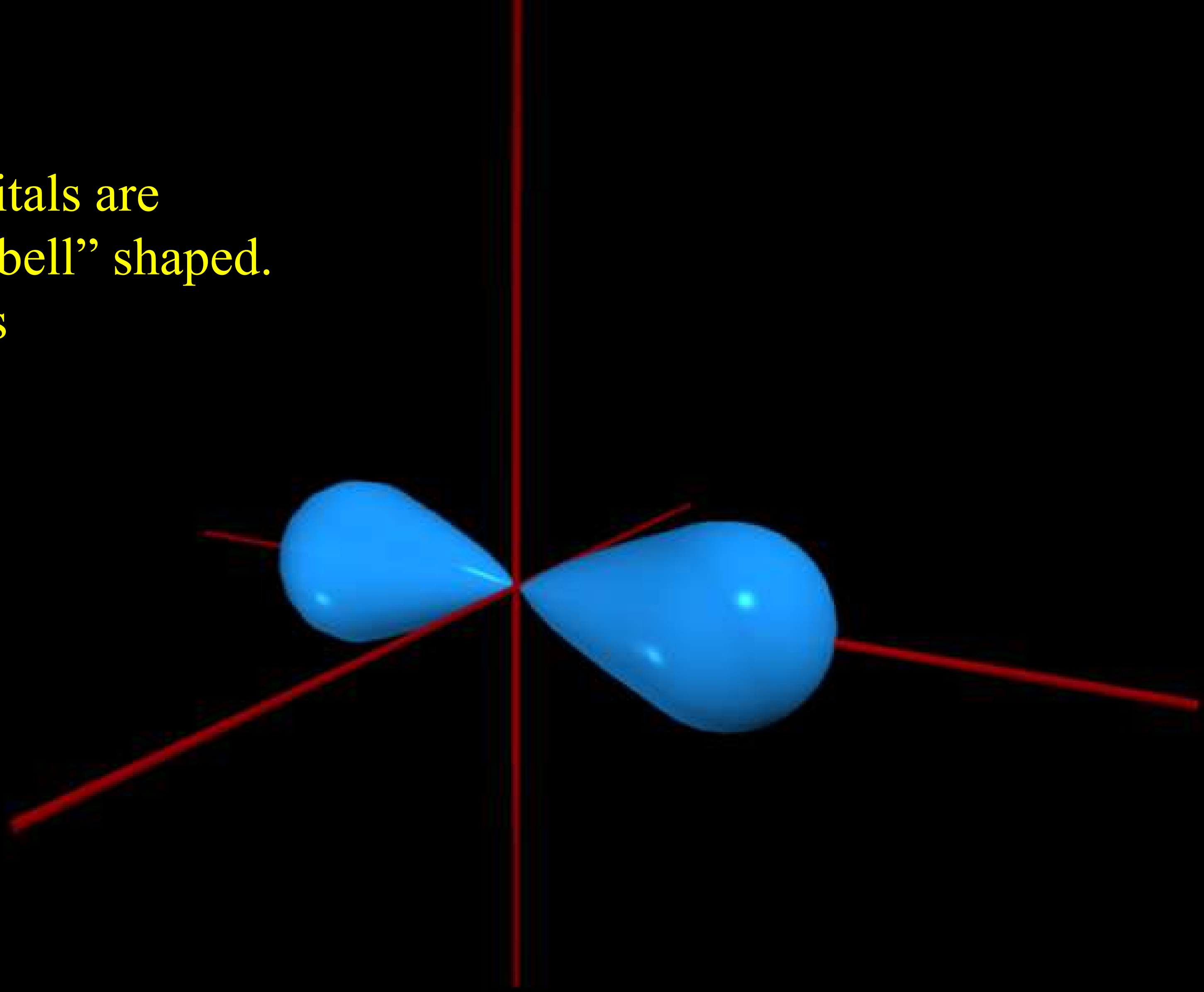




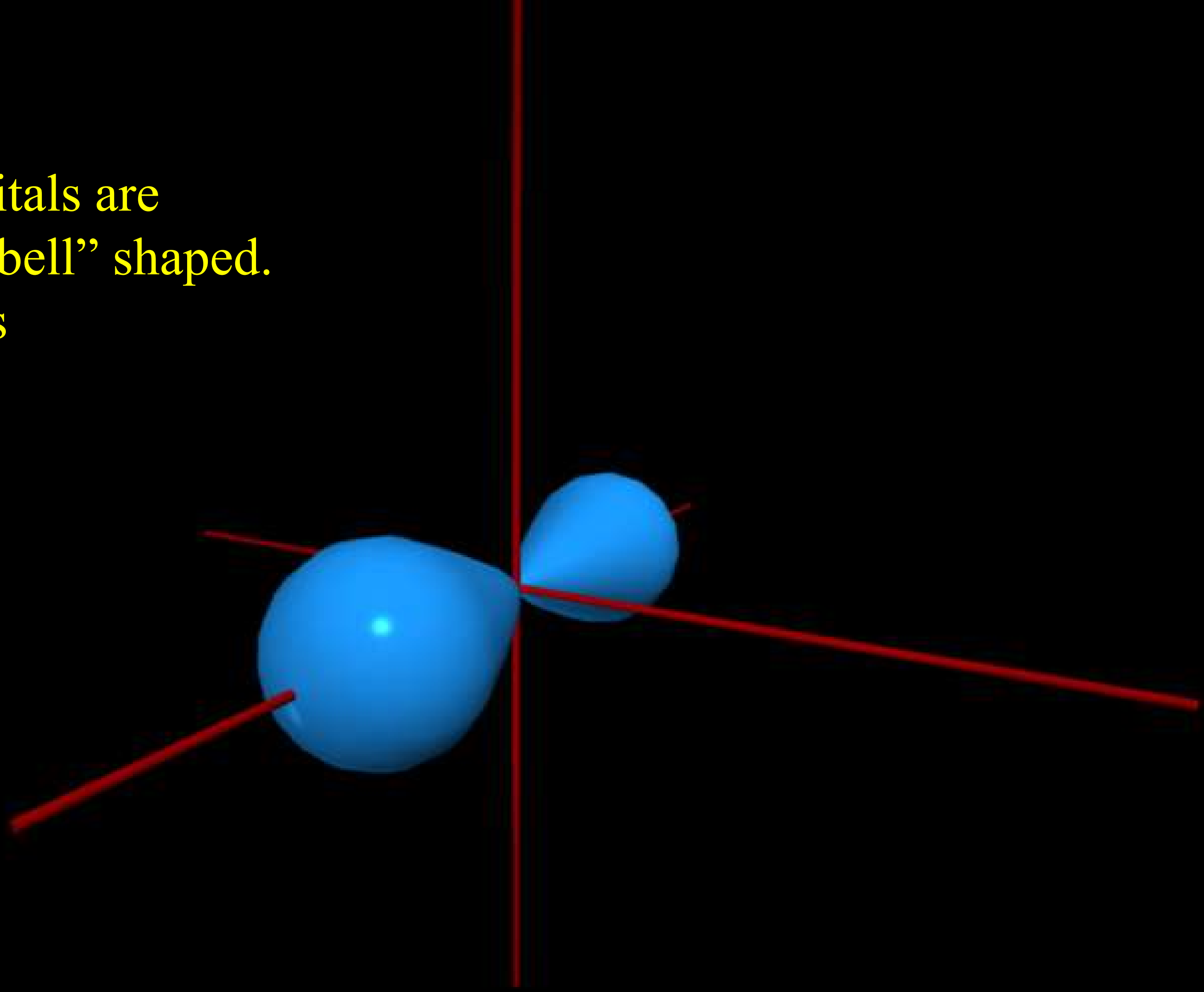
p-orbitals are
“dumbell” shaped.
z-axis



p-orbitals are
"dumbell" shaped.
x-axis



p-orbitals are
“dumbell” shaped.
y-axis



p-orbitals together
x, y, & z axes.

