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Physical Pharmacy

States of Matter, Molecular Structure and Binding Forces Between Molecules

Contents

In this lecture, you'll learn:

- What is “**Matter**” ?
- what is “**Matter made from**” ?
- What are the “**States of Matter**” ?
- What are the “**Forces which attach components of matter to each other** “?

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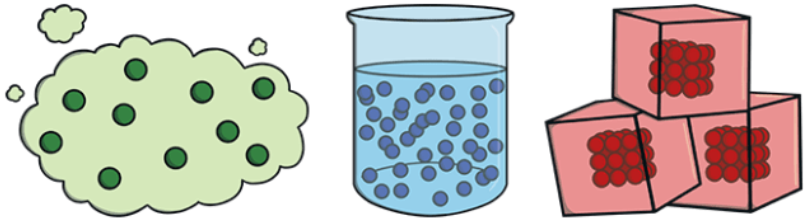
Matter

What is “**Matter**” ?

- **Matter** can be defined as anything that has a mass and a volume.

- There are four basic properties that should be used when we describe a matter, these are:



1. **Mass :** How much matter something contains
2. **Weight:** A measure of the pull of gravity on an object
3. **Volume**: How much space matter takes up
4. **Density**: How much matter is in a certain volume

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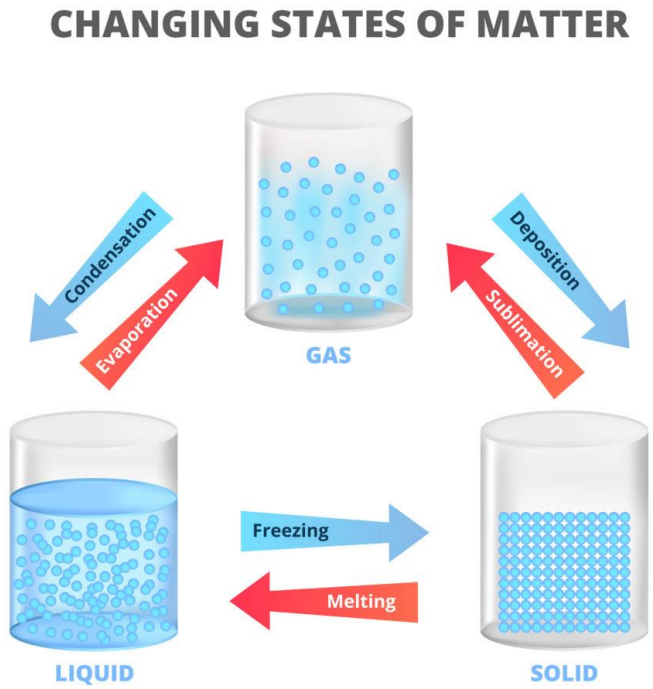
Matter

What are the "States of Matter"?

- States of matter are forms in which matter exists.
- It describe the qualities displayed by matter.

- **Fundamental States of Matter:** Basically, we have **3** different states of matter **(Solid, Liquid and Gas)** and these are characterized due to difference

1. Based upon particle arrangement
2. Based upon energy of particles
3. Based upon distance between particles



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PROPERTIES OF THE THREE STATES OF MATTER

Physical Property	Solids	Liquids	Gases
Shape	Has a fixed shape	Takes up the shape of the container	Takes up the shape of the container
Volume	Fixed volume	Fixed volume	Changes volume to fill its container
Fluidity	Does not flow easily	Flows easily	Flows easily
Compressibility	Not easy to compress	Not easy to compress	Easy to compress

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PROPERTIES OF THE THREE STATES OF MATTER

mass - stays the same

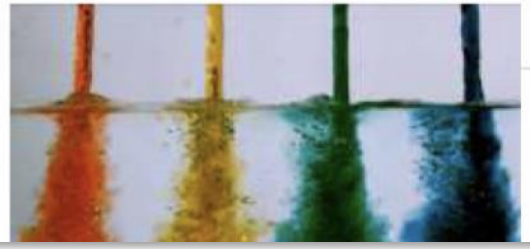
volume - stays the same

shape - stays the same

mass - stays the same

volume - stays the same

shape - changes



mass - stays the same

volume - changes

shape - changes

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Changes in Matter

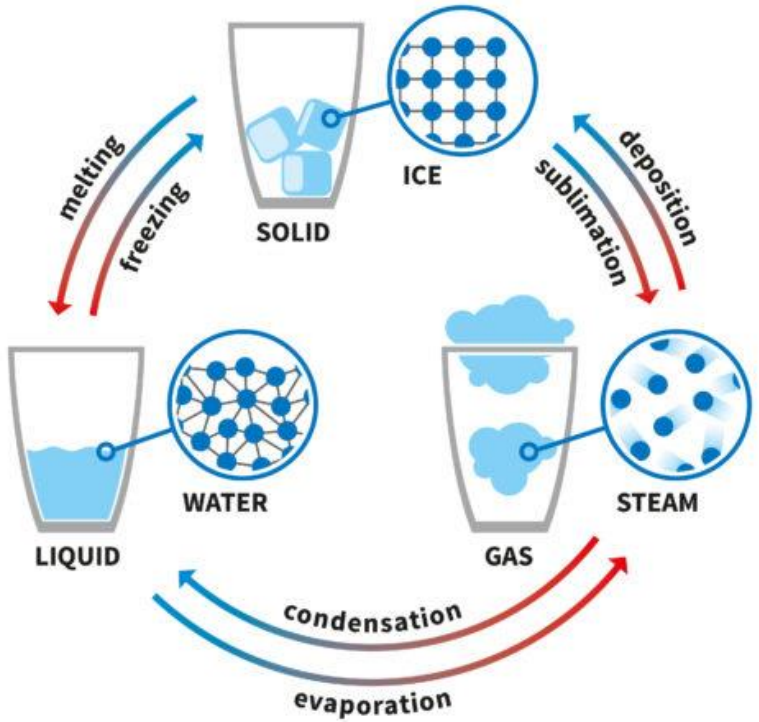
- Matter is constantly changing Into two types :

1. Physical Changes

- A change that alters a physical property of a substance (eg shape, state, temperature) but doesn't make a new substance.

- Usually reversible - can get the original substances back easily

- Examples - cutting paper, freezing water to form ice, dissolving sugar in water



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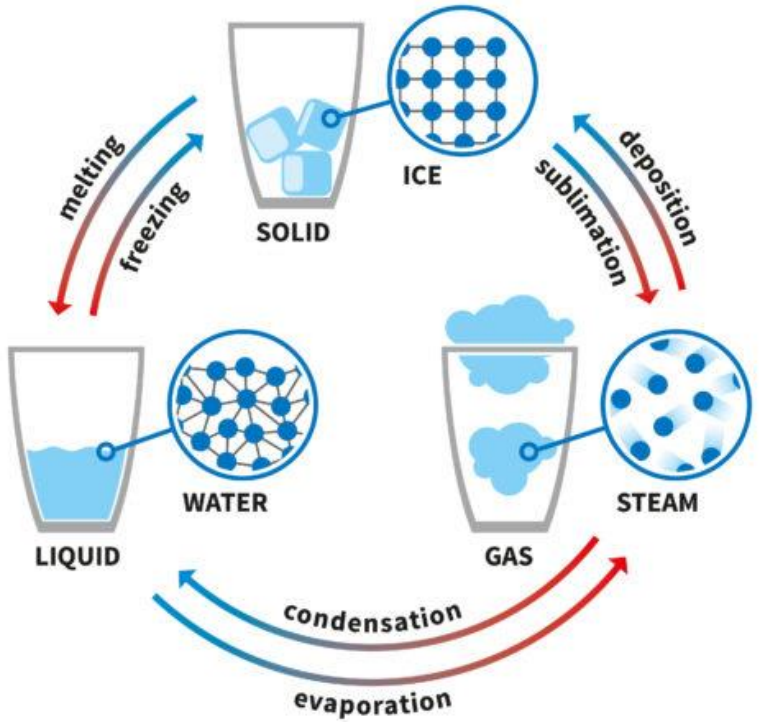
Changes in Matter

- Matter is constantly changing Into two types :

2. Chemical Changes

- A change that forms one or more new substances
- Usually irreversible - cannot get the original substances back.
- Examples - cooking an egg, burning paper, baking a cake



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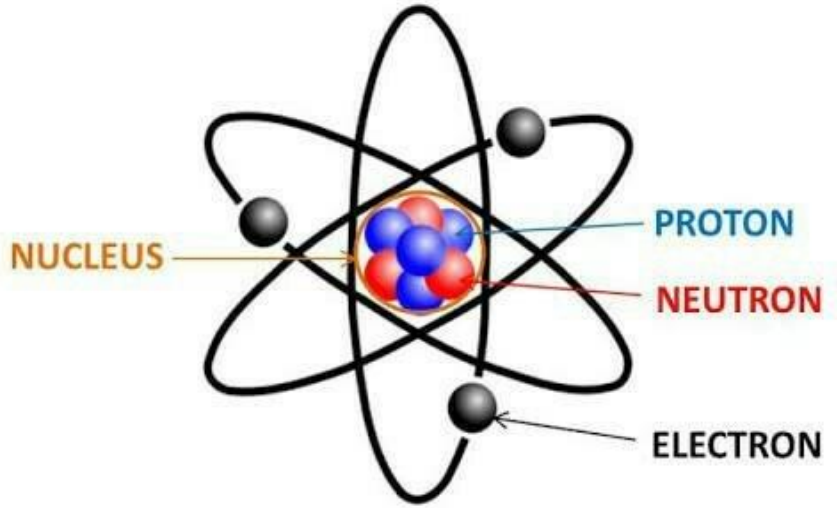
what is " Matter "made from?

- All matter is composed of small particles (atoms, molecules, or ions).

