Atomic Structure & Interatomic Bonding
Chapter Outline

• Review of Atomic Structure
• Atomic Bonding
Atomic Structure

Atoms are the smallest structural units of all solids, liquids & gases.

Atom: The smallest unit of an element that retains the chemical properties of the element. Atoms can exist alone or in combinations with other atoms forming molecules.

Element: One of less than 118 pure chemical substances. An element is a substance composed of atoms with identical atomic number.
**Molecule:** A particle formed by the chemical bonding of two or more atoms. The molecule is the smallest particle of a chemical compound that retains the chemical properties of the compound.

**Compound:** A material formed by the chemical combination of elements in defined proportions. Compounds can be chemically decomposed into simpler substances.
Proton: A sub-atomic particle with a positive charge of 1.60×10⁻¹⁹ coulombs and a mass of 1.672×10⁻⁷ kg. Protons are found in the nucleus of atoms.

Neutron: A sub-atomic particle with no charge and a mass of 1.675×10⁻²⁷ kg. Neutrons are found in the nucleus of atoms.

Electron: A sub-atomic particle with a negative charge of 1.60 × 10⁻¹⁹ coulombs and a mass of 9.11 × 10⁻³¹ kg. Electrons are generally found in orbit around the nucleus of an atom, but may be gained or lost during ion formation.
Atomic mass \((A)\) = Total number of nucleons (protons + neutrons) in the nucleus

Atomic number \((Z)\) = # protons (positively charged particles) which are in its nucleus, and in neutral atom the atomic number is also equal to the number of electrons in the charged cloud.

Avagadro’s Number \((N_o)\): Number of atoms of an element in one mole. \(N_o = 6.023 \times 10^{23}\)
INTERATOMIC BONDING

- Atoms link to form materials. When this linkage is self-sufficient, the resultant will be a gas, a liquid or a solid.

For example;

Atoms bond to form long chains → Polymers
Atoms bond in regular 3-D arrays → Metals

- The bonding b/w atoms is the result of the universal tendency of all systems to take up their lowest energy state. Atoms achieve their lowest energy level by the possession of 8 electrons in their outermost shell (except for the first shell which is stable only with 2e⁻)
Considering the periodic table, the elements having 8e- in their outermost shell are inert gases.
They are chemically inactive.
Electron Configuration of some elements

<table>
<thead>
<tr>
<th>Element</th>
<th>Symbol</th>
<th>Atomic Number</th>
<th>Electron Configuration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrogen</td>
<td>H</td>
<td>1</td>
<td>1s1</td>
</tr>
<tr>
<td>Helium</td>
<td>He</td>
<td>2</td>
<td>1s2</td>
</tr>
<tr>
<td>Carbon</td>
<td>C</td>
<td>6</td>
<td>1s2 2s2 2p2</td>
</tr>
<tr>
<td>Fluorine</td>
<td>F</td>
<td>9</td>
<td>1s2 2s2 2p5</td>
</tr>
<tr>
<td>Neon</td>
<td>Ne</td>
<td>10</td>
<td>1s2 2s2 2p6</td>
</tr>
<tr>
<td>Aluminium</td>
<td>Al</td>
<td>13</td>
<td>1s2 2s2 2p6 3s2 3p1</td>
</tr>
<tr>
<td>Iron</td>
<td>Fe</td>
<td>26</td>
<td>1s2 2s2 2p6 3s2 3p6 3d6 4s2</td>
</tr>
<tr>
<td>Copper</td>
<td>Cu</td>
<td>29</td>
<td>1s2 2s2 2p6 3s2 3p6 3d10 4s1</td>
</tr>
</tbody>
</table>

- **Valence Electrons** - electrons occupying outermost shells; most important as they participate in bonding between atoms and molecules.
- The rightmost elements in periodic table (Group VIII) are very stable and have only limited interaction at low temperatures (INERT GASES; rare gases, Ne, Ar, Kr, He)
Atoms of the elements having 5, 6, 7 e⁻ in their outermost shell accept 3, 2, 1 electrons respectively.

Those having 1, 2 or 3 e⁻ give up their outermost shell electrons to remain with 8 e⁻ in their underlaying shell.

Atoms having 4 valance electrons may behave in either way.

Valance electrons: The electrons at the outermost shell.
Valence Electrons (the electrons in the last shell) are responsible for most of the properties of the matter the atoms form.

