QUANTUM THEORY & ATOMIC STRUCTURE

GENERAL CHEMISTRY
by Dr. Istadi

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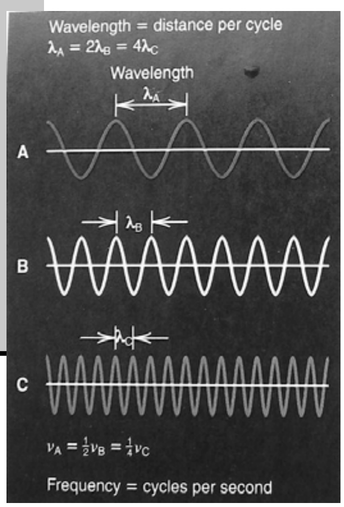
THE NATURE OF LIGHT



- Visible light is one type of electromagnetic radiation (electromagnetic radiation)
- The electromagnetic radiation has the wave properties:
  - **Frequency (ν)**: the number of cycles the wave undergoes per second ==> 1/second ≈ Hz
  - **Wavelength (λ)**: the distance between any point on a wave and the corresponding point on the next crest of the wave (the distance the wave travels during one cycle) ==> m, nm, Å (10^{-10} m)

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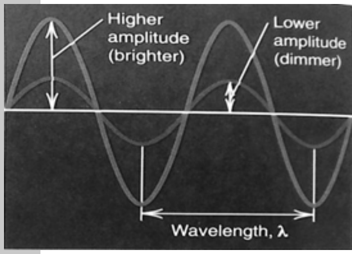

- Speed of light (c): 3 x 10^8 m/s ==> ***c = v x λ***
- where c is constant
- That's mean, radiation with a high frequency has a short wavelength, and vice versa
- Another characteristic of a wave is: **AMPLITUDE**
- Amplitude: the height of the crest of each wave or intensity of the wave/radiation
- The two waves shown have the same wavelength (color) but different amplitudes, and therefore different brightnesses (intensities)

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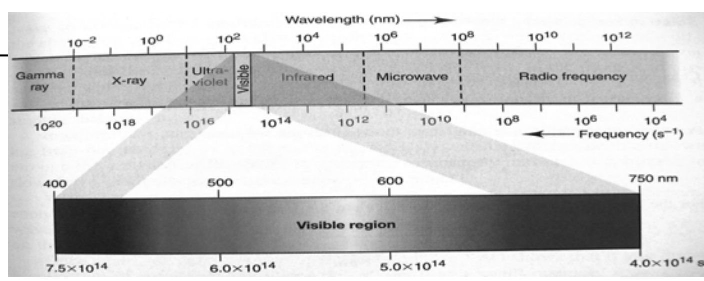
The Electromagnetic Spectrum



- Visible light represents a small portion of the continuum of radiant energy, known as **electromagnetic spectrum**
- **All the waves in the spectrum travel at the same speed through a vacuum but differ in frequency and therefore wavelength**
- **Wavelength of visible light as different colors: from red (λ=750 nm) to violet (λ=750 nm)**
- **Light of single wavelength is called MONOCHROMATIC**
- Light of many wavelength is called POLYCHROMATIC

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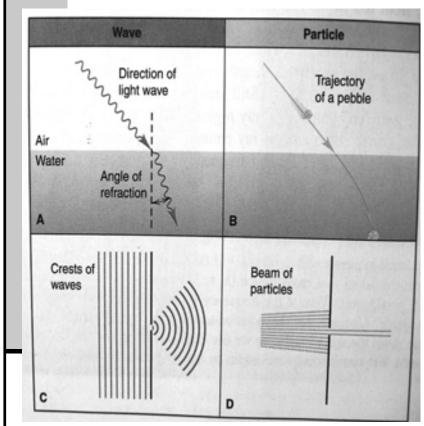
Distinction Between Energy and Matter



In contrast, a particle does not undergo refraction when passing a boundary

- when light wave passes from air to water, the speed of the wave changes ==> **refraction**
- After strikes the boundary, the light continues at a different angle, therefore change in speed and direction
- The new angle depends on the materials on either side of the boundary and the wavelength of the light
- White light is dispersed into its component colorsm when pass through a prism, because each incoming wavelength is refracted at a slightly different angle.