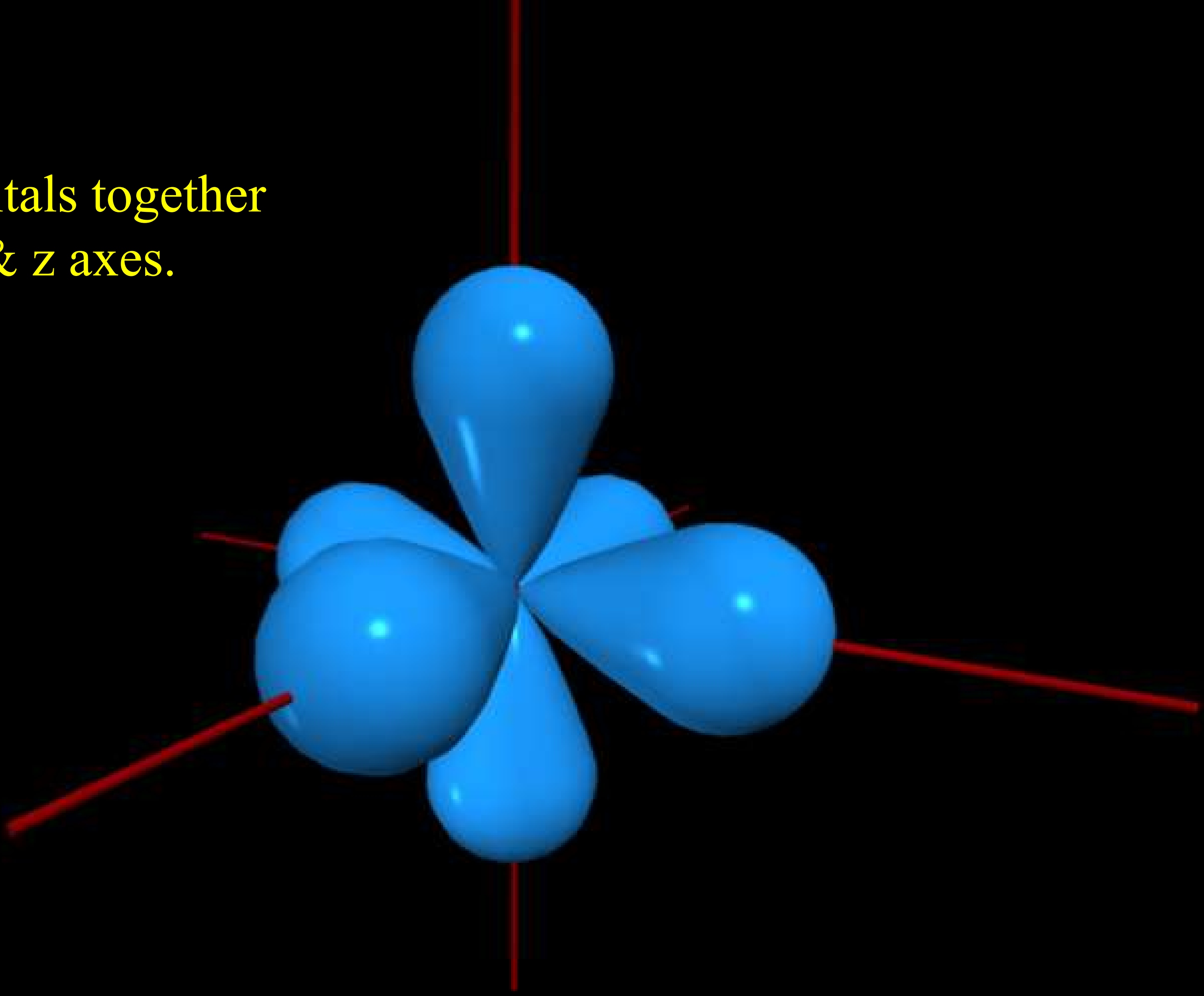
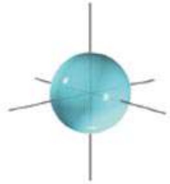
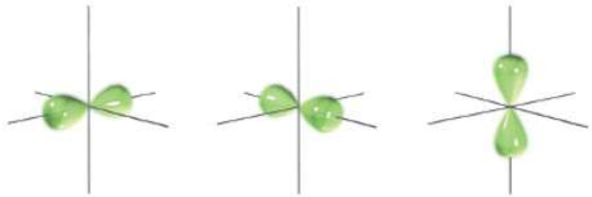