They Determine:
- Types of the atomic bond
- Interatomic distances
- Mechanical strength
- Electrical properties
- Chemical properties
- Thermal properties
In a neutral atom, if the number of valence electrons is less than 8, it can give or take electrons.

The elements in the left part of the Periodic table have low valencies. These can easily give electrons to form positive ions (CATİ ONS). Such elements are called ELECTROPOSI Tİ VE Elements.

The elements at the right of the periodic table have the tendency of gaining electrons easily to form negatively charged ions (ANİ ONS). These elements are named as ELECTRONEGATİ VE Elements.

Certain other elements in between may share pairs of electrons.
PRIMÁRY BONDS

Electrostatic forces between atoms result in strong interatomic bonds

1. Ionic Bonds.
2. Covalent Bonds.
3. Metallic Bonds.

The bond or linkage between atoms is a result of general tentency of all systems to take up their lowest energy states.
2. IONIC BONDING

The transfer of an electron(s) from an electropositive atom to an electronegative one, so that a strong electrostatic attraction is set up between resultant positive and negative ions.
The most common ionic bonds form by the electron transfer from a metallic atom to a non-metallic atom. (CaF$_2$, CaO, NaCl, KCl)

Example: **NaCl**
- **Na** has 11 electrons, 1 more than needed for a full outer shell
- **Cl** has 17 electrons, 1 less than needed for a full outer shell
Formation of an ionic bond between sodium Na and chloride Cl.
Electron transfer reduces the energy of the system of atoms, that is, electron transfer is energetically favorable

- Note relative sizes of ions: Na shrinks and Cl expands
Properties of Ionic Bonding

1. Force of attraction is electrostatic (coulombic)
2. Bond is non-directional (each + ion is surrounded by as many – ions as possible)
3. Bond is strong, stable, brittle
4. High melting point (as the # of e- involved in the bond increases, melting point increases)
5. Poor electrical conductivity
6. Forms between atoms of different electronegativity values (one high, one low). An obvious limitation is that it can form only b/w different atoms.
2. COVALENT BONDING

- **Covalent bond** is the bond in which e\(^{-}\) are shared b/w atoms.

The elements showing covalent bond obey (8-N) rule.

- **(8-N) rule**: The number of the closest neighbors to each atom is equal to (8-N)

  - N is the valance e\(^{-}\).

- When N=7, such as Cl

  \[ \text{Cl}^{-} + \text{Cl}^{+} \rightarrow \text{Cl}_2 \]

  8-7=1 → the atoms pair off as diatomic molecules.
Ex: \( \text{Cl}_2 \) molecule. \( Z_{\text{Cl}} = 17 \) \( (1S^2 \ 2S^2 \ 2P^6 \ 3S^2 \ 3P^5) \) 
\( N' = 7, \ 8 \ - \ N' = 1 \rightarrow \) can form only one covalent bond.
When \( N = 6 \) such as S

\[ _{16}S : 1s^2 \ 2s^2 \ 2p^6 \ 3s^2 \ 3p^4 \]

\[ 6 \quad 8-6=2 \]

- each atom has two closest neighbors so they form **long chains**.

O, Se, Te behave like S.
When \( N = 5 \), such as

\[
{_{33}}\text{As} : 1s^2 \ 2s^2 \ 2p^6 \ 3s^2 \ 3p^6 \ 3d^{10} \ 4s^2 \ 4p^3
\]

\( 8 - 5 = 3 \rightarrow \) They require 3 closest neighbors so they form *sheets of atoms*.

When \( N = 4 \), such as \( {_{6}}\text{C} : 1s^2 \ 2s^2 \ 2p^2 \)

\( 8 - 4 = 4 \rightarrow \) They form *3-D structures*. 
Ex: Carbon materials. $Z_C = 6 \ (1S^2 \ 2S^2 \ 2P^2)$ N’ = 4, 8 - N’ = 4 → can form up to four covalent bonds

ethylene molecule:

polyethylene molecule:

ethylene mer
Ex: Carbon materials. $Z_c = 6$ (1S2 2S2 2P2) $N = 4, 8 - N' = 4 \rightarrow$ can form up to four covalent bonds

**diamond:**
(each C atom has four covalent bonds with four other carbon atoms)
Properties of Covalent Bonding

1. It is based on electron sharing.
2. Bond is directional (each atom is surrounded by a definite amount of other atoms)
3. Bond is hard and strong (slightly less than ionic)
4. Very high melting point.
5. Poor electrical conductivity.
6. Forms b/w atoms with high electronegativity. Covalent bonding is not limited to elements; many compounds are covalent, like HCl, H₂O.
3. METALLIC BONDING

- Covalent bonding occurs in electronegative atoms where they want to give away electrons.
- Metallic bond can be considered as a special type of covalent bond in which instead of sharing particular valance electrons, general sharing of valance e\(^{-}\) is responsible for the bond.
- Valance electrons are detached from atoms, and spread in an “electron cloud” that holds the ions together.
The positive metal ions are arranged regularly in a "crystal lattice" and a cloud of valance electrons surround them.

