

Jacqueline Bennett • SUNY Oneonta

### **Chapter Objectives**

- Describe similarities and differences between various light sources.
- Describe waves in terms of frequency, wavelength, and amplitude.
- Interconvert between the frequency, wavelength, and amplitude of light and relate those those quantities to characteristics such as color and brightness.
- Describe the photoelectric effect by stating what sort of experiment is involved and what results are seen.

### **Chapter Objectives**

- Explain how the results of the photoelectric effect experiment are consistent with a photon model of light.
- Use Planck's equation to calculate the energy of a photon from its wavelength or frequency.
- Use ideas about conservation of energy to explain how the observation of atomic spectra implies that atoms have quantized energies.

### **Chapter Objectives**

- Use an energy-level diagram to predict the wavelengths or frequencies of light that an atom will absorb or emit, or use the observed wavelengths or frequencies to determine the allowed energy levels.
- Describe similarities and differences between the Bohr model and the quantum mechanical model of atomic structure.
- Recognize how quantum numbers arise as a consequence of the wave model.
- · Define the term orbital.

### **Chapter Objectives**

- Identify an orbital (as 1s, 3p, etc.) from its quantum numbers or vice versa.
- List the number of orbitals of each type (1s, 3p, etc.) in an atom.
- Sketch the shapes of *s* and *p* orbitals and recognize orbitals by their shapes.
- · Rank various orbitals in terms of size and energy.

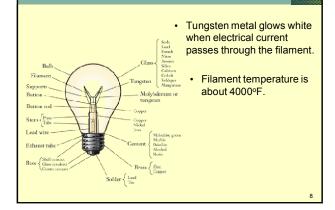
### Chapter Objectives

- Use the Pauli exclusion principle and Hund's rule to write electron configurations for atoms and ions of main group elements.
- Explain the connection between valence electron configurations and the periodic table.
- Define the following properties of atoms: atomic radius, ionization energy, and electron affinity.
- State how the above properties vary with position in the periodic table.

### Incandescent and Fluorescent Lights

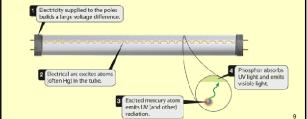
- When metals are heated, they glow (incandescence)
  - The specific color of light emitted depends on the temperature of the metal.
  - Low temperature emission is red, higher temperature emission is orange, and eventually the emission becomes white.
  - Light bulbs produce light by heating a metal filament with electricity.

### Incandescent and Fluorescent Lights



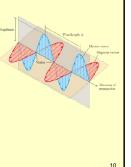
### Gases can be made to emit light when an arc of electricity

- Gases can be made to emit light when an arc of electricity passes through a poorly conducting gas.
  - The electrical arc excites gas molecules, which emit light that then interacts with the phosphor to reemit light of many different possible colors. (fluorescence)



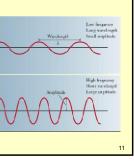
### The Electromagnetic Spectrum

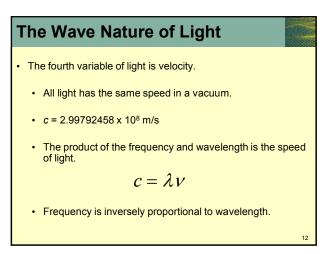
- Visible light is a small portion of the electromagnetic radiation spectrum detected by our eyes.
- Electromagnetic radiation includes radio waves, microwaves and Xrays.
  - Described as a wave traveling through space.
  - There are two components to electromagnetic radiation, an electric field and magnetic field.



### The Wave Nature of Light Wavelength, λ, is the distance

- between two corresponding points on a wave.
- Amplitude is the size or "height" of a wave.
- Frequency, v, is the number of cycles of the wave passing a given point per second, usually expressed in Hz.