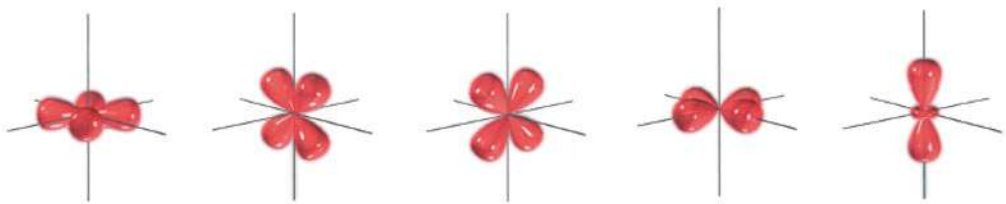
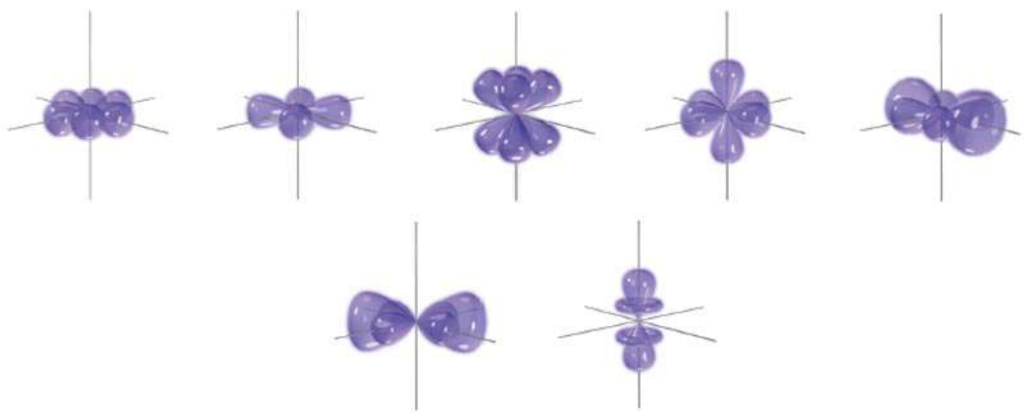
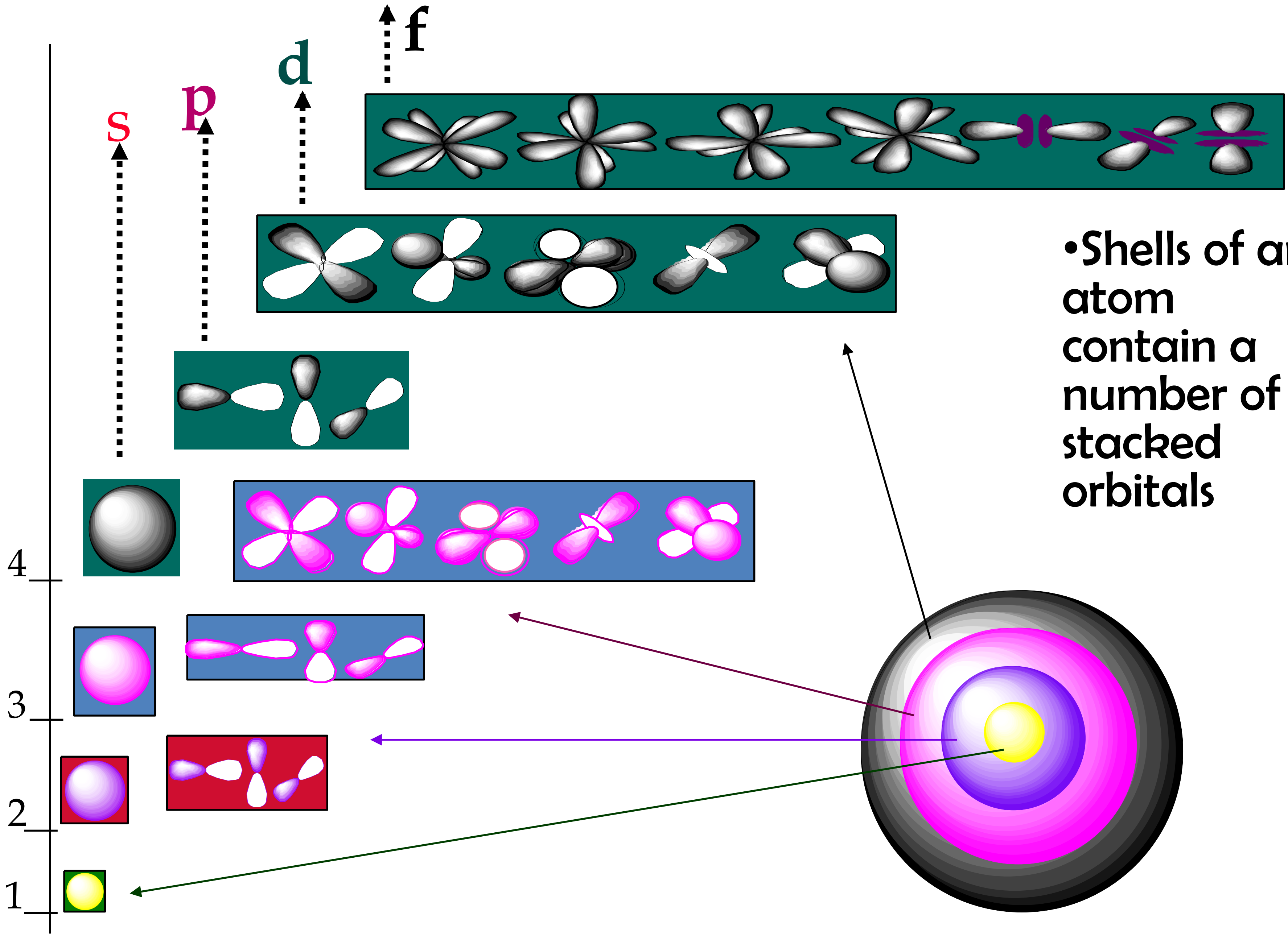