The electrostatic attraction between metal ions and free e\textsuperscript{-} provide the cohesive strength of the metal.
Properties of Metallic Bond

1. It is based on electron sharing. Electrons are shared among all atoms.
2. Non directionality - desire for the largest number of nearest neighbors.
3. High thermal and electrical conductivity.
4. Moderately lower melting point.
5. Weakest primary bond.
6. Ductile and Malleable.
7. .
High thermal and electrical conductivity

Since the valance $e^-$ are not bound to any particular atom, they can move through the lattice under the application of an electric potential causing a current flow. Also by a series of collisions with neighboring electrons they transmit thermal energy rapidly through the lattice.
SECONDARY BONDS
(VAN DER WAALS BONDS)

- Secondary bonds are universal to all atoms and molecules, but as it is a very weak bond, it may be neglected when primary bonds exist.
- It can also be termed as a physical bond as opposite to chemical bonding that involves e-transfer.
- Describes a dipolar attraction b/w neutral atoms.
- Since electrons move around nucleus (electronic charge is in motion), it is possible for electrons to be located **unsymmetrically** with respect to nucleus at a moment.
- In this way a dipole will be formed.
- Van der Waals bonding is a result of an attraction b/w opposite poles of these dipoles.

**Dipole**: Pair of equal and opposite electric charges.
Ex: HYDROGEN BOND

- As the valance electrons of water molecule spend more of its time around Oxygen atom than the Hydrogen atom, a dipole is formed.
  - The oxygen end of the molecule develops a partial negative charge (because of the negative charge on the electrons).
  - For the same reason, the hydrogen end of the molecule develops a partial positive charge.

- Negative end of each water molecule is attracted by a positive end of another water molecule.
- Ions are not formed; however, the molecule develops a partial electrical charge across it called a dipole.
A simulation of polar covalent bonding in the $\text{H}_2\text{O}$ molecule
(Only valence electrons are shown)
• Metals: Metallic bond
• Ceramics: Ionic / Covalent bonds
• Polymers: Covalent and Secondary bonds
• Semiconductors: Covalent or ionic / Ionic bonds
<table>
<thead>
<tr>
<th>Bonding Type</th>
<th>Substance</th>
<th>Bonding Energy</th>
<th>Melting Temperature</th>
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<tbody>
<tr>
<td></td>
<td></td>
<td>kJ/mol (kcal/mol)</td>
<td>eV/Atom, Ion, Molecule</td>
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<tr>
<td>Ionic</td>
<td>NaCl</td>
<td>640 (153)</td>
<td>3.3</td>
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<tr>
<td></td>
<td>MgO</td>
<td>1000 (239)</td>
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<tr>
<td>Covalent</td>
<td>Si</td>
<td>450 (108)</td>
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<tr>
<td></td>
<td>C (diamond)</td>
<td>713 (170)</td>
<td>7.4</td>
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<tr>
<td></td>
<td>Hg</td>
<td>68 (16)</td>
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<tr>
<td></td>
<td>Al</td>
<td>324 (77)</td>
<td>3.4</td>
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<tr>
<td>Metallic</td>
<td>Fe</td>
<td>406 (97)</td>
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</tr>
<tr>
<td></td>
<td>W</td>
<td>849 (203)</td>
<td>8.8</td>
</tr>
<tr>
<td>van der Waals</td>
<td>Ar</td>
<td>7.7 (1.8)</td>
<td>0.08</td>
</tr>
<tr>
<td></td>
<td>Cl₂</td>
<td>31 (7.4)</td>
<td>0.32</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>NH₃</td>
<td>35 (8.4)</td>
<td>0.36</td>
</tr>
<tr>
<td></td>
<td>H₂O</td>
<td>51 (12.2)</td>
<td>0.52</td>
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