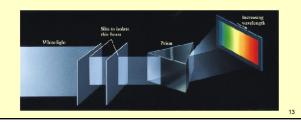




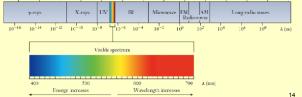
### The Wave Nature of Light

 Refraction is the bending of light when it passes from one medium to another of different density.

- Speed of light changes.
- Light bends at an angle depending on its wavelength.
- Light separates into its component colors.



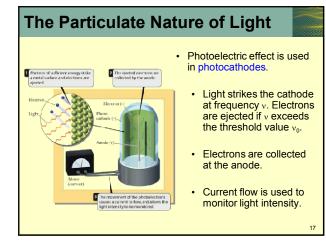
### The Wave Nature of Light Electromagnetic radiation can be categorized in terms of wavelength or frequency. Visible light is a small portion of the entire electromagnetic spectrum.

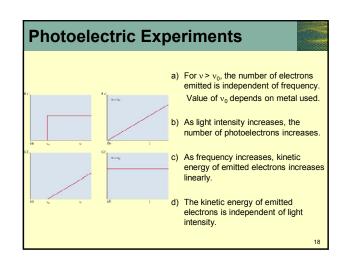


# Example Problem 6.1 • Neon lights emit an orange-red colored glow. This light has a wavelength of 670 nm. What is the frequency of this light?

### The Particulate Nature of Light

- Photoelectric effect: light striking a metal surface generates photoelectrons.
  - The light's energy is transferred to electrons in metal.
  - With sufficient energy, electrons "break free" of the metal.
  - Electrons given more energy move faster (have higher kinetic energy) when they leave the metal.





22

24

### The Particulate Nature of Light

- The photoelectric effect is not explained using a wave description but is explained by modeling light as a particle.
- Wave-particle duality depending on the situation, light is best described as a wave or a particle.
  - Light is best described as a particle when light is imparting energy to another object.
  - Particles of light are called photons.
  - Neither waves nor particles provide an accurate description of all the properties of light. Use the model that best describes the properties being examined.

### The Particulate Nature of Light

- The energy of a photon (*E*) is proportional to the frequency (v).
  - and is inversely proportional to the wavelength (λ).
  - h = Planck's constant = 6.626 x 10<sup>-34</sup> J s

$$E = hv = \frac{hc}{\lambda}$$

## The laser in a standard laser printer emits light with a wavelength of 780.0 nm. What is the energy of a photon of this light?

### The Particulate Nature of Light

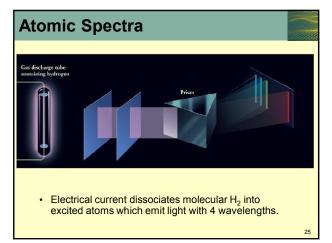
- · Binding Energy energy holding an electron to a metal.
  - Threshold frequency,  $v_0$  minimum frequency of light needed to emit an electron.
  - For frequencies below the threshold frequency, no electrons are emitted.
  - For frequencies above the threshold frequency, extra energy is imparted to the electrons as kinetic energy.
     *E*<sub>photon</sub> = Binding *E* + Kinetic *E*
  - · This explains the photoelectric effect.

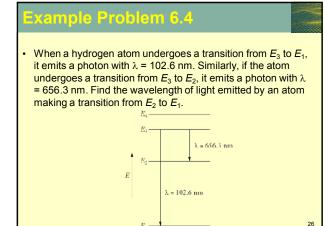
### Example Problem 6.3

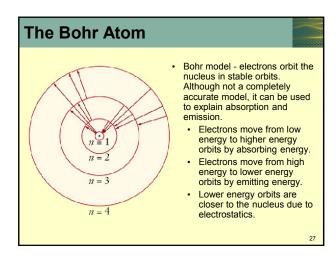
 In a photoelectric experiment, ultraviolet light with a wavelength of 337 nm was directed at the surface of a piece of potassium metal. The kinetic energy of the ejected electrons was measured as 2.30 x 10<sup>-19</sup> J. What is the electron binding energy for potassium?