TABLE 5.1 FOUR CATEGORIES OF ATOMIC ORBITALS: *s*, *p*, *d*, *f*

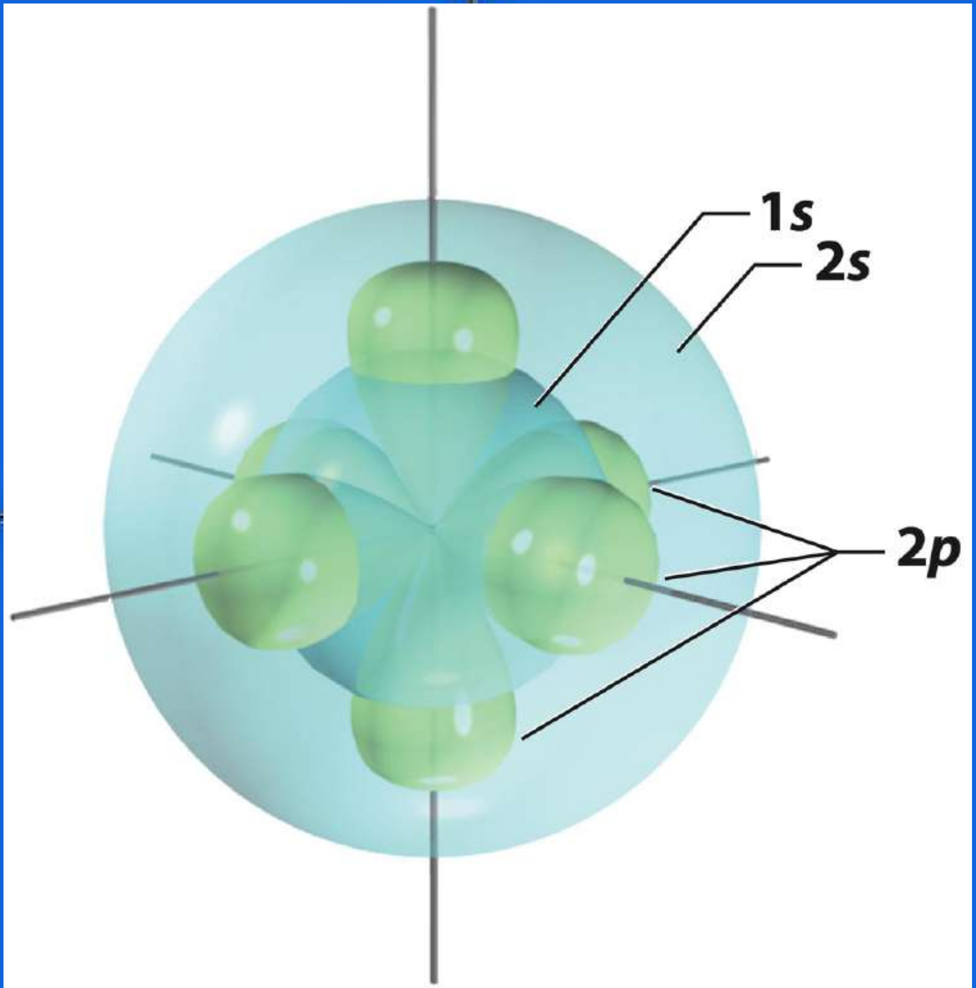
Orbital Type	Spatial Orientations
s The *s* orbital has only one shape, which is spherical.	
p There are three *p* orbitals. They differ by orientation.	
d There are five *d* orbitals.	
f There are seven *f* orbitals.	

Shells and Orbitals and Atomic Structure



- Shells of an atom contain a number of stacked orbitals

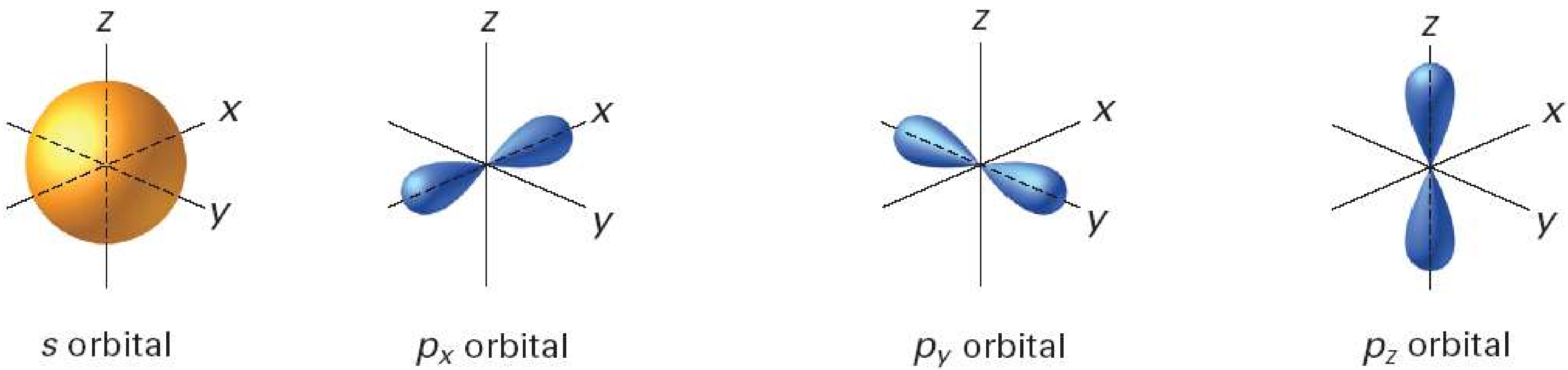
1st and 2nd level s-orbitals
and the p-orbitals all together.