- The smallest unit of any matter is called **Atom**



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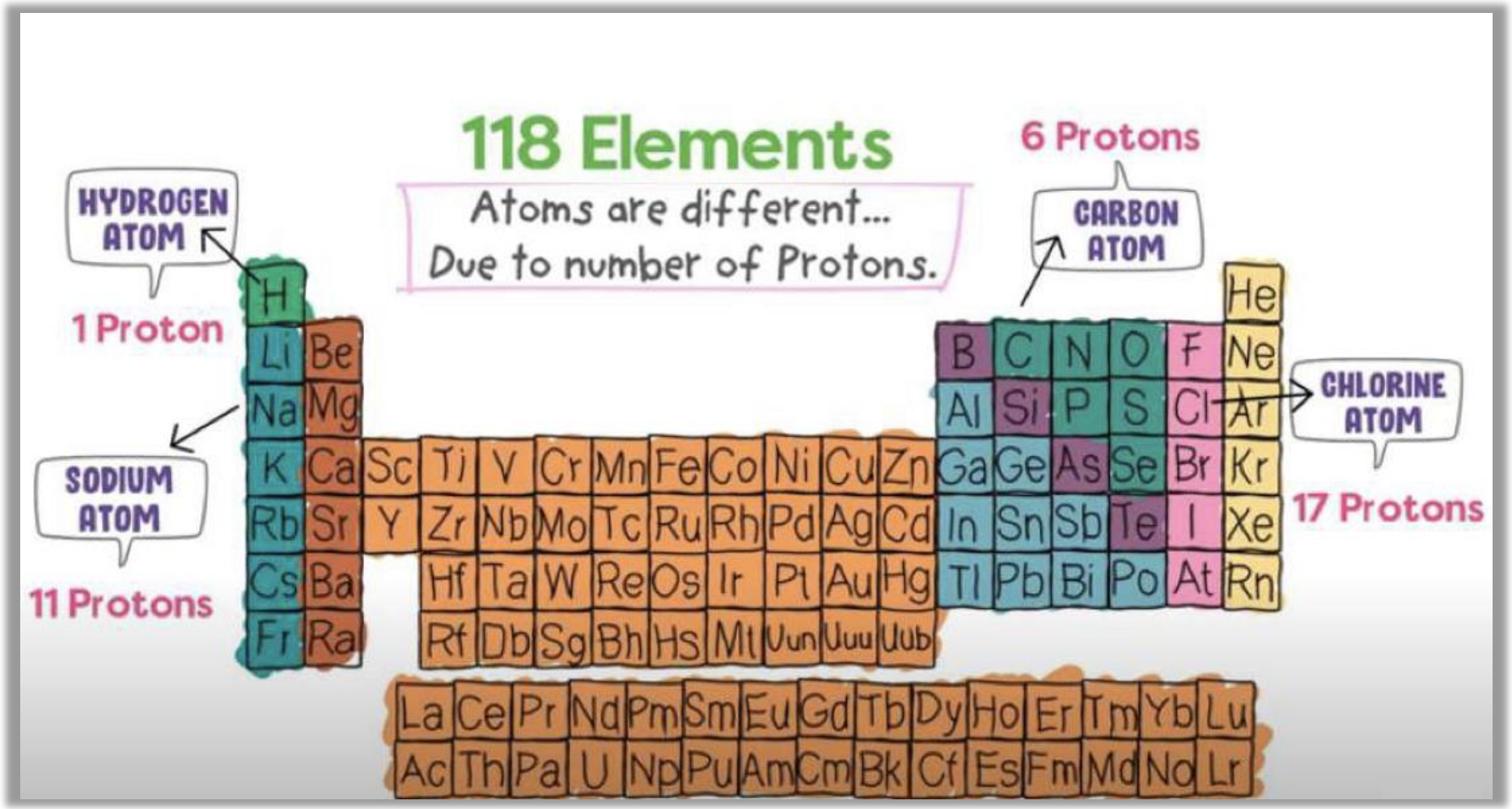

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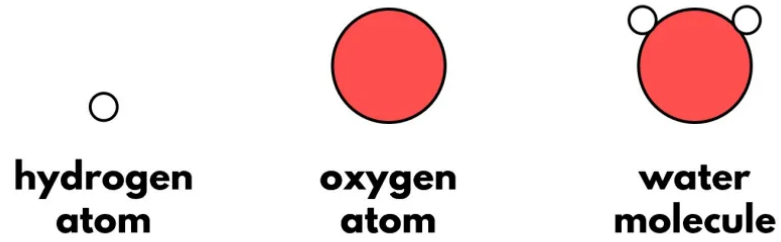
What binds Atoms and Molecules together?

- Atoms need to create bonds in order to become stable

- There are different types of forces which bind atoms and molecules
- What are **molecules**? When two or more atoms combine chemically together, they form a molecule
- Molecules can be:

1. **Pure elements:** when it is composed of same type of atoms. For example: Cl2
2. **Compound:** when it is composed of different type of atoms. For example: H2O



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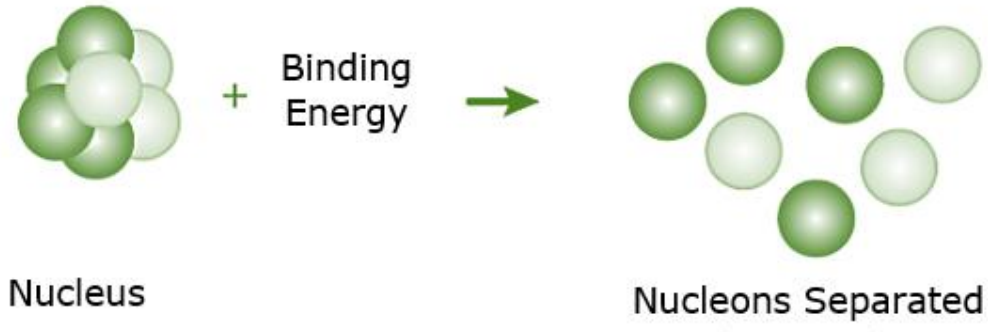
What binds **Atoms** and **Molecules** together?

- **Binding Force**

1. **Intra-molecular forces**
2. **Intermolecular forces**



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What binds Atoms and Molecules together?

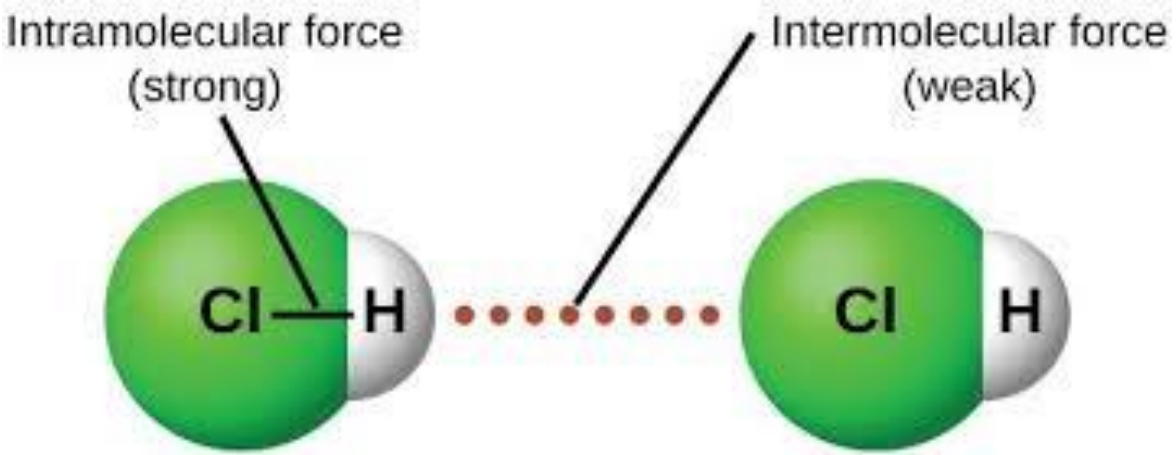
- **The difference between**
- **Intra-molecular forces**

1. Forces of attraction between the atoms that hold an individual molecule together

2. Bonding Forces

3. Exist within **Molecules**

4. Determine Chemical Properties...



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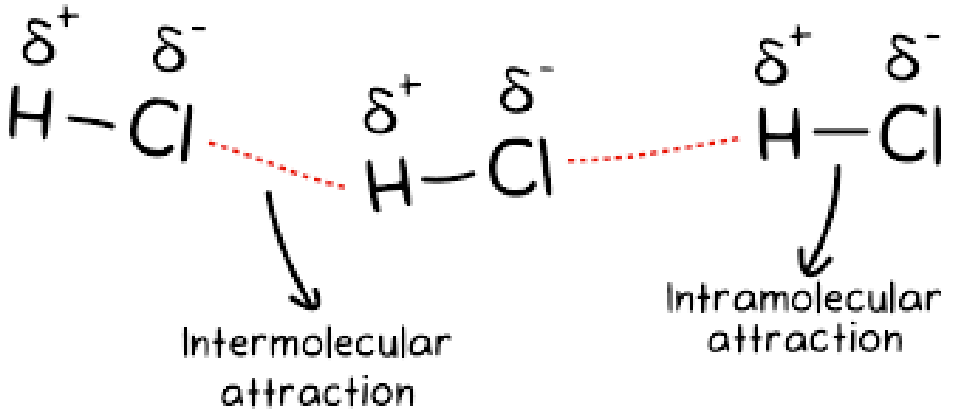
What binds Atoms and Molecules together?

- **The difference between**
- **Inter-molecular forces**

1. Forces of attractions between a molecule and its neighboring molecule
2. Attractive Forces **(Non-bonding Forces)**

3. Exist between **Molecules**

4. Determine Physical Properties...



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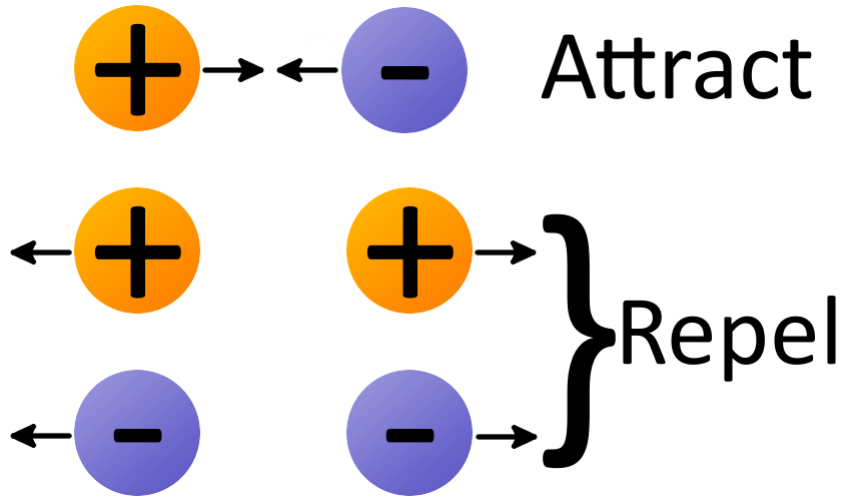
What type of forces exist between atoms and molecules?

- On the atomic or molecular scale, all particles exert both attractive and repulsive forces on each other.

- The nature of these forces dictate some of the important properties of matter.

Repulsive and Attractive Forces



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What type of forces attach components of matter to each other ?