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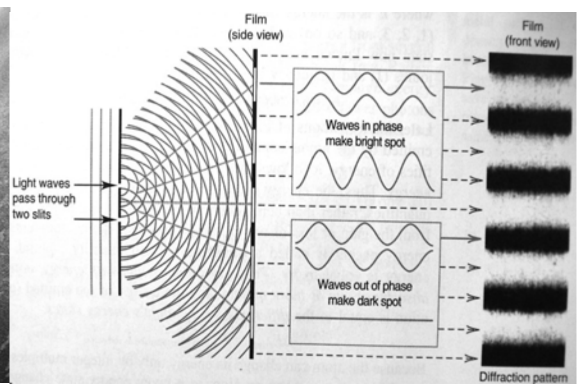

- If waves of light pass through two adjacent slits, the emerging circular waves interact with each other through the process of **interference**.
- If the crests of the waves coincide (in phase), they interfere **constructively** and the amplitudes add together.
- If the crests coincide with throughs (out of phase), they interfere **destructively** and the amplitudes cancel.
- the result is a diffraction pattern of **brighter** and **darker** regions

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The Particle Nature of Light

1. Blackbody Radiation
2. The Photoelectric effect
3. Atomic Spectra

Blackbody Radiation

- When a coal is heated to 1000 K ==> emit visible light (red glow)
- At 1500 K, the light is brighter and more orange, like that from an electric heating coil (*elemen pemanas listrik*)
- These changes in **intensity** and **wavelength** of emitted light as an object is heated are **characteristic of blackbody** radiation.
- In 1900, Max Planck ==> hot or glowing object could emit or absorb only certain quantities of energy:

$$E = nh\nu$$

- E: energy of radiation (J); ν : frequency (s^{-1}); n : positive integer of a quantum number; h : proportionality constant (Planck's constant in J.s)
- $h = 6.62606876 \times 10^{-34}$ J.s $= 6.626 \times 10^{-34}$ J.s

Quantum Energy

- If an atom itself can emit only certain quantities of energy ==> the atom itself can have only certain quantities of energy
- Thus, the energy of an atom is quantized
- Each change in the atom's energy results from the gain or loss of one or more "packet" (amount) of energy.
- Each energy packet is called a quantum (= $h\nu$)
- *An atom changes its energy state by emiting (or absorbing) one or more quanta*, and *the energy of the emitted (or absorbed) radiation is equal to the difference in the atom's energy states*:

$$\Delta E_{atom} = E_{emitted\ (or\ absorbed)\ radiation} = \Delta n h\nu$$

- The atom can change its energy only by integer multiples of $h\nu$ ==> the smallest changes occurs when an atom in a given energy state changes to an adjacent states when Δn=1

$$\boxed{\Delta E = h\nu}$$

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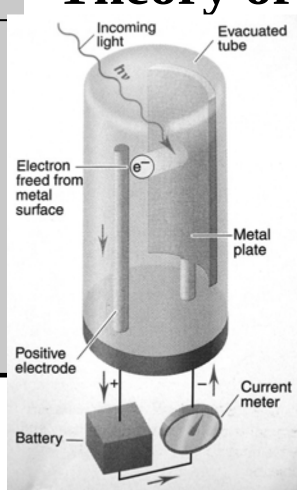
Photoelectric Effect and Photon Theory of Light



- When monochromatical light of high enough frequency strikes the metal plate, electrons are freed from the plate and travel to the positive electrode, creating a **current**
- **Plank's idea of quantized energy ==> Einstein: "*light itself is particulate, that is quantized into small bundles of electromagnetic energy*" ==> PHOTONS**
- **Planck ==> each atom changes its energyu whenever it absorbs or emits one photon, one particle of light, whose energy is fixed by its *frequency*:**

$$E_{photon} = h\nu = \Delta E_{atom}$$

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How Einstein's Photon Theory Explains the Photoelectric Effect?