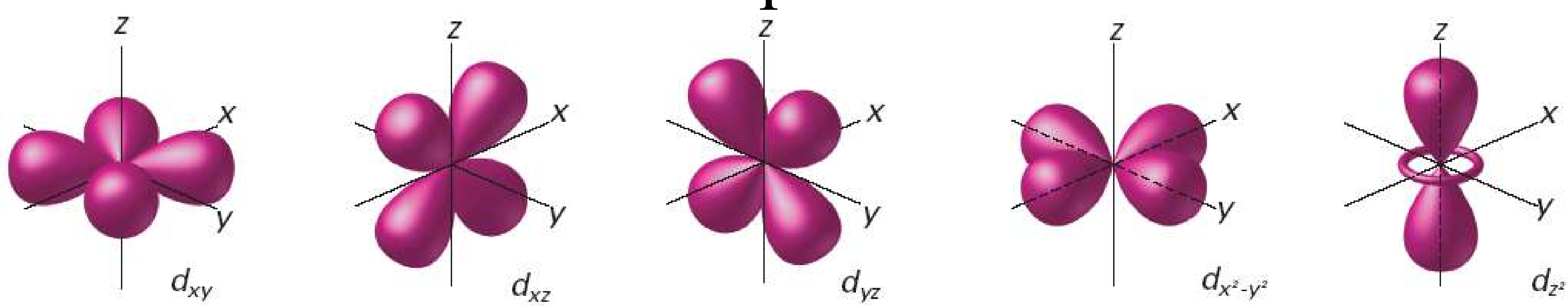
Why are Atoms Spherical?

Atomic Orbitals

- Different atomic orbitals are denoted by letters. The s orbitals are spherical, and p orbitals are dumbbell-shaped.



- Four of the five d orbitals have the same shape but different orientations in space.



Atomic Orbitals

- The numbers and kinds of atomic orbitals depend on the energy sublevel.

Energy Level, n	# of sublevels	Letter of sublevels	# of orbitals per sublevel	# of electrons in each orbital	Total electrons in energy level

Atomic Orbitals

- The numbers and kinds of atomic orbitals depend on the energy sublevel.

Energy Level, n	# of sublevels	Letter of sublevels	# of orbitals per sublevel	# of electrons in each orbital	Total electrons in energy level
1	1	s	1	2	2
2	2	s p	1 3	2 6	8
3	3	s p d	1 3 5	2 6 10	18
4	4	s p d f	1 3 5 7	2 6 10 14	32

Atomic Orbitals

- The number of electrons allowed in each of the first four energy levels are shown here.
  - A maximum of 2 electrons per orbital

Table 5.2 Maximum Numbers of Electrons	
Energy level *n*	Maximum number of electrons
1	2
2	8
3	18
4	32

Use this to find the # of electrons in an energy level $2n^2$

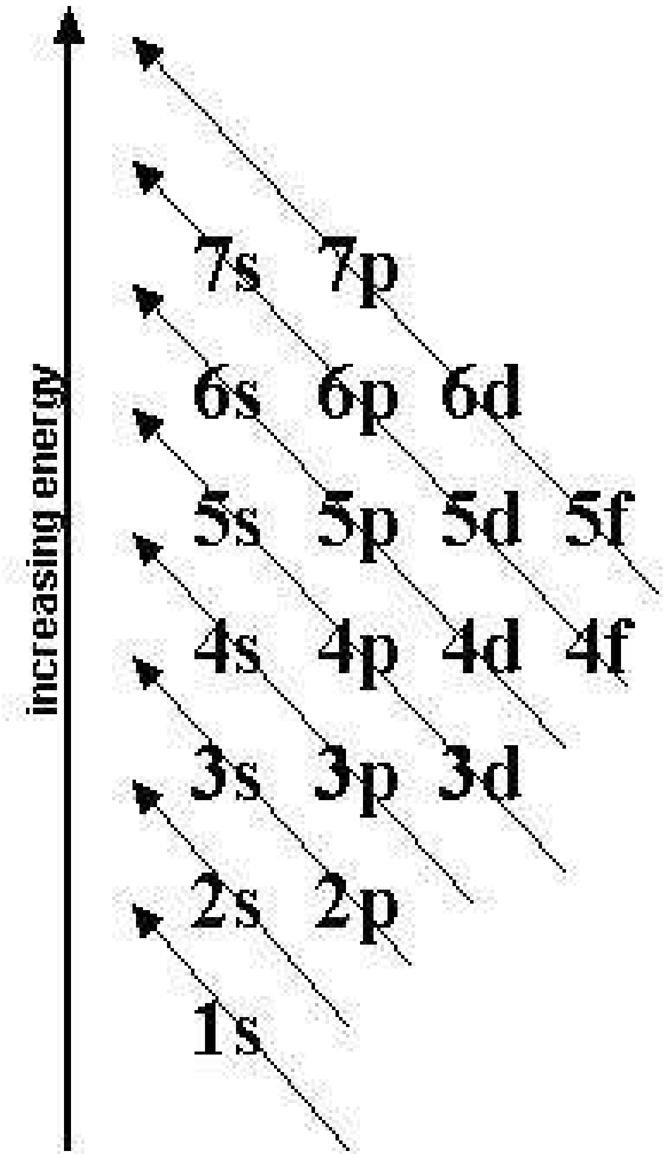
Electron Configurations

- The ways in which electrons are arranged in various orbitals around the nuclei of atoms are called **electron configurations.**
  - Three rules—the aufbau principle, the Pauli exclusion principle, and Hund's rule—tell you how to find the electron configurations of atoms.

Electron Configurations

- **Aufbau Principle**
  - According to the **aufbau principle**, electrons occupy the orbitals of lowest energy first. In the aufbau diagram below, each box represents an atomic orbital.
- **Pauli Exclusion Principle**
  - According to the **Pauli exclusion principle**, an atomic orbital may describe at most two electrons. To occupy the same orbital, two electrons must have opposite spins; that is, the electron spins must be paired.
- **Hund's Rule**
  - **Hund's rule** states that electrons occupy orbitals of the same energy in a way that makes the number of electrons with the same spin direction as large as possible.