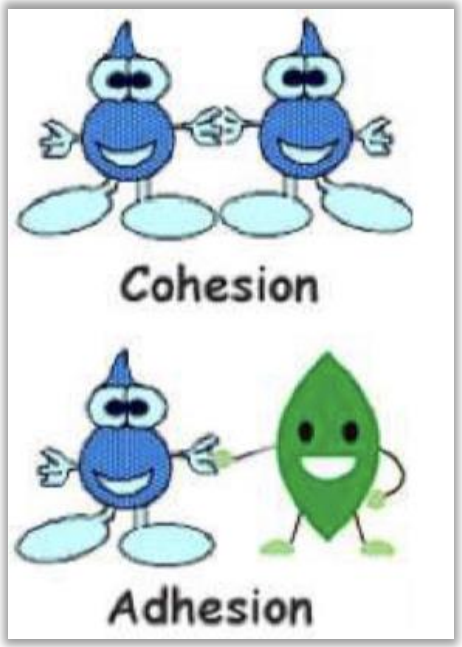
Attractive and Repulsive Forces

Attractive Forces

1. Bring atoms or molecules together and are necessary for molecules to cohere.
2. They are seen as two atoms or molecules with opposite charges are brought closer together
3. They are of two types:

   a) **Cohesion forces (attraction between molecules of the same substance)**
   b) **Adhesion forces (attraction between molecules of different substances)**

4. They are long range interactions



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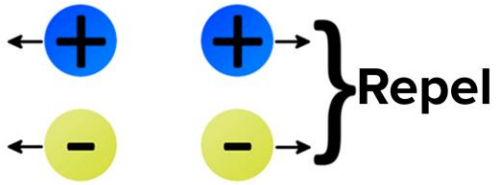
Repulsive Forces

1. Push atoms or molecules apart and prevent the molecules from interpenetrating with each other.

2. They are seen as the negatively charged electron clouds of the molecules are brought so close that the outer charge clouds touch, and hence the molecules will repel each other like rigid elastic bodies.

3. These are short range interactions.



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- Sharing of electrons by atoms make them more stable (have lower energy)
- When two atoms or molecules approach (come together)There is a gradual energy change and a combination of attractive and repulsive forces act on these two atoms.

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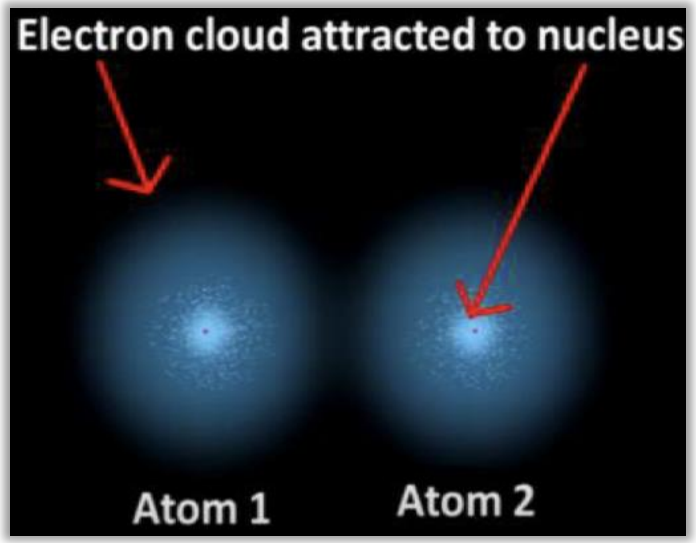
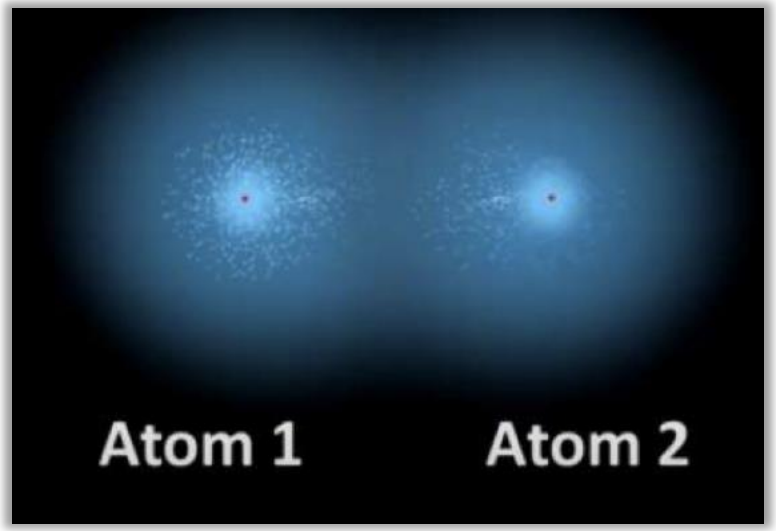
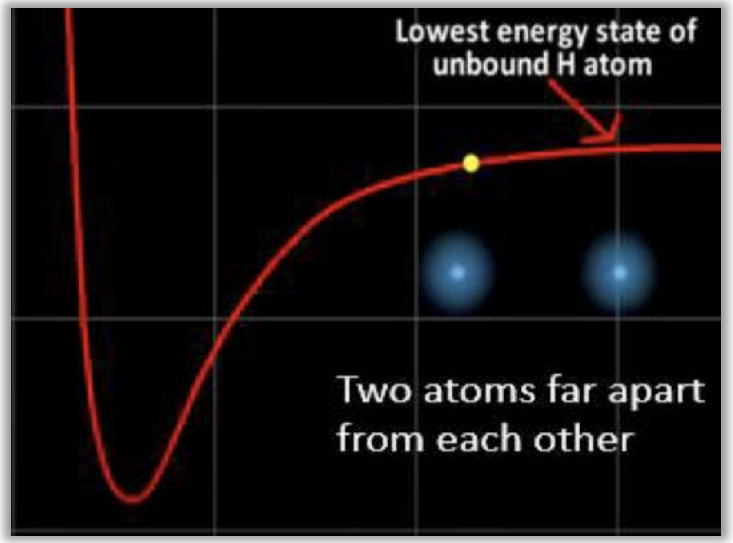
1. There are initially forces are attraction which act to pull the opposite charges of two molecules closer to a point of minimum energy.







- In a force responsive curve, as two atoms come together, the potential energy becomes increasingly negative.

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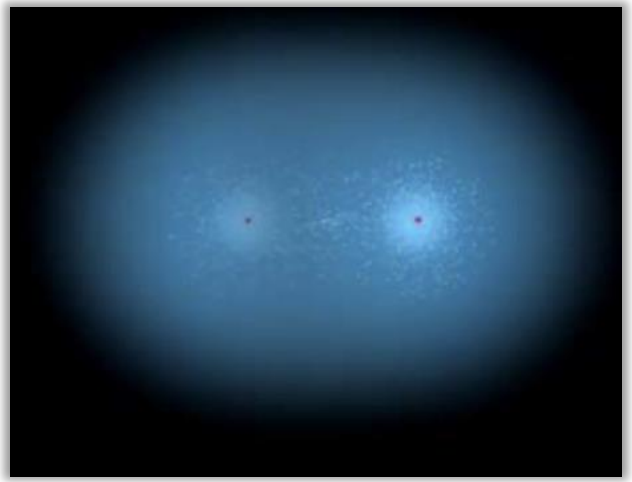
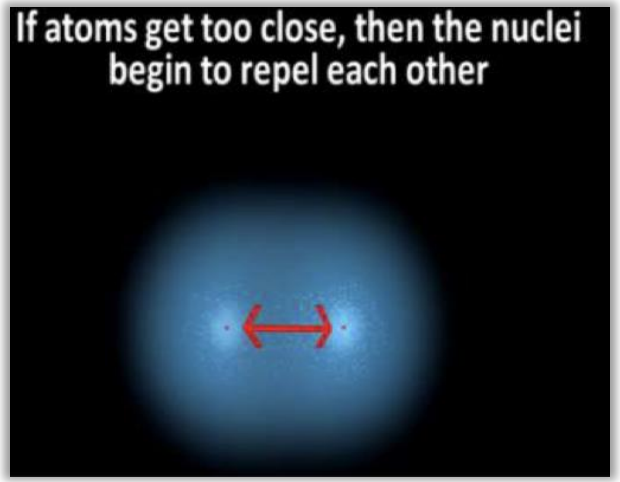
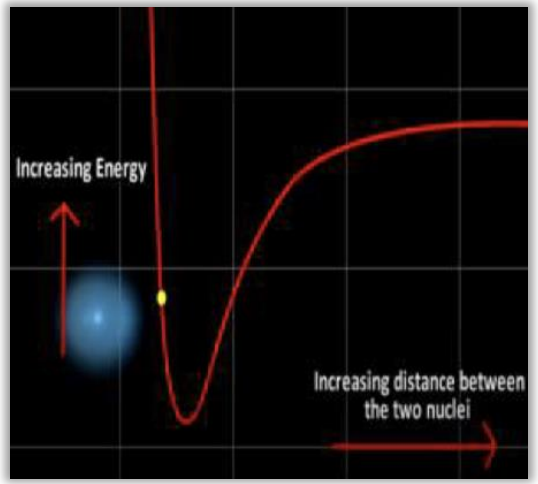
- **When two atoms or molecules approach (come together): Cont.'**
- **2 -** As the atoms or molecules become very close together, the electron clouds start to overlap, which leads to very strong **repulsive forces.**
- As the repulsive forces increase, the potential energy becomes increasingly positive







- The negatively charged electron clouds of the molecules largely govern the balance of forces between the two molecules

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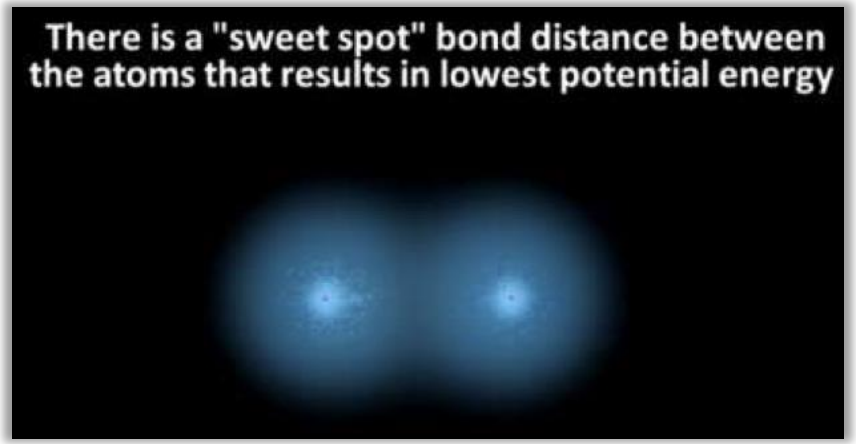
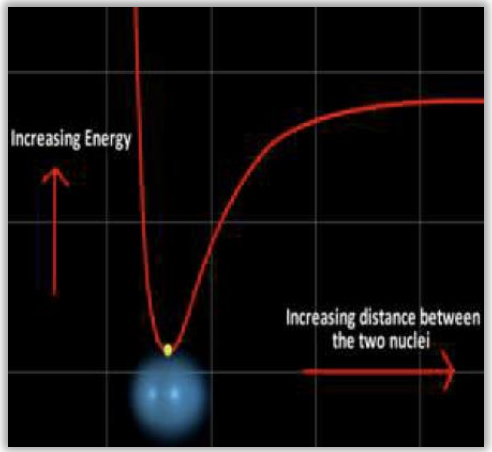
- **When two atoms or molecules approach (come together): Cont.'**
- 3. When a balance point is reached between attractive and repulsive forces, the atoms will have minimum potential energy.