- According to the photon theory, a beam of light consists of an enormous number of photons.
- Light intensity is related to the number of photons striking the surface per unit time, but not to their energy.
- Therefore, a photon of a certain minimum energy must be absorbed for an electron to be freed.
- Since energy depends on frequency ($h\nu$), the theory predicts a threshold frequency.
- An electron can not save up energy from several photons below the minimum energy until it has enough to break free.
- Rather, one electron breaks free the moment it absorbs one photon of enough energy.
- The current is weaker in dim light than in bright light because fewer photons of enough energy are present, so fewer electrons break free per unit time.
- But some current flows the moment photons reach the metal plate

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Examples of Energy Radiation

- A cook uses a microwave oven to heat a metal. The wavelength of the radiation is 1.20 cm. What is energy of one photon of this microwave radiation?
- Solution:
- $E = h\nu = hc/\lambda$
- $$= \frac{(6.626 \times 10^{-34}\ \text{J.s})(3.00 \times 10^{8}\ \text{m/s})}{(1.20\ \text{cm})(10^{-2}\ \text{m/cm})}$$
- $= 1.66 \times 10^{-23}$ J

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ATOMIC SPECTRA

- What happen when an element is vaporized and then electrically excited?
- Light from excited Hydrogen atoms pases through a narrow slit and is then refracted by a prism.
- This light does not create a continuous spectrum, or rainbow, as sunlight does
- Instead, it creates a **line spectrum**, a series of fine lines of individual colors separated by colorless spaces (black)
- The wavelength of these spectral lines are characteristic of the element producing them
- Next the figure ==>

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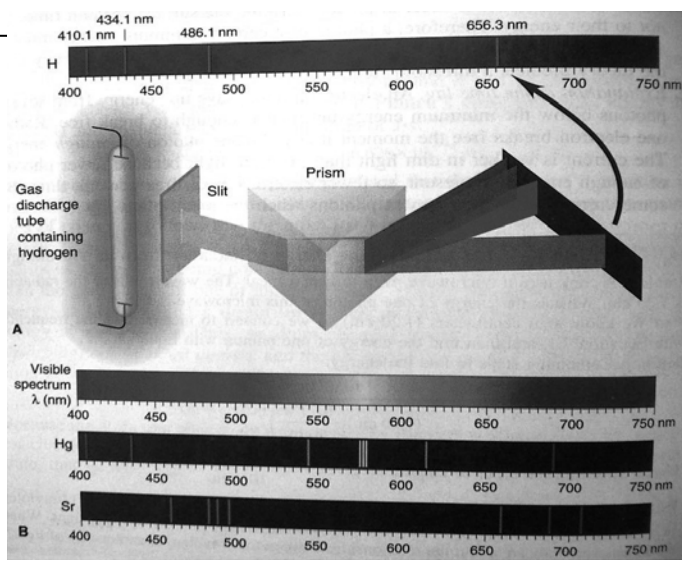
Example: The line spectra of hydrogen



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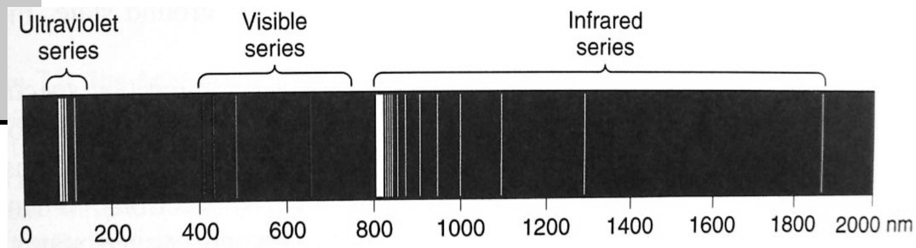
Spectral Lines of Hydrogen Atom

- Spectroscopist studying the spectrum of atomic hydrogen had identified several series of such lines in different regions of the electromagnetic spectrum
- Three series of spectral lines of atomic hydrogen:



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Rydberg Equation

- Rydberg Equation ==> to predict the position and wavelength of any lines in a given series:

$$\frac{1}{\lambda} = R * \left(\frac{1}{n_1^{\ 2}} - \frac{1}{n_2^{\ 2}} \right)$$

- where λ is the wavelength of a spectral line, n_1 and n_2 are positive integers with $n_2 > n_1$, and R is the Rydberg constant (1.096776×10^7 m^{-1})
- For the visible series of lines, $n_1=2$:

$$\frac{1}{\lambda} = R * \left(\frac{1}{2^2} - \frac{1}{n_2^{\ 2}} \right), with n_2 = 3,4,5,...$$

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The Bohr Model of The Hydrogen Atom

- **Niels Bohr** (1885-1962) suggested a model for the H atom that predicted the existence of ***line spectra***.
- In this model, Bohr used Planck's and Einstein's ideas about quantized energy and proposed three postulates:
  - *The H atom has only certain allowable energy levels* ==> **stationary states**. Each of these states is associated with a fixed circular orbit of the electron around the nucleus
  - *The atom does not radiate energy while in one of its stationary states*. That is, even though it violates the ideas of classical physics, the atom does not change energy while the electron moves within an orbit.
  - *The atom changes to another stationary state (the electron moves to another orbit) only by absorbing or emitting a photon* whose energy equals the difference in energy between the two states:

$$E_{photon} = E_{state\ A} - E_{state\ B} = h\nu$$

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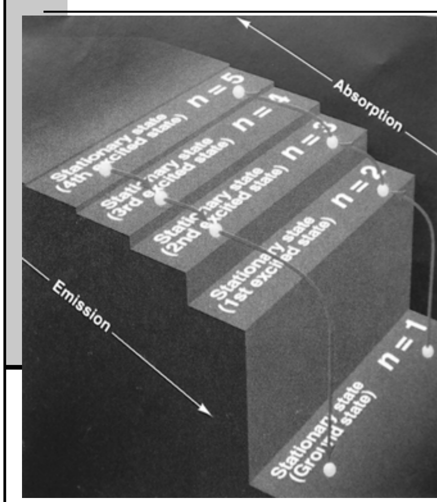
Quantum staircase of Hydrogen Atom



- Analogy for the energy levels of the hydrogen atom
- An electron can absorb a photon and jump to a higher step (stationary state)
- or emit a photon and jump down to a lower one
- But the electron cannot lie between two steps

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Bohr's Model

- A spectral line results when a photon of specific energy (and frequency) is emitted as the electron moves from a higher energy state to a lower one
- Therefore, Bohr's model explains that *the atomic spectrum is not continuous because the atom's energy has only certain discrete levels or states*
- *In Bohr's model, the quantum number n is associated with the radius of an electron orbit, which is related to the electron's energy*

  the lower the n value, the smaller the radius of the orbit, and the lower the energy level
- *When the electron is in the first orbit (n=1), the orbit closest to the nucleus, the H atom is in its lowest energy level ==>* ***GROUND STATE***

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Cont'd ....

- If the H atom absorbs a photon whose energy equals the difference between the first and second energy levels, the electron moves to the second orbit (n=2), the next orbit out from the nucleus.
- When the electron is in the second or any higher orbit, the atom is said to be in an **EXCITED STATE**
- If the H atom in the first excited state (electron in second orbit) emits a photon of that same energy, it returns to the **ground state**.
- When electron drops from an outer orbit to an inner one, the atom emits a photon of specific energy that give rise to a spectral line ==> *look at the next Figure*

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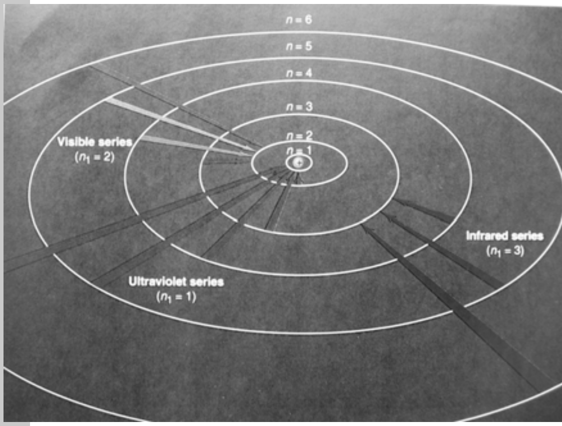