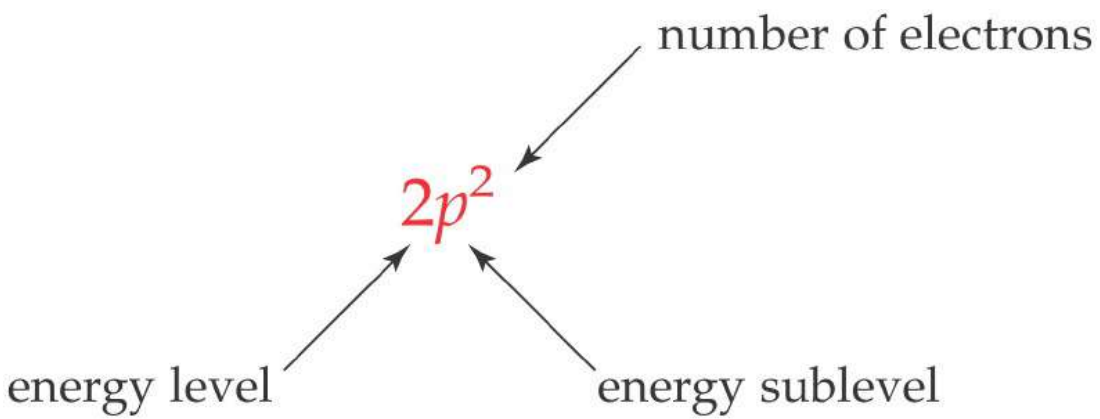
Filling Diagram for Sublevels



Aufbau Principle

Electron Configurations

- The ***electron configuration*** of an atom is a shorthand method of writing the location of electrons by sublevel.
- The sublevel is written followed by a superscript with the number of electrons in the sublevel.
  - If the $2p$ sublevel contains 2 electrons, it is written $2p^2$



Writing Electron Configurations

- First, determine how many electrons are in the atom. Iron has 26 electrons.
- Arrange the energy sublevels according to increasing energy:
  - $1s\ \ 2s\ \ 2p\ \ 3s\ \ 3p\ \ 4s\ \ 3d$ ...
- Fill each sublevel with electrons until you have used all the electrons in the atom:
  - Fe: $1s^2\ \ 2s^2\ \ 2p^6\ \ 3s^2\ \ 3p^6\ \ 4s^2\ \ 3d^6$
- The sum of the superscripts equals the atomic number of iron (26)

Electron Configuration Practice

- Write a ground state electron configuration for a neutral atom

K

Ne

Electron Configuration Practice

- Write a ground state electron configuration for these ions.

O^{2-}

Na^{+}

Electron Configuration Practice

- An excited atom has an electron or electrons which are not in the lowest energy state. Excited atoms are unstable energetically. The electrons eventually fall to a lower level. * is used to indicate an excited atom. For example: *Li $1s^2$ $3p^1$. (The ground state for Li is $1s^2$ $2s^1$.)

- Write an excited electron configuration for the following atoms.