- Thus:The total force between atoms or molecules is the sum of attractive and repulsive forces.
- The net energy represents a function of the distance between the molecules.
- The repulsion forces increase exponentially with a decrease in distance (r) between the molecules.

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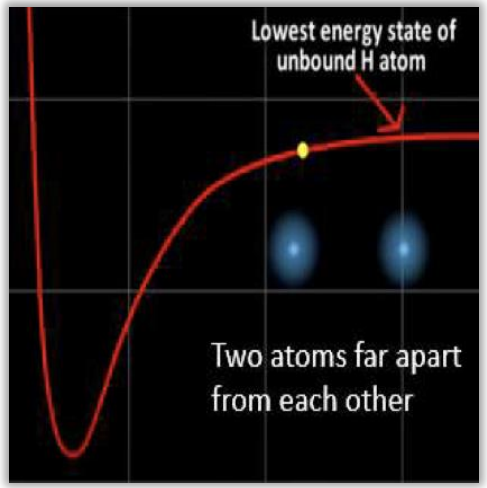
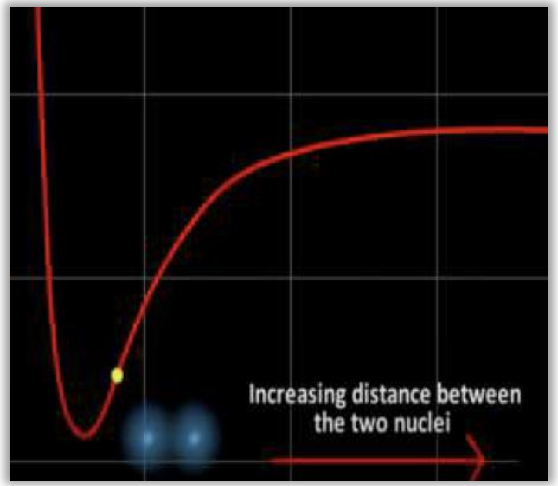
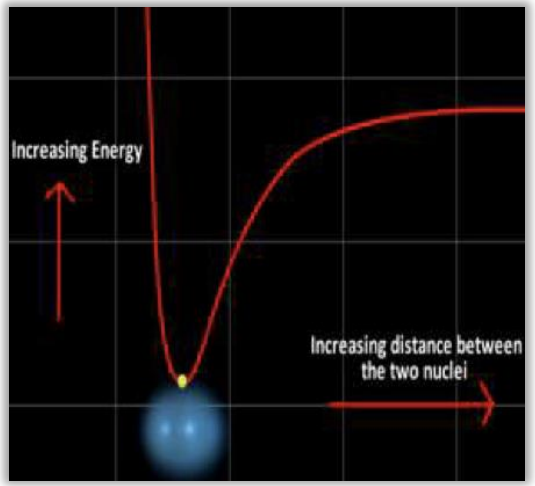
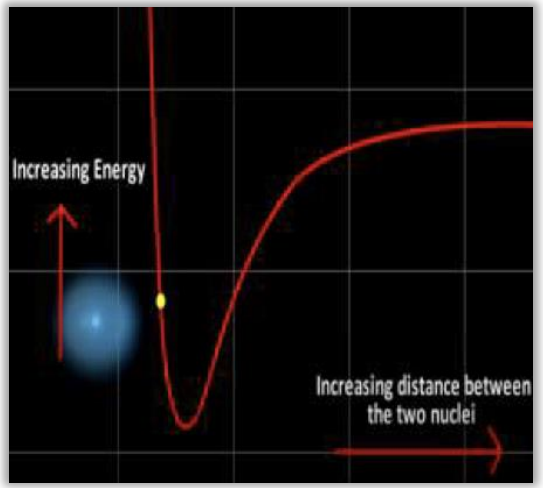
- **Using a potential energy diagram (Force Response Curve):**
- In the figures: as we move from right to left: There is gradual energy change; as the attractive forces increase, the potential energy becomes increasingly negative.
- As the repulsive forces increase, the potential energy becomes increasingly positive









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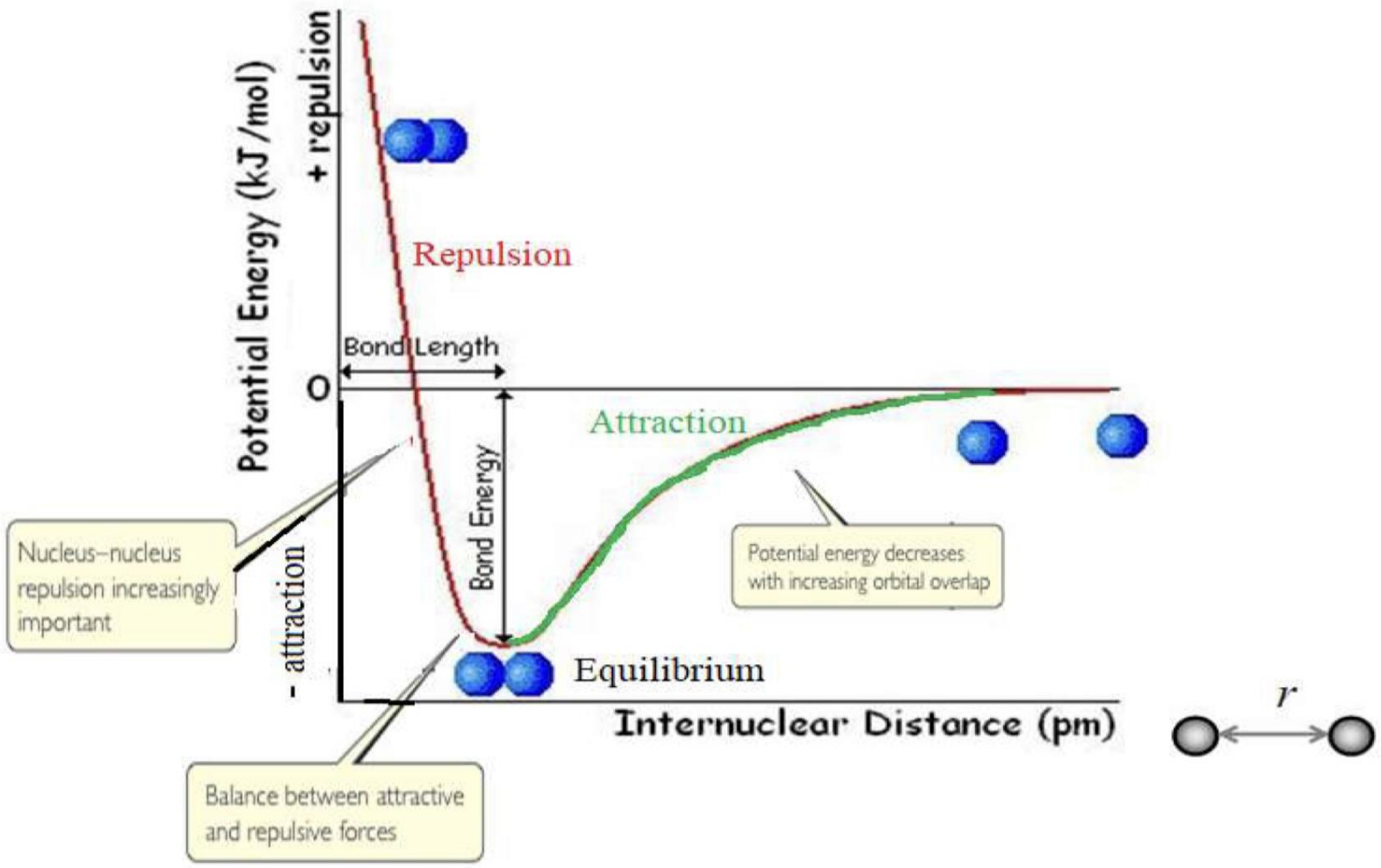
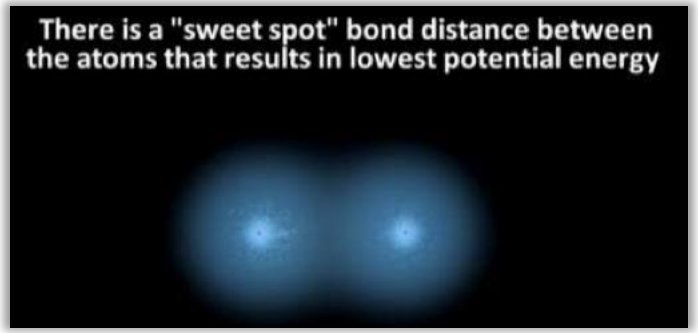


Force Response Curve



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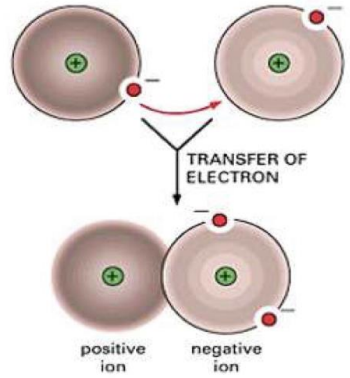
Forces within molecules: inter-molecular force

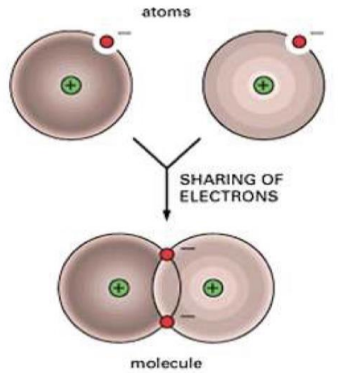
- **Ionic Bonds :** Are bonds formed between two oppositely charged ions due to complete transfer of valence electrons from one atom to another.