### **Atomic Spectra**

- Atomic Spectra: the particular pattern of wavelengths absorbed and emitted by an element.
  - · Wavelengths are well separated or discrete.
  - · Wavelengths vary from one element to the next.
- Atoms can only exist in a few states with very specific energies.
  - When light is emitted, the atom goes from a higher energy state to a lower energy state.







### The Bohr Atom

- Excited state: grouping of electrons that is not at the lowest possible energy state.
- Ground state: grouping of electrons that is at the lowest possible energy state.
  - Atoms return to the ground state by emitting energy as light.

### The Quantum Mechanical Model of the Atom

- Quantum mechanical model replaced the Bohr model of the atom.
  - Bohr model depicted electrons as particles in circular orbits of fixed radius.
  - Quantum mechanical model depicts electrons as waves spread through a region of space (delocalized) called an orbital.

29

• The energy of the orbitals is quantized like the Bohr model.

### The Quantum Mechanical Model of the Atom

- Diffraction of electrons shown in 1927.
  - · Electrons exhibit wave-like behavior.
- Wave behavior described using a wave function, the Schrödinger equation.
  - *H* is an operator, *E* is energy and  $\psi$  is the wave function.

 $H\psi = E\psi$ 

28

34

### **Potential Energy and Orbitals**

- Total energy for electrons includes potential and kinetic energies.
  - Potential energy more important in describing atomic structure; associated with coulombic attraction between positive nucleus and negative electrons.
- Multiple solutions exist for the wave function for any given potential interaction.
  - *n* is the index that labels the different solutions.

 $H\psi_n = E\psi_n$ 

31

33

### Potential Energy and Orbitals

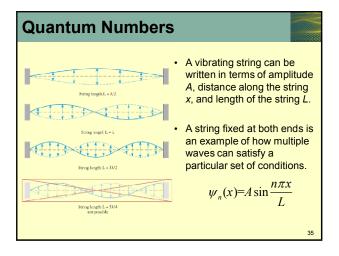
- $\psi_n$  can be written in terms of two components.
  - Radial component, depends on the distance from the nucleus.
  - Angular component, depends on the direction or orientation of electron with respect to the nucleus.

### **Potential Energy and Orbitals**

- The wave function may have positive and negative signs in different regions.
  - Square of the wave function, ψ<sup>2</sup>, is always positive and gives probability of finding an electron at any particular point.
- · Each solution of the wave function defines an orbital.
  - Each solution labeled by a letter and number combination: 1*s*, 2*s*, 2*p*, 3*s*, 3*p*, 3*d*, etc.
  - An orbital in quantum mechanical terms is actually a region of space rather than a particular point.

### **Quantum Numbers**

- Quantum numbers solutions to the functions used to solve the wave equation.
  - Quantum numbers used to name atomic orbitals.
  - Vibrating string fixed at both ends can be used to illustrate a function of the wave equation.



### **Quantum Numbers**

- When solving the Schrödinger equation, three quantum numbers are used.
  - Principal quantum number, *n* (*n* = 1, 2, 3, 4, 5, ...)
  - Secondary quantum number, I
  - Magnetic quantum number, m

### **Quantum Numbers**

- The principal quantum number, *n*, defines the shell in which a particular orbital is found.
  - *n* must be a positive integer
  - n = 1 is the first shell, n = 2 is the second shell, etc.
  - · Each shell has different energies.

