

### The History of the Atom

#### Democritus (300 B.C.)

First person to conceive the idea of **tiny, indivisible particles** called **atoms**

#### John Dalton (1805) - The billiard ball model

**Pure substances** are made up of atoms

Atoms of the **same element** are **exactly alike**

Atoms **cannot** be **created, destroyed**, or **divided** into smaller particles

Compounds are formed by **joining 2 or more elements**

#### William Crookes (1875) - Discovery of the electron

Created an **electric discharge tube** (a **cathode ray tube**) with a screen and magnet

Discovered the bar magnet could deflect/move the cathode rays (they have a **charge**)

If he added a paddle wheel inside the tube, it moved (the rays had **mass**)

#### J.J. Thomson (1897) - The raisin bun model

Using Crooke's cathode ray tube, determined rays were **made up of negatively charged particles** called **electrons**

Electrons were **2000x lighter** than hydrogen, the lightest known element

#### Ernest Rutherford (1903) - The beehive model

Conducted the **gold foil experiment**; if the atom was like Thomson proposed, any alpha particles sent through it would **pass straight through**

Most of the particles went through, but **some were scattered**

Determined that atoms were **mostly empty space**, with a **small, dense, positively charged nucleus** in the centre with  $e^-$  scattered around it

### The History of the Atom (cont)

**1932** - determined with James Chadwick that the mass of the nucleus **did not equal the mass of the protons only**, i.e. electrically neutral **neutrons**

#### Niels Bohr (1913) - The planetary model

Proposed that electrons are **not allowed to orbit anywhere**, but rather they occupy certain **defined (fixed) orbits**

Based off experiments with hydrogen atoms and spectroscopes

Electrons can **jump to higher orbits** when they are given energy in **quantized amounts (no partial amounts)**, usually in the form of **photons** (light particles)

### Quantum Mechanical Model of the Atom

**Louis de Broglie** (1924) proposed that if light waves properties of particles, then **particles can have properties of waves**

**Erwin Schrodinger** (1933) realized that a **wave theory** and mathematical equations were needed to **explain atoms with more than 2  $e^-$**

#### Schrodinger's Wave Function

Contains 3 variables called **quantum numbers** ( $n, l, m_l$ ) to help determine a **region in space** where the electron spends **90%** of its time (the **atomic orbital**)

A fourth number ( $m_s$ ) was added so that all characteristics of atoms could be explained

**Heisenberg's Uncertainty Principle**: it is **impossible** to know both the **exact location and speed** of an  $e^-$  at a given time

### Quantum Theory and Chemical Bonding

**Valence Bond Theory**: atomic orbitals of one atom can overlap with atomic orbitals of another atom to **share a common region of space**

**Molecular Orbital Theory**: when orbitals overlap, they **combine to form new orbitals** called **molecular orbitals (hybridization)**; the **greater** the overlap, the **more stable** the bond

**Double/Triple Bonds: Sigma ( $\sigma$ ) bonds** (**end-to-end** overlap of orbitals) and **pi ( $\pi$ ) bonds** ("**sideways**" orbitals—usually  $p$  orbitals—overlap **above and below** the plane of the bond)

**Single bond** = 1  $\sigma$  bond; **Double bond** = 1  $\sigma$  bond + 1  $\pi$  bond; **Triple bond** = 1  $\sigma$  bond + 2  $\pi$  bonds

### Quantum Numbers

| Quantum number           | Symbol | Meaning               | Possibilities                                |
|--------------------------|--------|-----------------------|--|
| Principal quantum number | $n$    | Energy level          | $n \in \mathbb{N}$ (any whole number $> 0$ ) |
| Secondary quantum number | $l$    | Shape of orbital      | $0 \leq l \leq n - 1$                        |
| Magnetic quantum number  | $m_l$  | Direction/orientation | $-l \leq m_l \leq l$                         |
| Spin quantum number      | $m_s$  | Spin                  | $\pm 1/2$                                    |

### Shape of Electron Orbitals ( $l$ and $m_l$ )

| Value of $l$ | Symbol | Shape          | # of suborbitals ( $m_l$ ) |
|--------------|--------|----------------|----------------------------|
| 0            | $s$    | Sphere (sharp) | 1 ( $m_l = 0$ )            |



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### Shape of Electron Orbitals (l and ml) (cont)

|   |                      |               |                                      |
|---|----------------------|---------------|--------------------------------------|
| 1 | $p$<br>(principal)   | Dumbbell      | 3 ( $m_l = -1, 0, 1$ )               |
| 2 | $d$ (diffuse)        | Flower/petal  | 5 ( $m_l = -2, -1, 0, 1, 2$ )        |
| 3 | $f$<br>(fundamental) | Double flower | 7 ( $m_l = -3, -2, -1, 0, 1, 2, 3$ ) |

### VSEPR Theory

#### VSEPR: Valence Shell Electron Pair Repulsion

Helps determine the structure around an atom by **minimizing the repulsive force** between  $e^-$  pairs

Bonded and lone pair  $e^-$  position themselves **as far away as possible** from each other

Lone pairs of  $e^-$  on a central atom **repels a little more** than bonding pairs; they **push the bonding pairs closer together**