Example: NaCl



- **Covalent Bonds:** Are bonds formed between two atoms (same or different) due to sharing of electrons.

Example: H2, CCl4



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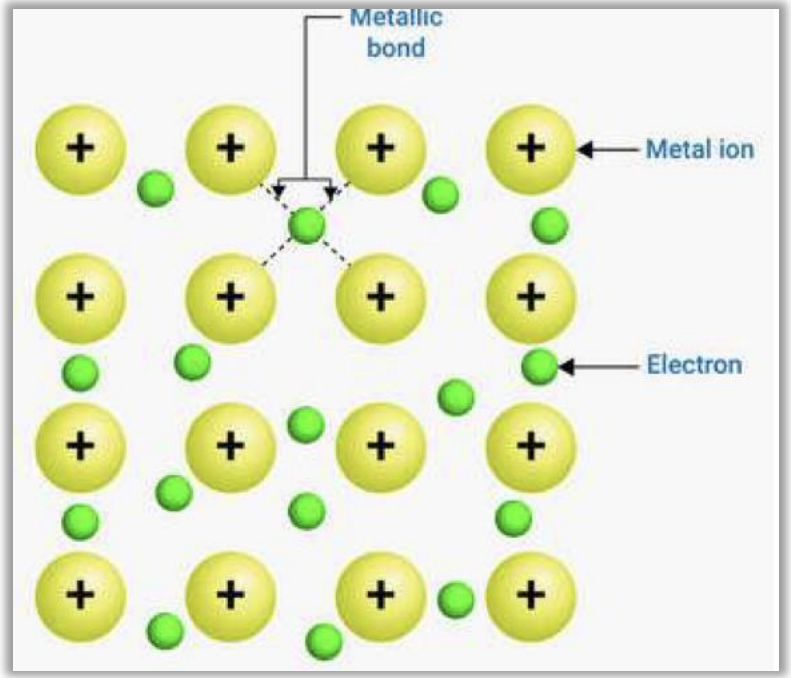
Forces within molecules: inter-molecular force

- **Metallic Bonds:** Are bonds formed due to sharing of free valence electrons between a group of positively charged metal ions.

Example: Gold, silver, copper



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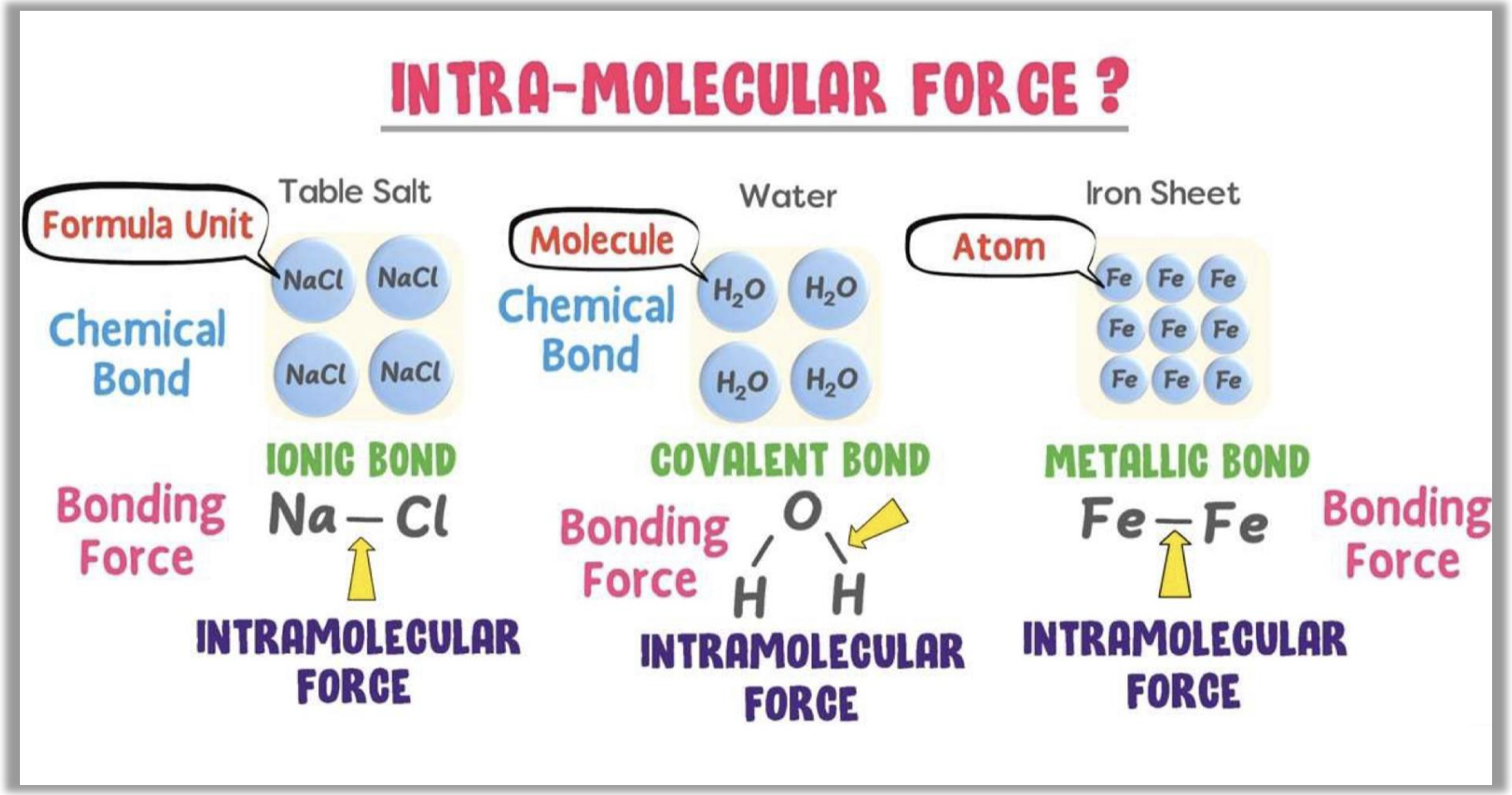

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Forces within molecules: inter-molecular force

- An **intermolecular force** (or secondary force) is the force that mediates interaction between molecules.
- These forces must exist between molecules so that such molecules can form aggregates in gases, liquids, and solids.
- The intermolecular forces may involve weak attractive forces due to the electron distribution in the molecules or involve specific intermolecular bonds – such as hydrogen bonds.
- The common types of attractive intermolecular forces are categorized into the following classes:

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Forces within molecules: inter-molecular force

- Van der Waals forces

a) Keesom forces
b) Debye forces
c) London forces

- Hydrogen bonding
- Ion–dipole forces
- Ion–induced dipole forces

Before discussing intermolecular forces ,you need to understand the concept of a dipole.(see supplementary slides 55,56,57,58 if required)

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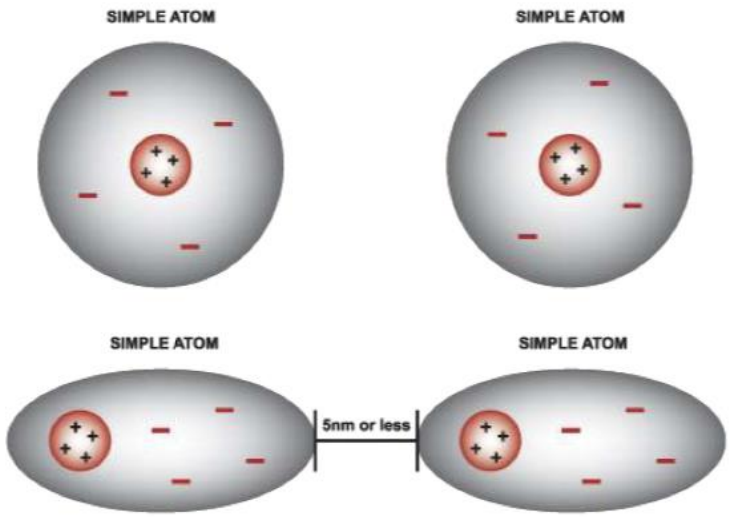
Inter-molecular force

- **Van der Waals forces:** Van der Waals Forces are relatively weak attractive forces that arise because of fluctuation in the electron density of all molecules and these cause sma dipoles within the molecules.

- The electric polarization will attract one molecule to another.

- When two atoms come within 5 nanometers of each othe there will be a transient shift in electron density to one side of the nucleus, thus causing polarity and a slight attraction between the atoms.



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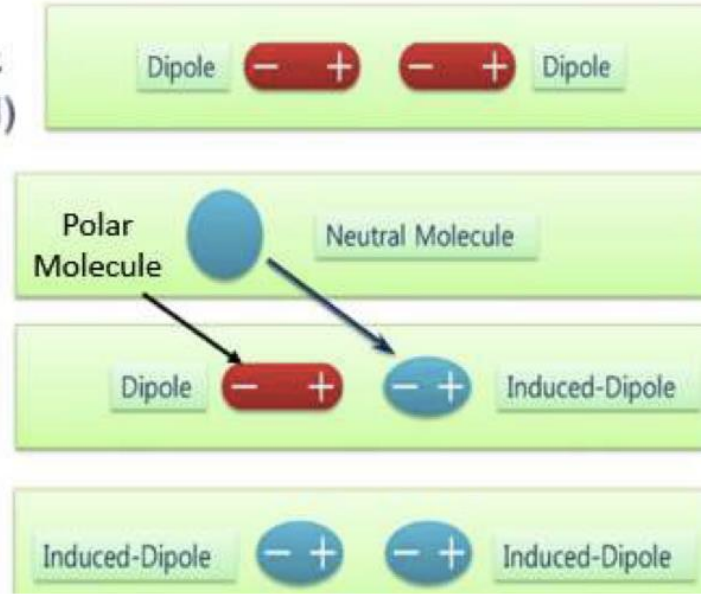
Inter-molecular force

van der Waals forces

- Keesom forces: permanent dipole - permanent dipole
  (water, hydrochloric acid, alcohol, phenol)
  → hydrogen bond
- Debye forces: permanent dipole – induced dipole
  (ethylacetate, methylene chloride, ether)
- London forces: instantaneous dipole- induced dipole
  (carbon disulfide, carbon tetrachloride, hexane)



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Van der Waals Forces : 1- Dipole–Dipole Forces (Keesom forces)

- Are electrostatic attractive forces that occur between two polar molecules (molecules which have permanent dipoles, where molecules have an asymmetric distribution of electrons, i.e., they contain polar bonds)

- Dipolar molecules frequently tend to align themselves with their neighbors to lower the energy of the assembled molecules so that the negative pole of one molecule (d-) points toward the positive pole (d+) of the next.