### **Quantum Numbers**

- The secondary quantum number, I, indexes energy differences between orbitals in the same shell in an atom.
- I has integral values from 0 to n-1.
  - I specifies subshell
  - Each shell contains as many I values as its value of *n*.
  - Table 6.1

37

39

Letter designations for the secondary quantum number

3

f

4

g

40

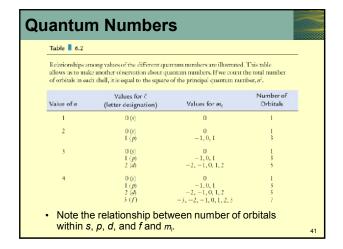
<i>ℓ</i> -value	0	1	2
Letter Designation	\$	Þ	d

### Quantum Numbers

- The energies of orbitals are specified completely using only the *n* and I quantum numbers.
  - In magnetic fields, some emission lines split into three, five, or seven components.
  - · A third quantum number describes splitting.

### **Quantum Numbers**

- The third quantum number is the magnetic quantum number,  $m_{\rm l}$ .
  - *m*<sub>I</sub> has integer values.
  - *m*<sub>I</sub> may be either positive or negative.
  - $m_{\rm l}$ 's absolute value must be less than or equal to I.
  - For I = 1, m<sub>I</sub> = -1, 0, +1



### Example Problem 6.5

 Write all of the allowed sets of quantum numbers (n, I, and m<sub>i</sub>) for a 3p orbital.

### **Visualizing Orbitals**

### Table 📕 6.3

Wive functions for the n = 1 and n = 2 shells of a hydrogen atom are listed. There is no need to memorize these functions they are shown a merely to point out that they are made up of ordinary methematical terms.

### Orbital Wave Function

- $\psi_{1r} = \pi^{-1/2} a_{\xi}^{-3/2} e^{-(r/q_0)}$
- $2s \qquad \psi_{2s} = (4\pi)^{-1/2} (2a_0)^{-3/2} \left(2 \frac{r}{a_0}\right) e^{-ir/2a_0}$
- $2p_{*} \qquad \psi_{2p_{*}} = (4\pi)^{-1/2} (2a_{0})^{-3/2} \frac{r}{a_{0}} e^{-(r/2a)} \sin\theta \cos\phi$
- $2p_j \qquad \psi_{2p_j} = (4\pi)^{-1/2} (2a_0)^{-3/2} \frac{r}{a_0} e^{-(r/2a_j)} \sin\theta \sin\phi$
- $2p_z = \psi_{2p_z} = (4\pi)^{-1/2} (2a_0)^{-1/2} \frac{r}{a_0} e^{-(r/2a_0)} \cos\theta$

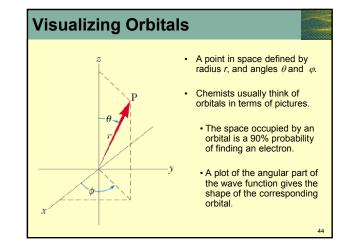
 Wave functions for the first five orbitals of hydrogen.

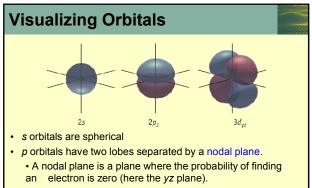
The wave function is written in spherical polar coordinates with the nucleus at the origin.

- Point in space defined by radius *r*, and angles *θ* and *φ*.
- *r* determines the orbital size.
  θ and φ determine the orbital shape.

43

45

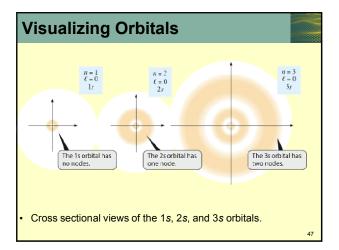


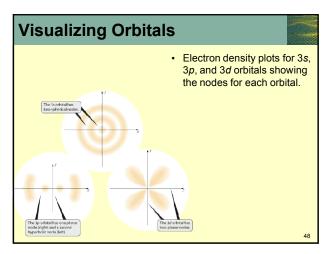


• *d* orbitals have more complicated shapes due to the presence of two nodal planes.