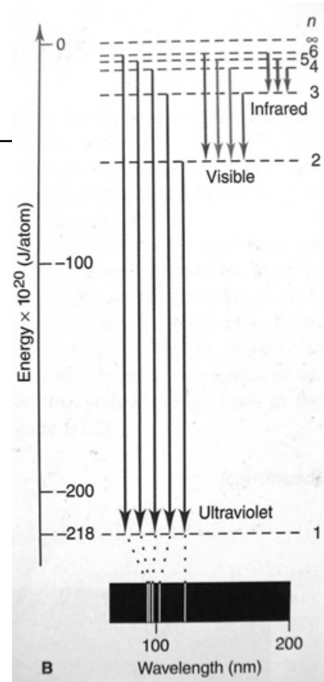

Limitations of the Bohr's Model

- The Bohr Model failed to predict the spectrum of any other atom, even that of helium, the next simplest element.
- It suitable for H atom and for other one-electron species
- But, it does not work for atoms with more than one electron because in these systems, additional nucleus-electron attractions and electron-electron repulsions are present
- As a picture of the atom, the Bohr model is incorrect, but we still use the terms "**ground state**" and "**excited state**".
- and retain one of Bohr's central ideas that: "***the energy of an atom occurs in discrete levels***"

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The Energy States of the Hydrogen Atom

- Bohr's work ==> calculation of energy levels of an atom (which derived from principles of electrostatic attraction and circular motion):
$$E = \left(-2.18\text{x}10^{-18} J\right)\left(\frac{Z^2}{n^2}\right)$$
- where Z is the charge of the nucleus.
- For H atom with Z=1: $E = \left(-2.18\text{x}10^{-18} J\right)\left(\frac{1^2}{n^2}\right) = \left(-2.18\text{x}10^{-18} J\right)\left(\frac{1}{n^2}\right)$
- Therefore, the energy of the ground state (n=1) is:
$$E = \left(-2.18\text{x}10^{-18} J\right)\left(\frac{1}{1^2}\right) = -2.18\text{x}10^{-18} J$$
- The negative sign appears because we define the zero point of the atom's energy when the electron is completely removed from the nucleus
- Thus, E=0 when n=∞, so E<0 for any smaller n.

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$$E = \left(-2.18\text{x}10^{-18} J\right)\left(\frac{Z^2}{n^2}\right)$$

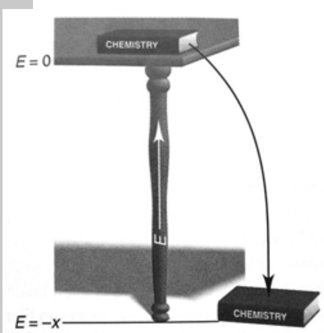

Figure 7.12 A tabletop analogy for the H atom's energy.

- Since n is in the denominator of the energy equation, as the electron moves closer to the nucleus (n decreases), the atom becomes more stable (less energetic)
- its energy becomes a larger negative number.
- As the electron moves away from the nucleus (n increases), the atom's energy increases (becomes a smaller negative number)

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- The energy difference between any two levels:

$$\Delta E = E_{final} - E_{initial} = \left(-2.18\text{x}10^{-18} J\right)\left(\frac{1}{n_{final}^2} - \frac{1}{n_{initial}^2}\right)$$

- We can predict the wavelengths of the spectral lines of H atom:

$$\Delta E = hv = hc/\lambda = \left(-2.18\text{x}10^{-18} J\right)\left(\frac{1}{n_{final}^2} - \frac{1}{n_{initial}^2}\right)$$