- Thus, a large groups of molecules may be associated through weak attractions.

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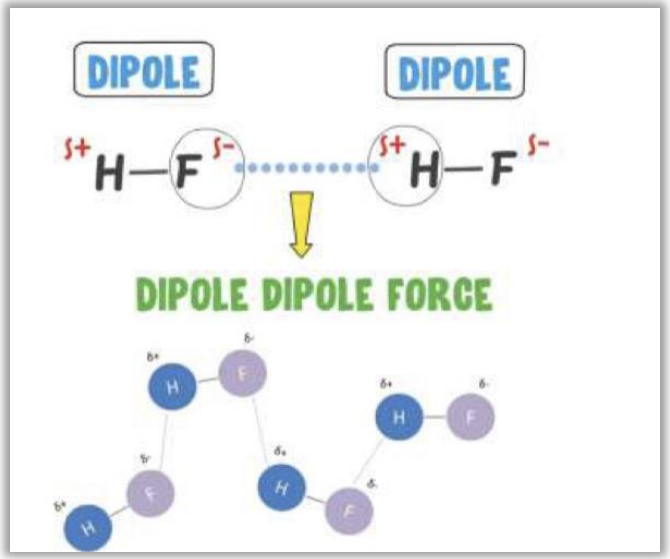
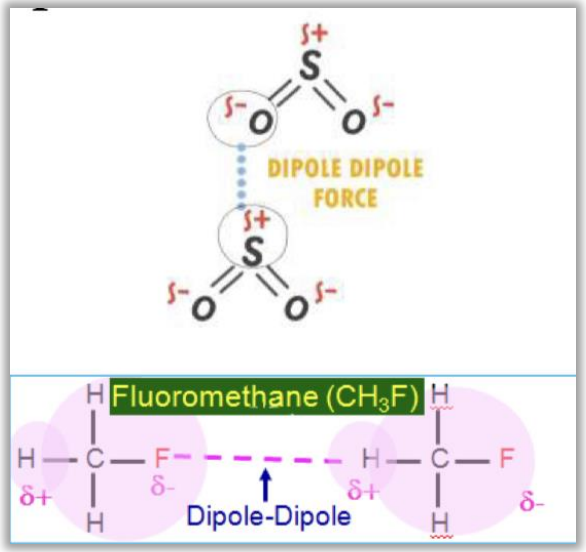
Van der Waals Forces : 1- Dipole–Dipole Forces (Keesom forces)

- **Energy of attraction: 1-7 Kcal/mole**





a) Dipole Dipole Force is not a Chemical Bond
b) Dipole Dipole Force exists only in Polar Covalent... HCL , So2
c) Dipole Dipole Force does not exsit in No Polar Covalent...Cl2, 02

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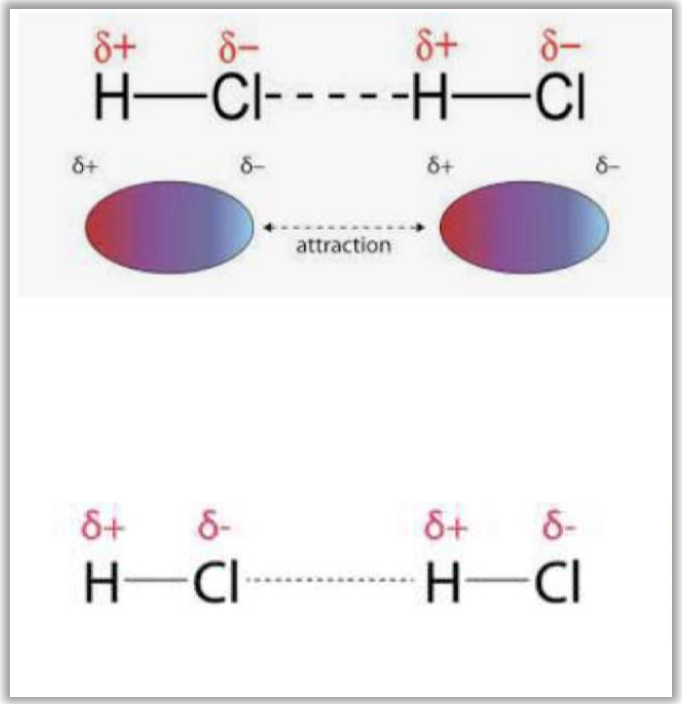
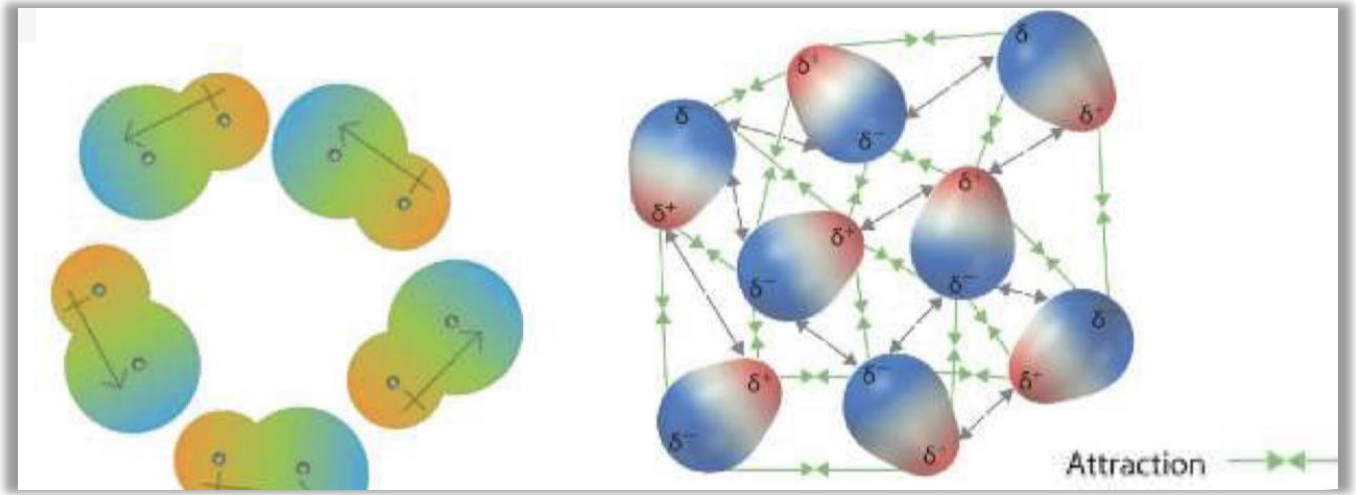
Van der Waals Forces : 1- Dipole–Dipole Forces (Keesom forces)

- The alignment could be end-to-end, resulting in a stronger interaction than a side-by-side alignment.





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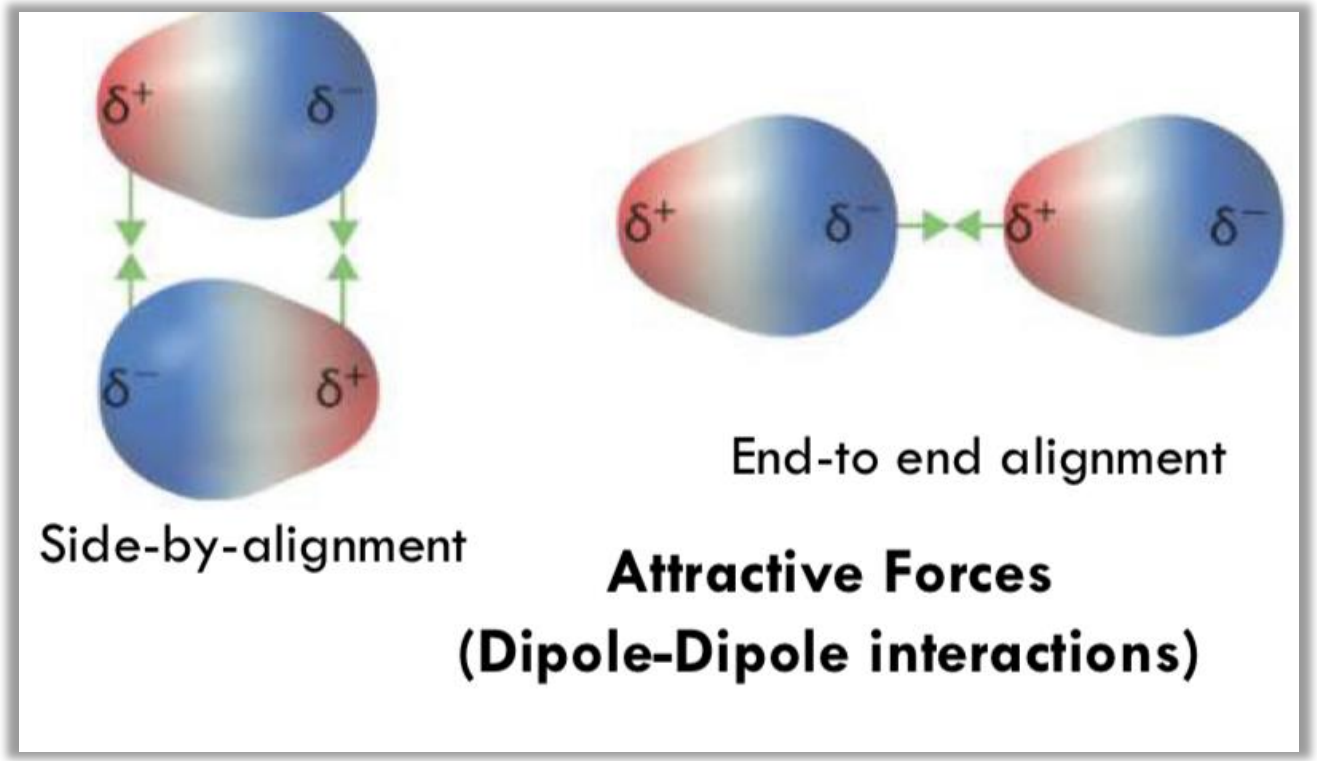
Van der Waals Forces : 1- Dipole–Dipole Forces (Keesom forces)



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Van der Waals Forces : 2- Dipole–Induced dipole Forces (Debye forces)

- Permanent dipoles (polar molecules) are capable of inducing a temporary electric dipole in normally non-polar molecules (easily polarizable), and thus produce a net attractive force between the two particles.