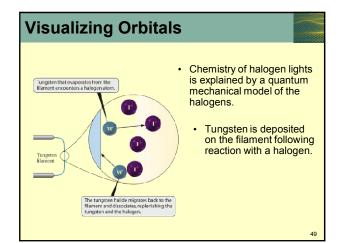
### Visualizing Orbitals

- Nodes are explained using the Uncertainty Principle.
  - It is impossible to determine both the position and momentum of an electron simultaneously and with complete accuracy.
  - An orbital depicts the probability of finding an electron.
- The radial part of the wave function describes how the probability of finding an electron varies with distance from the nucleus.
  - Spherical nodes are generated by the radial portion of the wave function.





52



### The Pauli Exclusion Principle and Electron Configurations

- The spin quantum number,  $m_{\rm s}$ , determines the number of electrons that can occupy an orbital.
  - $m_s = \pm 1/2$
  - Electrons described as "spin up" or "spin down".
  - An electron is specified by a set of four quantum numbers.

### The Pauli Exclusion Principle and Electron Configurations

- Pauli Exclusion Principle no two electrons in an atom may have the same set of four quantum numbers.
  - Two electrons can have the same values of n, I, and  $m_{\rm l}$ , but different values of  $m_{\rm s}$ .
  - · Two electrons maximum per orbital.
  - Two electrons occupying the same orbital are spin paired.

51

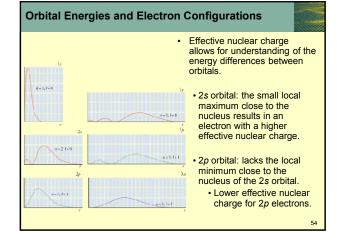
53

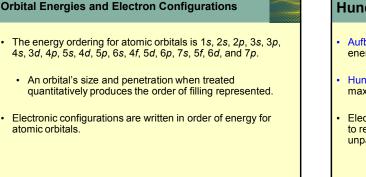
### **Orbital Energies and Electron Configurations**

- Electrons in smaller orbitals are held more tightly and have lower energies.
  - Orbital size increases as the value of *n* increases.
  - True for hydrogen atoms, but not entirely true for multielectron atoms.
    - As nuclear charge increases, orbital size decreases.
    - Electrons interact with other electrons as well as the positively charged nucleus.

### Orbital Energies and Electron Configurations

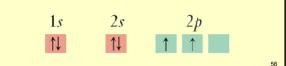
- For electrons in larger orbitals, the charge "felt" is a combination of the actual nuclear charge and the offsetting charge of electrons in lower orbitals.
  - The masking of the nuclear charge is called shielding.
  - Shielding results in a reduced, effective nuclear charge.

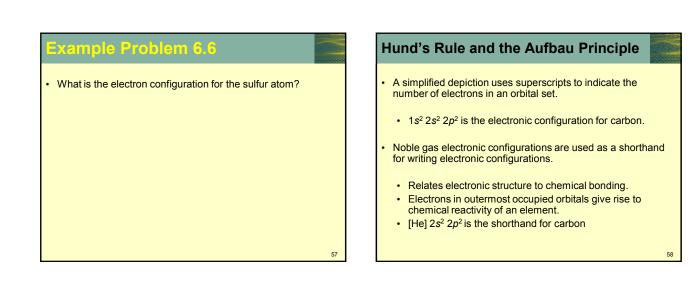




### Hund's Rule and the Aufbau Principle

- Aufbau principle when filling orbitals, start with the lowest energy and proceed to the next highest energy level.
- Hund's rule within a subshell, electrons occupy the maximum number of orbitals possible.
- Electron configurations are sometimes depicted using boxes to represent orbitals. This depiction shows paired and unpaired electrons explicitly.