- *Al

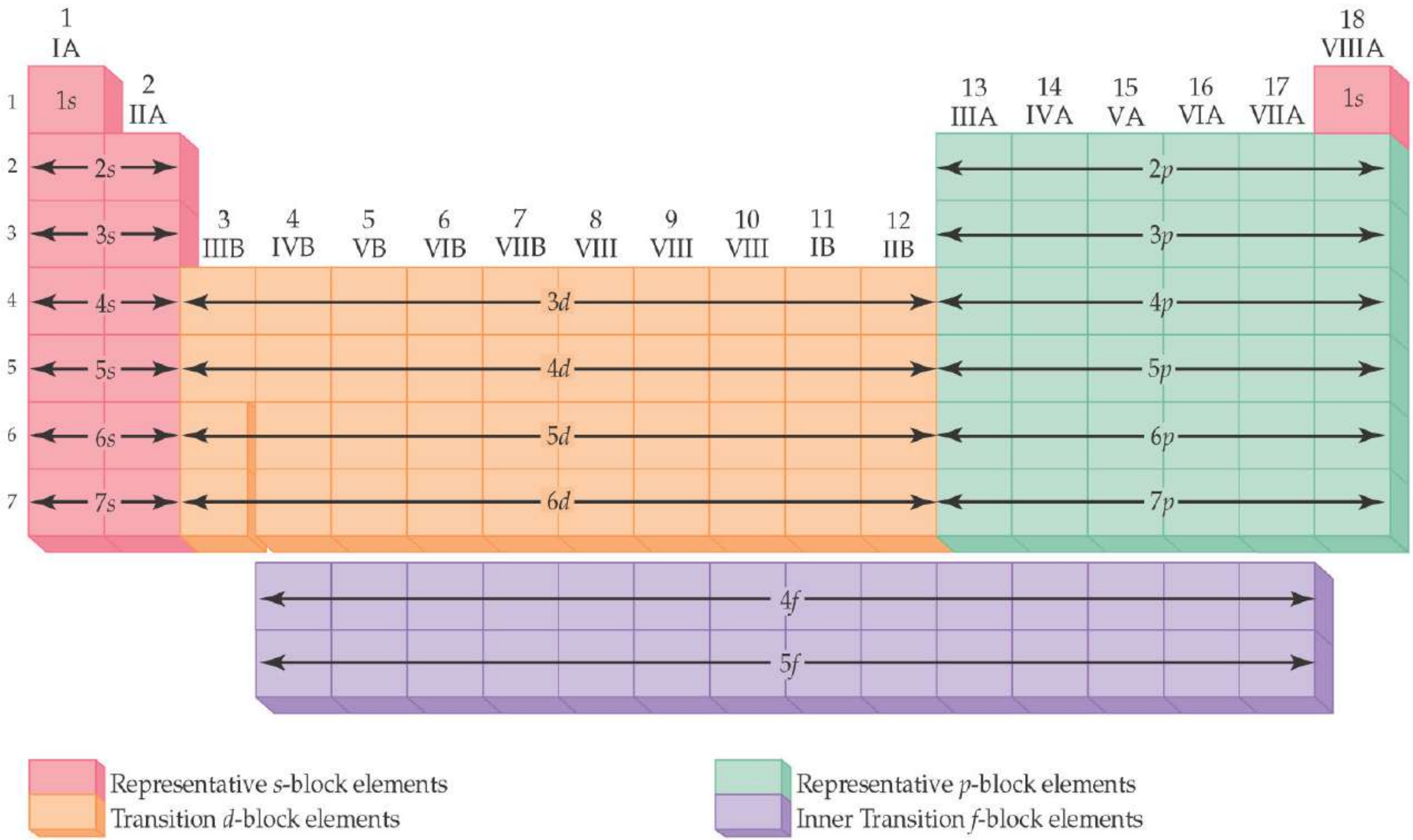
- *K

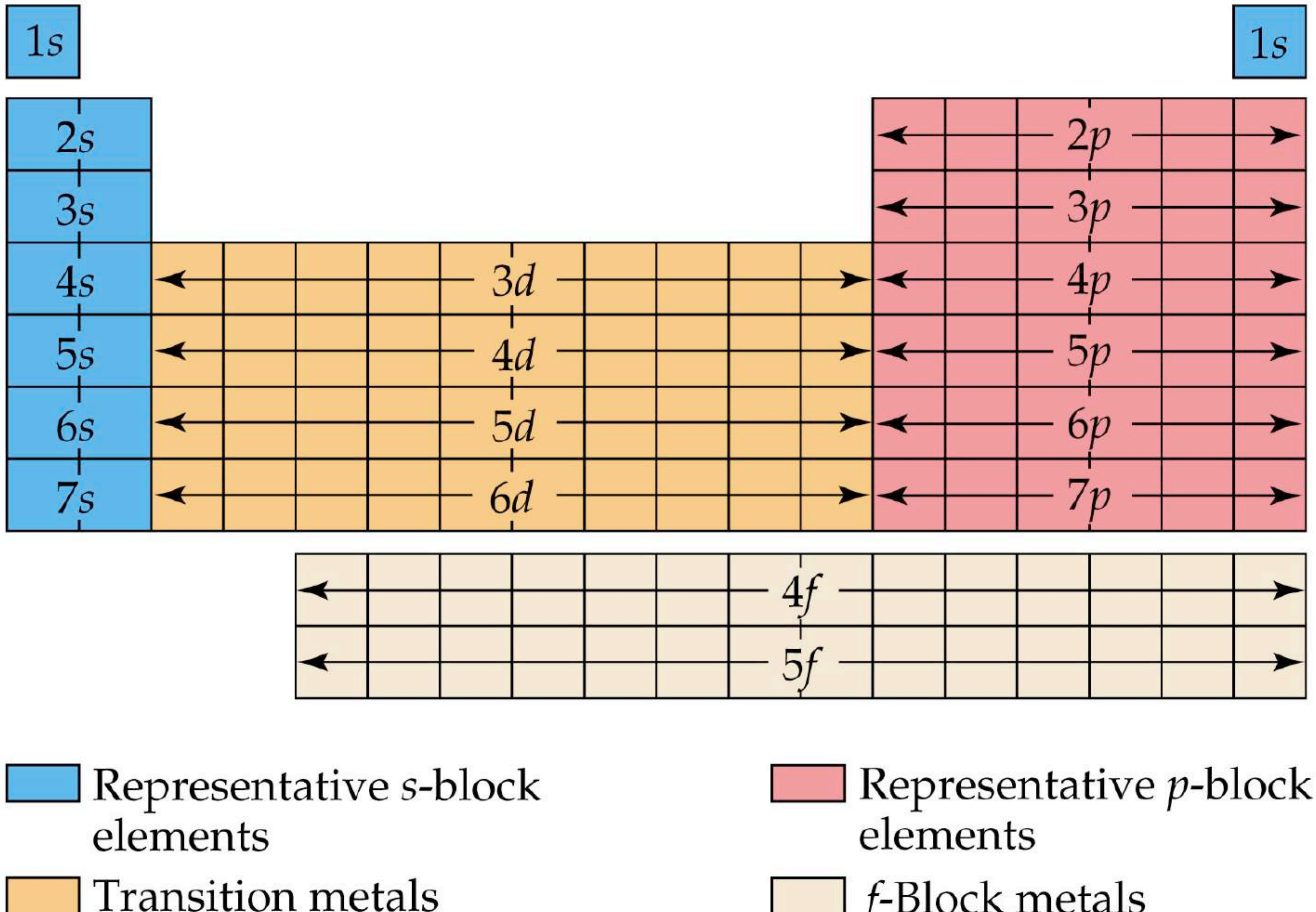
Electron Configurations and the Periodic Table

- The periodic table can be used as a guide for electron configurations.
- The period number is the value of *n*.
- Groups 1A and 2A have the *s*-orbital filled.
- Groups 3A - 8A have the *p*-orbital filled.
- Groups 3B - 2B have the *d*-orbital filled.
- The lanthanides and actinides have the *f*-orbital filled.

Blocks and Sublevels

- We can use the periodic table to predict which sublevel is being filled by a particular element.




1s
1s
2s
2p
3s
3p
4s
3d
4p
5s
4d
5p
6s
5d
6p
7s
6d
7p
4f
5f
Representative s-block elements
Representative p-block elements
Transition metals
f-Block metals

Noble Gas Core Electron Configurations

- Recall, the electron configuration for Na is:

  Na: $1s^2\ 2s^2\ 2p^6\ 3s^1$

- We can abbreviate the electron configuration by indicating the innermost electrons with the symbol of the preceding noble gas.

- The preceding noble gas with an atomic number less than sodium is neon, Ne. We rewrite the electron configuration:

  Na: [Ne] $3s^1$

Electron Configurations

Condensed Electron Configurations

- Neon completes the $2p$ subshell.
- Sodium marks the beginning of a new row.
- So, we write the condensed electron configuration for sodium as

$$\text{Na: [Ne] } 3s^1$$

- [Ne] represents the electron configuration of neon.
- **Core electrons:** electrons in [Noble Gas].
- **Valence electrons:** electrons outside of [Noble Gas].