- This attraction is usually rather weak (about half of dipole-dipole forces), but in a few cases it can lead to the formation of loosely-bound compounds.

- This effect explains the observation that a wide variety of neutral molecules such as hydrocarbons, and even some of the noble gas elements, form stable hydrate compounds with water.

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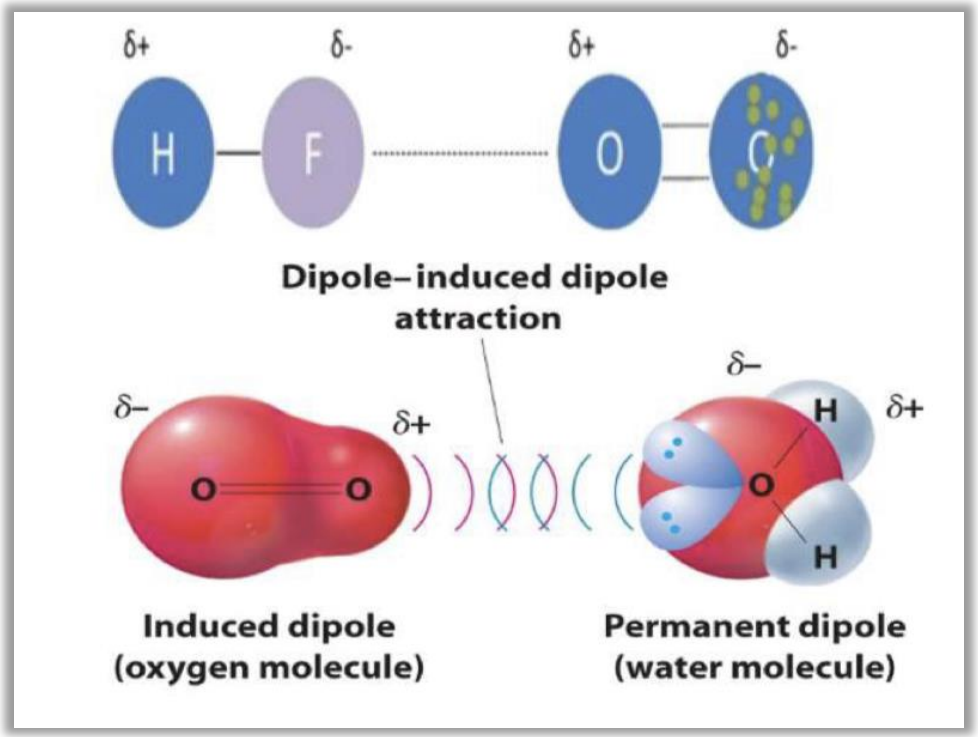
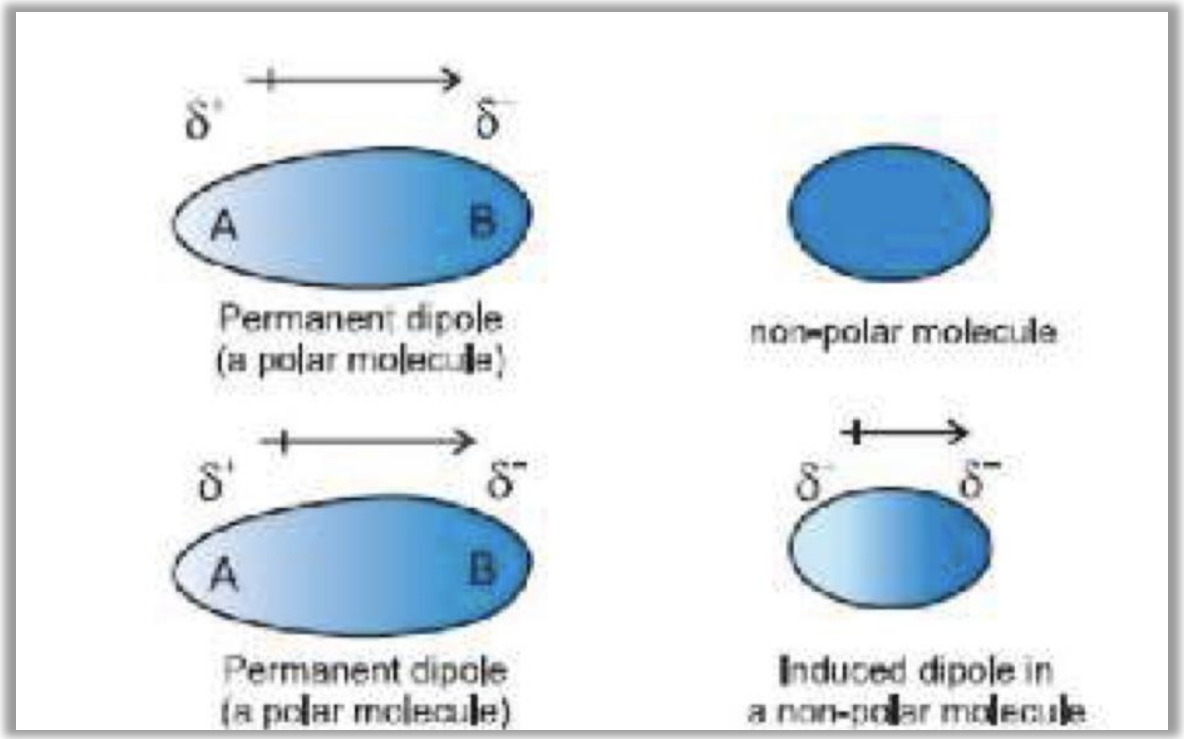
Van der Waals Forces : 2- Dipole–Induced dipole Forces (Debye forces)

- **Energy of attraction: 1-3 Kcal/mole**





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Van der Waals Forces : 3- Induced Dipole–Induced Dipole Forces (London forces)

- **Non polar molecules can induce polarity in one another.**
- This can be explained as follows:there is no guarantee that the distribution of negative charge around the center of an atom will be perfectly symmetrical at every instant.
- On a very short time scale, every atom therefore has a weak, fluctuating dipole moment that is continually disappearing and reappearing in another direction.

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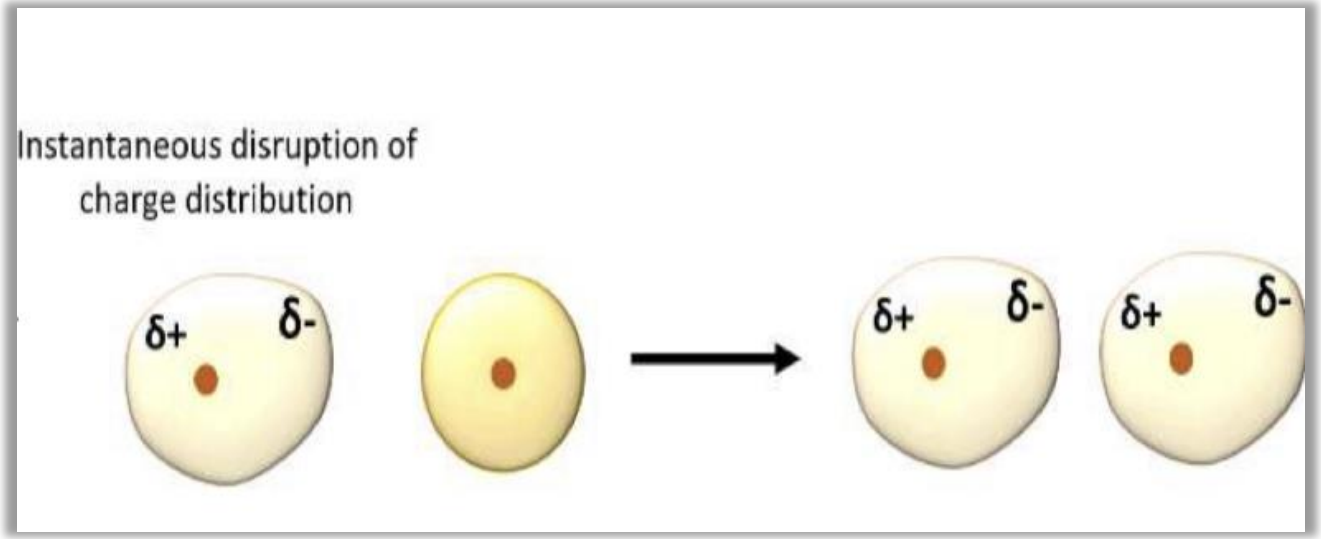
Van der Waals Forces : 3- Induced Dipole–Induced Dipole Forces (London forces)

- Although these extremely short-lived fluctuations quickly average out to zero, they can still induce new dipoles in a neighboring atom or molecule, which helps sustain the original dipole and gives rise to a weak attractive force known as the dispersion or London force.



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Van der Waals Forces : 3- Induced Dipole–Induced Dipole Forces (London forces)

- London forces are “the only kind of intermolecular interaction forces seen in non-polar molecules”.

- Unlike the other two types of Van der Wasls forces they are present in all molecules and are the weakest of all intermolecular forces.

- **Energy of attraction: 0.5-1 Kcal/mole**

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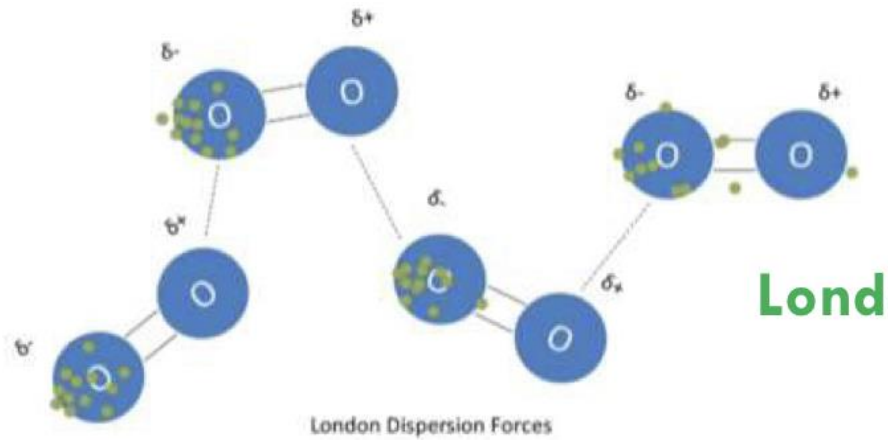
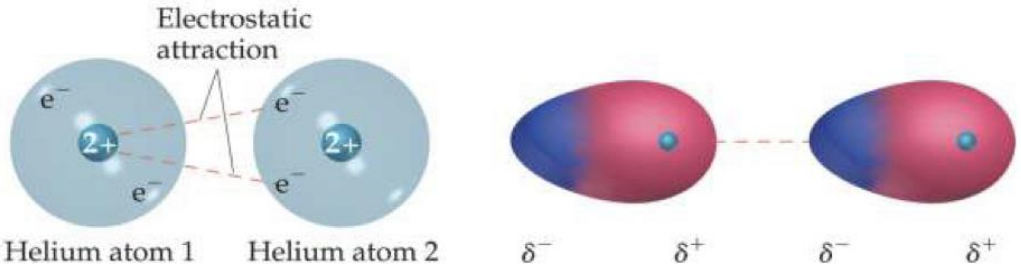
Van der Waals Forces : 3- Induced Dipole–Induced Dipole Forces (London forces)



London Forces

Between Non-polar molecules.