### VSEPR Molecule Shapes

| # of $e^-$ groups | $e^-$ configuration  | AXE formula                    | Molecular shape      |
|-------------------|----------------------|--------------------------------|----------------------|
| 2                 | Linear               | AX <sub>2</sub>                | Linear               |
| 3                 | Trigonal planar      | AX <sub>3</sub>                | Trigonal planar      |
|                   |                      | AX <sub>2</sub> E              | Bent                 |
| 4                 | Tetrahedral          | AX <sub>4</sub>                | Tetrahedral          |
|                   |                      | AX <sub>3</sub> E              | Trigonal pyramidal   |
|                   |                      | AX <sub>2</sub> E <sub>2</sub> | Bent                 |
| 5                 | Trigonal bipyramidal | AX <sub>5</sub>                | Trigonal bipyramidal |
|                   |                      | AX <sub>4</sub> E              | See-saw              |
|                   |                      | AX <sub>3</sub> E <sub>2</sub> | T-shape              |
|                   |                      | AX <sub>2</sub> E <sub>3</sub> | Linear               |
| 6                 | Octahedral           | AX <sub>6</sub>                | Octahedral           |

### VSEPR Molecule Shapes (cont)

|                                |                  |
|--------------------------------|------------------|
| AX <sub>5</sub> E              | Square pyramidal |
| AX <sub>4</sub> E <sub>2</sub> | Square planar    |

See a visual table here.

### Bond vs Molecular Polarity

**Bond Polarity:** the even/uneven distribution of  $e^-$  across **one bond** (can be single/double/triple); determined by  $\Delta EN$  (difference in electronegativity)

**Molecular Polarity:** the even/uneven distribution of  $e^-$  across an **entire molecule**; determine many properties of the substance

3 important factors to molecular polarity: **presence/absence of polar bonds**, **shape** of the molecule, and **presence/absence of lone  $e^-$  pairs**

It is possible to have a non-polar molecule with polar bonds within, if the shape cancels out any vectors created by the bonds.

### Ionic Crystals

Solids in which **positive and negative ions** are arranged in a **crystal lattice**

|   |                                    |
|---|------------------------------------|
| <b>Boiling/melting point</b>              | High                               |
| <b>Malleability</b>                       | Brittle                            |
| <b>Conductivity</b>                       | Poor as solid, high as solution    |
| <b>Solubility in water</b>                | Very soluble                       |
| <b>Hardness</b>                           | Very hard (very scratch-resistant) |
| <b>Types of forces acting on molecule</b> | Ionic bonds                        |

**Examples:** NaCl (table salt), K<sub>3</sub>PO<sub>4</sub> (potassium phosphate), CuSO<sub>4</sub> (copper (II) sulfate)

### Metallic Crystals

Solids composed of **individual molecules** held together by **intermolecular forces (IMFs)**; "**neutral**" molecules that form **complex crystal lattice** in solid state

|   |                         |
|---|-------------------------|
| <b>Boiling/melting point</b>              | Vary widely             |
| <b>Malleability</b>                       | Ductile (very flexible) |
| <b>Conductivity</b>                       | High as a solid         |
| <b>Solubility in water</b>                | Slightly soluble        |
| <b>Hardness</b>                           | Varied                  |
| <b>Types of forces acting on molecule</b> | Metallic bonds          |

**Examples:** Au (gold), Ag (silver), Ni (nickel), Fe (iron), Co (cobalt), Cu (copper), Zn (zinc), Cr (chromium)

### Ionic vs Metallic Bonds

**Ionic Bond:** Highly electropositive ion (**cation**) **gives up extra  $e^-$**  and gives them to highly electronegative ion (**anion**), then bond through **very strong electrostatic attraction** between the two ions, creating an **ionic crystal** structure

**Metallic Bond:** Many metal atoms shed a "**sea**" of  $e^-$  that engulf the metal ions ( $e^-$  are **delocalized**); pulled from all directions, the metal ions can barely move and **pack tightly together** in crystalline structures

Both ionic and metallic crystals take an immense amount of energy to break the bonds between ions; however, since the metal ions are inside the "sea" of  $e^-$ , metallic crystals are **much more malleable** than normal ionic crystals (the  $e^-$  mitigate the effect of shifting and sudden repulsion between the ions).



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## Molecular Crystals

Solids composed of **individual molecules** held together by **intermolecular forces (IMFs)**; "**neutral**" molecules that form **complex crystal lattice** in solid state

|   |   |
|---|---|
| <b>Boiling/melting point</b>              | Low                                     |
| <b>Malleability</b>                       | N/A                                     |
| <b>Conductivity</b>                       | Poor as solids                          |
| <b>Solubility in water</b>                | Varied                                  |
| <b>Hardness</b>                           | Soft (easy to scratch)                  |
| <b>Types of forces acting on molecule</b> | IMFs - weaker than ionic/metallic bonds |

**Examples:** I<sub>2</sub> (s) (iodine), At<sub>2</sub> (s) (astatine)

## Covalent Network Crystals

Solids in which the atoms **form covalent bonds** in an **interwoven network**; most contain **C** or **Si atoms**

|   |   |
|---|---|
| <b>Boiling/melting point</b>              | Very high   |
| <b>Malleability</b>                       | N/A   |
| <b>Conductivity</b>                       | Poor as solids  |
| <b>Solubility in water</b>                | Varied  |
| <b>Hardness</b>                           | Extreme hardness or softness  |
| <b>Types of forces acting on molecule</b> | Covalent bonds (strength increases with more bonds); sometimes IMFs (usually LDF) |

**Examples:** Diamond, graphite, silicone (**not** Si (silicon)), semiconductors, buckyballs, nanotubes



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