Atomic Structure

1. Idea of de Broglie Matter Waves

Concept:

Louis de Broglie proposed that matter (like electrons) exhibits wave-like properties. This concept bridges the gap between particles and waves, introducing the wave-particle duality of matter.

Derivation of de Broglie Wavelength:

1. From Einstein's energy equation for photons:

$$E = h\nu$$

   Where h is Planck's constant, and ν is the frequency.

2. For a photon, energy is also related to momentum p:

$$E = pc \quad (\text{where } c \text{ is the speed of light}).$$

3. Equating these two expressions for energy:

$$pc = h\nu$$

4. Substituting $\nu = \frac{c}{\lambda}$, we get:

$$p = \frac{h}{\lambda}$$

5. Extending this concept to particles:
   - Momentum $p = mv$ for a particle of mass m and velocity v.
   - Thus, de Broglie wavelength is:

$$\lambda = \frac{h}{mv}$$

Significance:

For macroscopic objects, the wavelength is negligibly small, making wave properties undetectable. For subatomic particles (e.g., electrons), λ becomes significant and measurable.

Example:

An electron ($m = 9.1 \times 10^{-31}\,\text{kg}$) moving at $10^6\,\text{m/s}$:

$$\lambda = \frac{6.626 \times 10^{-34}}{(9.1 \times 10^{-31})(10^6)} \approx 7.27\,\text{nm}$$

2. Heisenberg Uncertainty Principle

Statement:

It is impossible to simultaneously measure the exact position (x) and momentum (p) of a particle with absolute certainty. The principle is mathematically expressed as:

$$\Delta x \cdot \Delta p \geq \frac{h}{4\pi}$$

Where:

- Δx = Uncertainty in position
- $\Delta p = m \cdot \Delta v$, uncertainty in momentum
- h = Planck's constant

Derivation:

1. From wave-particle duality, momentum p is related to wavelength:

$$p = \frac{h}{\lambda}$$

2. A wave packet representing a particle has a spread in wavelengths ($\Delta\lambda$) due to wave superposition:

$$\Delta p = \frac{h}{\Delta\lambda}$$

3. The spread in position (Δx) is inversely proportional to the spread in wavelength:

$$\Delta x \cdot \Delta\lambda \approx 1$$

4. Combining the above equations:

$$\Delta x \cdot \Delta p \geq \frac{h}{4\pi}$$

Significance:

The uncertainty principle limits the precision of measurements, implying that electrons do not follow deterministic paths (as suggested by Bohr's model).

3. Schrödinger Wave Equation

The Schrödinger equation provides a mathematical framework for quantum mechanics. It describes the wave behavior of particles in terms of their energy and position.

Time-Independent Schrödinger Equation:

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

Where:

- $\hat{H}$ = Hamiltonian operator (total energy operator)
- ψ = Wave function (describes the quantum state of a system)
- E = Total energy

The Hamiltonian operator is expressed as:

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(r)$$

Where:

- $-\frac{\hbar^2}{2m}\nabla^2$ = Kinetic energy operator
- $V(r)$ = Potential energy

Interpretation:

- ψ gives the probability amplitude of finding an electron in a region.
- $|\psi|^2$ gives the probability density.

4. Quantum Numbers

Principal Quantum Number (n):

Defines the energy level of an electron and its average distance from the nucleus.

- Example: For $n = 1$, the electron is in the first energy level.

Azimuthal Quantum Number (l):

Determines the shape of the orbital:

$$l = 0, 1, 2, ..., (n-1)$$

- Example: $l = 0$ (s-orbital), $l = 1$ (p-orbital).

Magnetic Quantum Number (m_l):

Specifies the orientation of the orbital:

$$m_l = -l, ..., 0, ..., +l$$

Spin Quantum Number (m_s):

Represents the electron's spin:

$$m_s = +\frac{1}{2} \text{ or } -\frac{1}{2}$$

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5. Shapes of Orbitals

s-Orbitals:

- Spherical in shape.
- Example: Hydrogen's $1s$ orbital.

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p-Orbitals:

- Dumbbell-shaped.
- Three orientations (p_x, p_y, p_z).

d-Orbitals:

- Complex shapes (cloverleaf and donut).
- Five orientations (d_{xy}, d_{yz}, etc.).

6. Aufbau Principle

Electrons occupy orbitals in the order of increasing energy.

Order of Filling:

$$1s \rightarrow 2s \rightarrow 2p \rightarrow 3s \rightarrow 3p \rightarrow 4s \rightarrow 3d \rightarrow 4p \rightarrow 5s \rightarrow \ldots$$

Example:

- Carbon ($6e^-$): $1s^2 2s^2 2p^2$.

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7. Effective Nuclear Charge (Z_{eff})

The net positive charge experienced by an electron:

$$Z_{\text{eff}} = Z - S$$

Where:

- Z = Atomic number (total protons)
- S = Shielding constant (due to inner electrons).

Trends:

- Increases across a period (due to higher nuclear charge).
- Decreases down a group (due to increased shielding).