- Therefore (n_{final}=n_2, $n_{initial}$ = n_1):

$$\frac{1}{\lambda} = \frac{\left(-2.18\text{x}10^{-18} J\right)}{hc}\left(\frac{1}{n_{final}^2} - \frac{1}{n_{initial}^2}\right)$$

$$. = \frac{\left(-2.18\text{x}10^{-18} J\right)}{\left(6.626\text{x}10^{-34} J.s\right)\left(3.00\text{x}10^{8} m/s\right)}\left(\frac{1}{n_{final}^2} - \frac{1}{n_{initial}^2}\right)$$

$$. = -1.10\text{x}10^{7} m^{-1}\left(\frac{1}{n_{final}^2} - \frac{1}{n_{initial}^2}\right)$$

- Energy needed to completely remove the electron from an H atom:

  H(g) → H^+(g) + e^- ΔE=?

- n_{final}=∞ and $n_{initial}$=1, and obtain:

$$\Delta E = E_{final} - E_{initial} = \left(-2.18\text{x}10^{-18} J\right)\left(\frac{1}{\infty^2} - \frac{1}{1^2}\right)$$

$$\rightarrow \Delta E = \left(-2.18\text{x}10^{-18} J\right)\left(0-1\right) = 2.18\text{x}10^{3} kJ/mol$$

- *ΔE is positive because energy is absorbed to remove the electron from the vicinity of the nucleus.*
- *For 1 mol of H atoms:*

$$\Delta E = \left(-2.18\text{x}10^{-18} J/atom\right)\left(6.022\text{x}10^{23} atoms/mol\right)\left(\frac{1kJ}{10^3 J}\right)$$

$$\Delta E = 1.31\text{x}10^{3} kJ/mol$$

- *This is the ionization energy of the H atom, the energy required to form 1 mol of gaseous H^+ ions from 1 mol of gaseous H atoms*

de Broglie Wavelength

- From $E=mc^2$ and $E=h\nu=hc/\lambda$ ==> *de Broglie: wavelength of any particles:*

  $$\lambda = h/mu$$

- *Example: Find the de Broglie wavelength of an electron with a speed of 1.00x10^6 m/s (electron mass=9.11x10^{-31} kg; h=6.626x10^{-34} kg.m^2/s)*

$$\lambda = \frac{h}{mu} = \frac{6.626\text{x}10\ -34 kg.m^{2}/s}{(9.11\text{x}10\ -31 kg)(1.00\text{x}10^{6} m/s)} = 7.27\text{x}10^{-10} m$$

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The Heisenberg Uncertainty Principle

- Werner Heisenberg (1927) postulated **the uncertainty principle**.

  $$\Delta x.m\Delta\Delta \geq \frac{h}{4\pi}$$

- Δ*x*: the uncertainty in position; Δ*u*: the uncertainty in speed.
- **Example**: An electron moving near an atomic nucleus has a speed of 6x10^6 m/s ± 1%. What is uncertainty in its position (Δ*x)?*
- **Solution**: Finding uncertainty in speed, Δ*u:*

  Δu = 1% of u = (0.01)(6x10^6 m/s) = 6x10^4 m/s

- *Calculating the uncertainty in position, Δx:* $\Delta x.m\Delta\Delta \geq \frac{h}{4\pi}$

$$\Delta x \geq \frac{h}{4\pi m\Delta u} \geq \frac{6.626\text{x}10^{-34} kg.m^{3}/s}{4\pi(9.11\text{x}10^{-31} kg)(6\text{x}10^{4} m/s)} \geq 1\text{x}10^{-9} m$$

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Summary

- ***Blackbody radiation*** ==> Planck: Energy is quantized; only certain values allowed
- ***Photoelectric effect*** ==> Einstein: Light has particulate behavior (photons)
- ***Atomic line spectra*** ==> Bohr: Energy of atoms is quantized; photon emitted when electron changes orbit
- ***de Broglie***: All matter travels in waves: energy of atom is quantized due to wave motion of electrons
- According to the ***uncertainty principle***, we cannot know simultaneously the exact position and speed of an electron

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