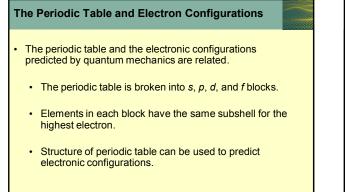
59

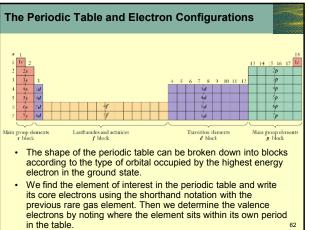
## Hund's Rule and the Aufbau Principle The inner electrons, which lie closer to the nucleus, are referred to as core electrons. Core electrons can be represented by the noble gas with the same electronic configuration. The outer electrons are usually referred to as valence electrons.

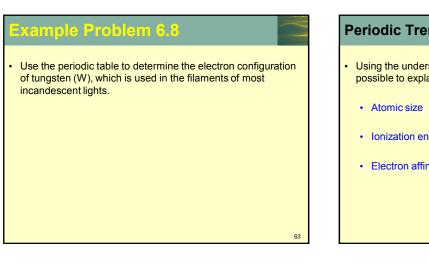
- Valence electrons are shown explicitly when a noble gas shorthand is used to write electronic configurations.
- Valence electrons determine reactivity.

### Example Problem 6.7

• Rewrite the electron configuration for sulfur using the shorthand notation.







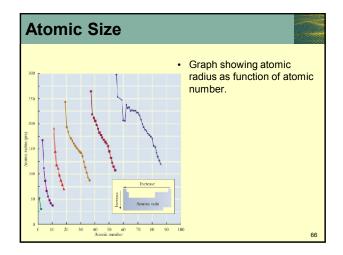
65

### **Periodic Trends in Atomic Properties**

- Using the understanding of orbitals and atomic structure, it is possible to explain some periodic properties.
  - Ionization energy
  - Electron affinity

### **Atomic Size**

- The shell in which the valence electrons are found affects atomic size.
  - The size of the valence orbitals increases with n, so size must increase from top to bottom for a group.
- The strength of the interaction between the nucleus and the valence electrons affects atomic size.
  - The effective nuclear charge increases from left to right across a period, so the interaction between the electrons and the nucleus increases in strength.
  - As interaction strength increases, valence electrons are drawn closer to the nucleus, decreasing atomic size.



### Example Problem 6.9

• Using only the periodic table, rank the following elements in order of increasing size: Fe, K, Rb, S, and Se.

### **Ionization Energy**

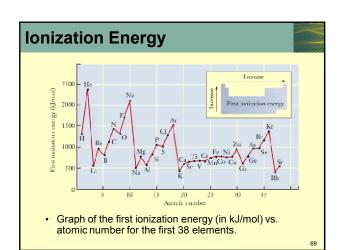
67

lonization energy - the energy required to remove an electron from a gaseous atom, forming a cation.

 Formation of X<sup>+</sup> is the first ionization energy, X<sup>2+</sup> would be the second ionization energy, etc.

$$X(g) \longrightarrow X^+(g) + e^{-g}$$

- Effective nuclear charge increases left to right across a period.
- The more strongly held an electron is, the higher the ionization energy must be.
- As valence electrons move further from the nucleus, they become easier to remove and the first ionization energy becomes smaller.

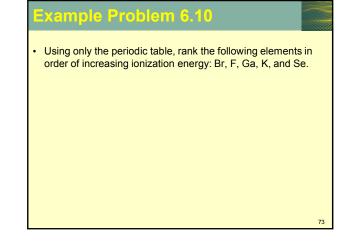


lor	nization Energy
io • •	rom nitrogen to oxygen, there is a slight decrease in nization energy. Nitrogen has a half-filled <i>p</i> subshell. Oxygen has a pair of <i>p</i> electrons in one 2 <i>p</i> orbital. Ionization of oxygen relieves electron-electron repulsion, lowering its ionization energy.
gi	nization energies increase with successive ionizations for a ven element. Effective nuclear charge for valence electrons is larger for the ion than the neutral atom.

 Filled subshells of electrons are difficult to break up, which is why it is difficult to remove electrons from noble gases.