Core	1A 1	2A 2	3B 3	4B 4	5B 5	6B 6	7B 7	8B 8	8B 9	8B 10	1B 11	2B 12	3A 13	4A 14	5A 15	6A 16	7A 17
Core	1 **H** $1s^1$																
[He]	3 **Li** $2s^1$	4 **Be** $2s^2$											5 **B** $2s^2 2p^1$	6 **C** $2s^2 2p^2$	7 **N** $2s^2 2p^3$	8 **O** $2s^2 2p^4$	9 **F** $2s^2 2p^5$
[Ne]	11 **Na** $3s^1$	12 **Mg** $3s^2$											13 **Al** $3s^2 3p^1$	14 **Si** $3s^2 3p^2$	15 **P** $3s^2 3p^3$	16 **S** $3s^2 3p^4$	17 **Cl** $3s^2 3p^5$
[Ar]	19 **K** $4s^1$	20 **Ca** $4s^2$	21 **Sc** $3d^1 4s^2$	22 **Ti** $3d^2 4s^2$	23 **V** $3d^3 4s^2$	24 **Cr** $3d^5 4s^1$	25 **Mn** $3d^5 4s^2$	26 **Fe** $3d^6 4s^2$	27 **Co** $3d^7 4s^2$	28 **Ni** $3d^8 4s^2$	29 **Cu** $3d^{10} 4s^1$	30 **Zn** $3d^{10} 4s^2$	31 **Ga** $3d^{10} 4s^2 4p^1$	32 **Ge** $3d^{10} 4s^2 4p^2$	33 **As** $3d^{10} 4s^2 4p^3$	34 **Se** $3d^{10} 4s^2 4p^4$	35 **Br** $3d^{10} 4s^2 4p^5$
[Kr]	37 **Rb** $5s^1$	38 **Sr** $5s^2$	39 **Y** $4d^1 5s^2$	40 **Zr** $4d^2 5s^2$	41 **Nb** $4d^3 5s^2$	42 **Mo** $4d^5 5s^1$	43 **Tc** $4d^5 5s^2$	44 **Ru** $4d^7 5s^1$	45 **Rh** $4d^8 5s^1$	46 **Pd** $4d^{10}$	47 **Ag** $4d^{10} 5s^1$	48 **Cd** $4d^{10} 5s^2$	49 **In** $4d^{10} 5s^2 5p^1$	50 **Sn** $4d^{10} 5s^2 5p^2$	51 **Sb** $4d^{10} 5s^2 5p^3$	52 **Te** $4d^{10} 5s^2 5p^4$	53 **I** $4d^{10} 5s^2 5p^5$
[Xe]	55 **Cs** $6s^1$	56 **Ba** $6s^2$	71 **Lu** $4f^{14} 5d^1 6s^2$	72 **Hf** $4f^{14} 5d^2 6s^2$	73 **Ta** $4f^{14} 5d^3 6s^2$	74 **W** $4f^{14} 5d^4 6s^2$	75 **Re** $4f^{14} 5d^5 6s^2$	76 **Os** $4f^{14} 5d^6 6s^2$	77 **Ir** $4f^{14} 5d^7 6s^2$	78 **Pt** $4f^{14} 5d^9 6s^1$	79 **Au** $4f^{14} 5d^{10} 6s^1$	80 **Hg** $4f^{14} 5d^{10} 6s^2$	81 **Tl** $4f^{14} 5d^{10} 6s^2 6p^1$	82 **Pb** $4f^{14} 5d^{10} 6s^2 6p^2$	83 **Bi** $4f^{14} 5d^{10} 6s^2 6p^3$	84 **Po** $4f^{14} 5d^{10} 6s^2 6p^4$	85 **At** $4f^{14} 5d^{10} 6s^2 6p^5$
[Rn]	87 **Fr** $7s^1$	88 **Ra** $7s^2$	103 **Lr** $5f^{14} 6d^1 7s^2$	104 **Rf** $5f^{14} 6d^2 7s^2$	105 **Db** $5f^{14} 6d^3 7s^2$	106 **Sg** $5f^{14} 6d^4 7s^2$	107 **Bh** $5f^{14} 6d^5 7s^2$	108 **Hs** $5f^{14} 6d^6 7s^2$	109 **Mt** $5f^{14} 6d^7 7s^2$	110	111	112		114		116	

Core	Series														
[Xe]	Lanthanide series	57 **La** $5d^1 6s^2$	58 **Ce** $4f^1 5d^1 6s^2$	59 **Pr** $4f^3 6s^2$	60 **Nd** $4f^7 6s^2$	61 **Pm** $4f^5 6s^2$	62 **Sm** $4f^6 6s^2$	63 **Eu** $4f^7 6s^2$	64 **Gd** $4f^7 5d^1 6s^2$	65 **Tb** $4f^9 6s^2$	66 **Dy** $4f^{10} 6s^2$	67 **Ho** $4f^{11} 6s^2$	68 **Er** $4f^{12} 6s^2$	69 **Tm** $4f^{13} 6s^2$	70 **Yb** $4f^{14} 6s^2$
[Rn]	Actinide series	89 **Ac** $6d^1 7s^2$	90 **Th** $6d^2 7s^2$	91 **Pa** $5f^2 6d^1 7s^2$	92 **U** $5f^3 6d^1 7s^2$	93 **Np** $5f^4 6d^1 7s^2$	94 **Pu** $5f^6 7s^2$	95 **Am** $5f^7 7s^2$	96 **Cm** $5f^7 6d^1 7s^2$	97 **Bk** $5f^9 7s^2$	98 **Cf** $5f^{10} 7s^2$	99 **Es** $5f^{11} 7s^2$	100 **Fm** $5f^{12} 7s^2$	101 **Md** $5f^{13} 7s^2$	102 **No** $5f^{14} 7s^2$

Metals Metalloids Nonmetals

Electron Configurations

- **Orbital Filling Diagram**

Table 5.3

Electron Configurations for Some Selected Elements

Element	Orbital filling 1s	2s	$2p_x$	$2p_y$	$2p_z$	3s	Electron configuration
H	↑						$1s^1$
He	↑↓						$1s^2$
Li	↑↓	↑					$1s^2 2s^1$
C	↑↓	↑↓	↑	↑			$1s^2 2s^2 2p^2$
N	↑↓	↑↓	↑	↑	↑		$1s^2 2s^2 2p^3$
O	↑↓	↑↓	↑↓	↑	↑		$1s^2 2s^2 2p^4$
F	↑↓	↑↓	↑↓	↑↓	↑		$1s^2 2s^2 2p^5$
Ne	↑↓	↑↓	↑↓	↑↓	↑↓		$1s^2 2s^2 2p^6$
Na	↑↓	↑↓	↑↓	↑↓	↑↓	↑	$1s^2 2s^2 2p^6 3s^1$

Exceptional Electron Configurations

- Some actual electron configurations differ from those assigned using the aufbau principle because half-filled sublevels are not as stable as filled sublevels, but they are more stable than other configurations.

Exceptional Electron Configurations

- Exceptions to the aufbau principle are due to subtle electron-electron interactions in orbitals with very similar energies.
- Copper has an electron configuration that is an exception to the aufbau principle.