Table 🛚 6.4								
Those is last elec	t four ionization c onizations with val tron from a partic stable filled shell, a	lucs shown in sha ular shell. Further	ded cells with bol ionization requir	d print involve re res removing an el	moving the lectron from			
Z	Element	IE,	IE <sub>2</sub>	IE <sub>2</sub>	IE4			
1	н	1,312	_	-	-			
2	Hc	2,372	5,250	_	_			
3	Li	520.2	7,298	11,815	_			
4	Be	899.4	1,757	14,848	21,007			
5	в	800.6	2,427	3,650	25,026			
6	С	1,086	2,353	4,620	6,223			
7	Ν	1,402	2,856	4,578	7,475			
8	0	1,314	3,388	5,300	7,469			
9	F	1,681	3,374	6,050	8,408			

Table	6.4				
Those last ele	st four ionization e ionizations with val stron from a partic stable filled shell, a	lucs shown in sha alar shell. Further	ded cells with bol rionization requi	ld print involve re res removing an e	moving the lectron from
z	Element	IE <sub>1</sub>	IE <sub>2</sub>	IE3	IE4
10	Ne	2,081	3,952	6,122	9,370
11	Na	495.6	4,562	6,912	9,544
12	Mg	737.7	1,451	7,733	10,540
13	Al	577.6	1,817	2,745	11,578
14	Si	786.4	1,577	3,232	4,356
15	P	1,012	1,908	2,912	4,957
15	5	999.5	2,251	3,357	4,564
17	a	1,251	2,297	3,822	5,158
18	Ar	1,520	2,666	3,931	5,771

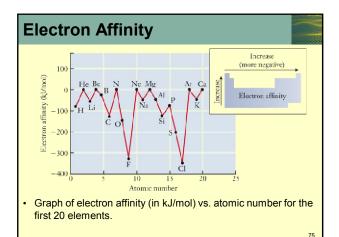


### **Electron Affinity**

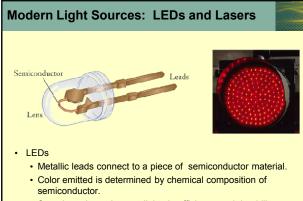
• Electron affinity - energy required to place an electron on a gaseous atom, forming an anion.

$$X(g) + e^{-} \longrightarrow X^{-}(g)$$

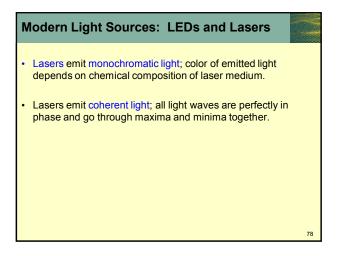
- Electron affinities may have positive or negative values.
   Negative values energy released
  - · Positive values energy absorbed
- Electron affinities increase (numerical value becomes more negative) from left to right for a period and bottom to top for a group.
- The greater (more negative) the electron affinity, the more stable the anion will be.



# Modern Light Sources: LEDs and Lasers Light Emitting Diodes (LEDs) emit monochromatic light. Monochromatic light - light of a single wavelength or color. LEDs are solid-state devices. Simply a piece of solid material. Color emitted depends on identity of solid material.



• Superior to incandescent lights in efficiency and durability.



### Modern Light Sources: LEDs and Lasers

Lasers - a direct result of the emergence of the quantum mechanical model of the atom.

- An understanding of energy levels within the laser medium is needed.
- Laser operation relies on stimulated emission, where the electron population of higher energy level is greater than a lower energy level.
- Emission occurs as electrons return to lower energy states.
- "Population inversion" in lasers established by solids, liquids or gases.

79

• Solid-state lasers are used in electronics.

### Modern Light Sources: LEDs and Lasers



Bright blue light emitted by an organic light emitting diode (OLED).

Holds promise of an entirely new class of paper-thin flexible color displays.