H_2 F_2 Cl_2 O_2



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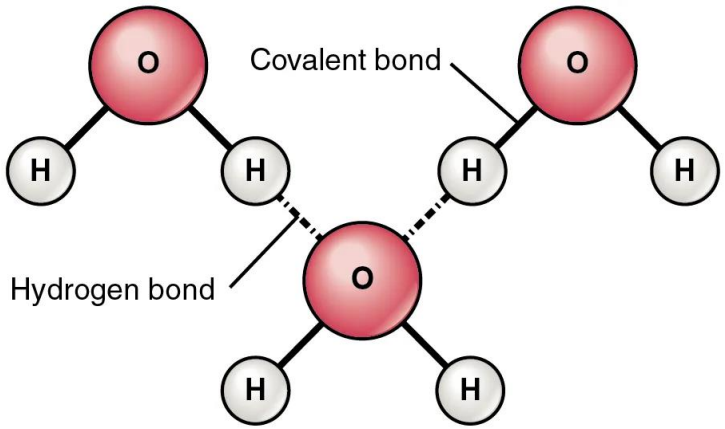
Intermolecular Forces: Hydrogen Bonding

- Hydrogen bonding occurs when a hydrogen atom bonded to an electronegative atom **(Z)** such as **(O, N, or F)** is attracted to a lone pair of electrons on an atom in another molecule.
- To emphasize this one more time; hydrogen bonding is not a covalent bond within the molecule, but it is a specific type of dipole-dipole interaction.
- Hydrogen bonds are shown with dotted lines connecting a lone pair with the hydrogen.



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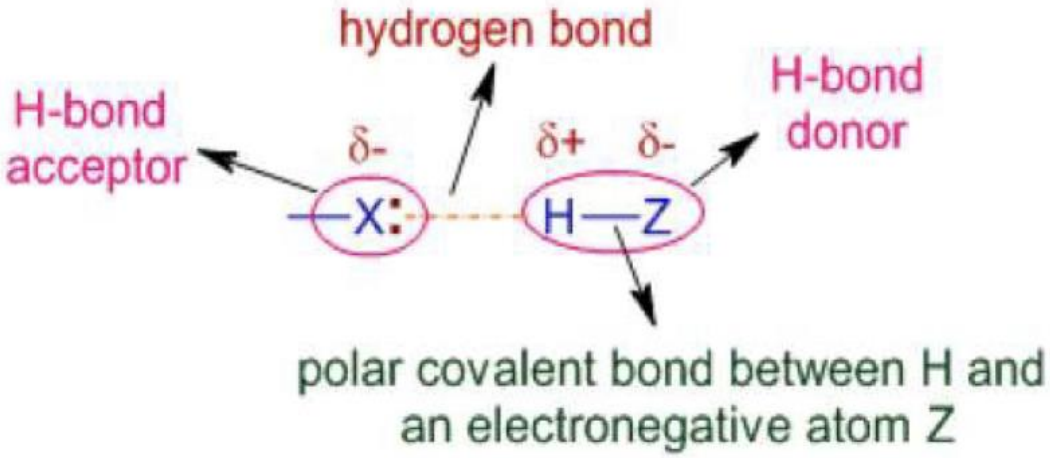
Intermolecular Forces : Hydrogen Bonding

- Hydrogen bonding is very common in nature starting from water and going to complex biological systems like **DNA** and proteins.
- The hydrogen bond is stronger than Van der Waals interaction, but weaker than covalent c ionic bonds.
- **Energy of attraction: 2-8 Kcal/mole**



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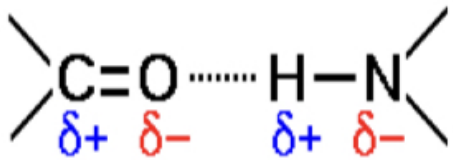
Hydrogen Bonding：Examples on Hydrogen Bonding

- Simple hydrogen bonding between two diatomic molecules

- As in hydrogen fluoride in the vapor state which exist as a hydrogen bonded polymer **(F-H....)n** where can be as large as **6**.



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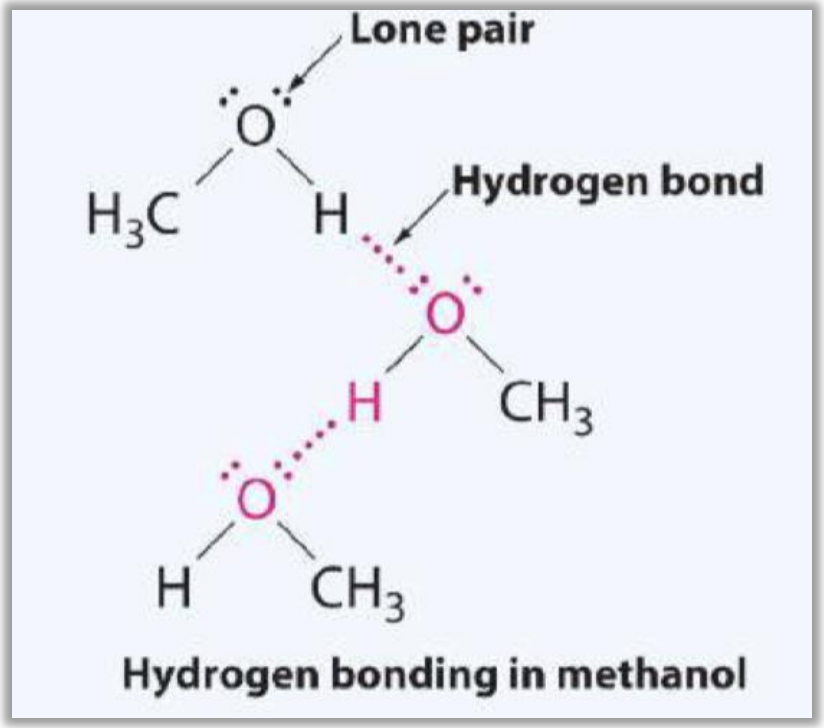
Hydrogen Bonding：Examples on Hydrogen Bonding

- Hydrogen bonding between carbonyl and amide group
- Hydrogen bonds can also exist between **alcohol molecules, carboxylic acids, aldehydes, esters, and polypeptides**



Hydrogen bonding in methanol

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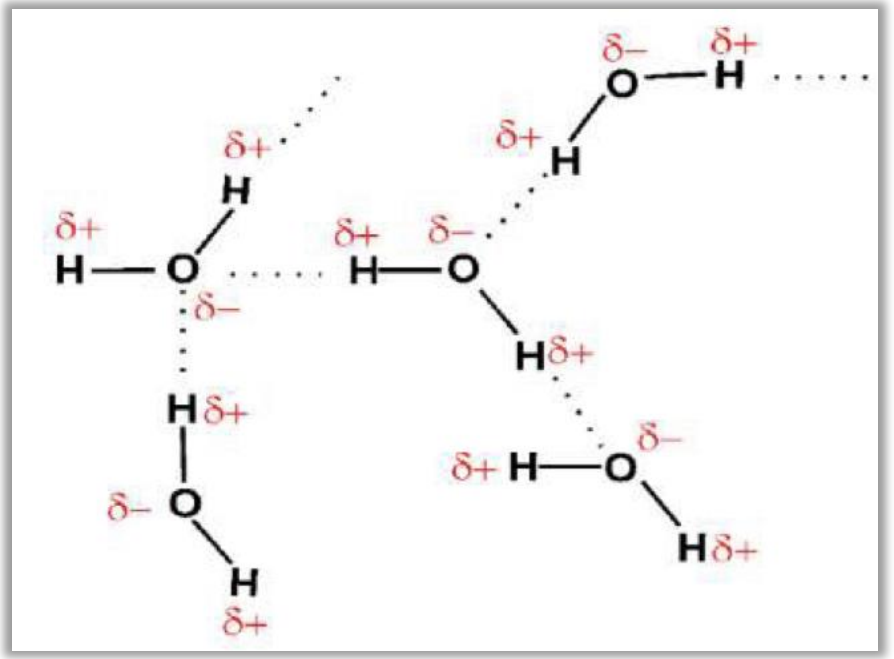
Hydrogen Bonding in water

- Hydrogen bond exists in ice and in liquid water; it accounts for many of the unusual properties of water including its high dielectric constant, abnormally low vapor pressure, and high boiling point.
- Ice has the very unusual property that its solid state is less dense than its liquid state.
- As a result, ice floats in liquid water.



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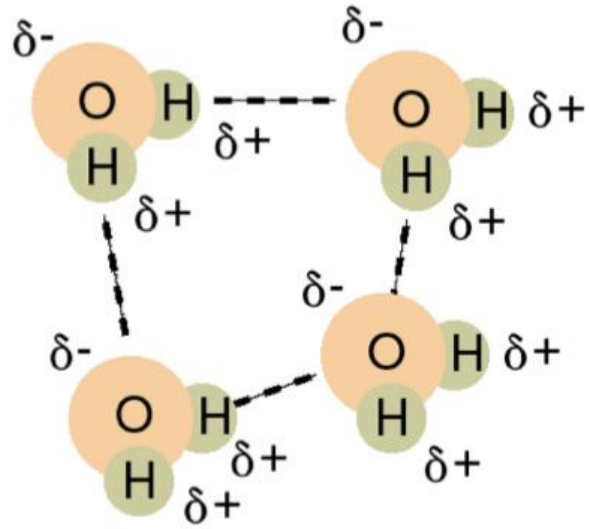
Hydrogen Bonding in water

- The expansion of water when freezing also explains why unprotected pipes in houses break if they are allowed to freeze.
- Ice is well ordered **3-dimensional** array of regular tetrahedra with oxygen in the center and **H** atom at each corner **(H-atoms are not exactly midway between the oxygens)**



Water as liquid

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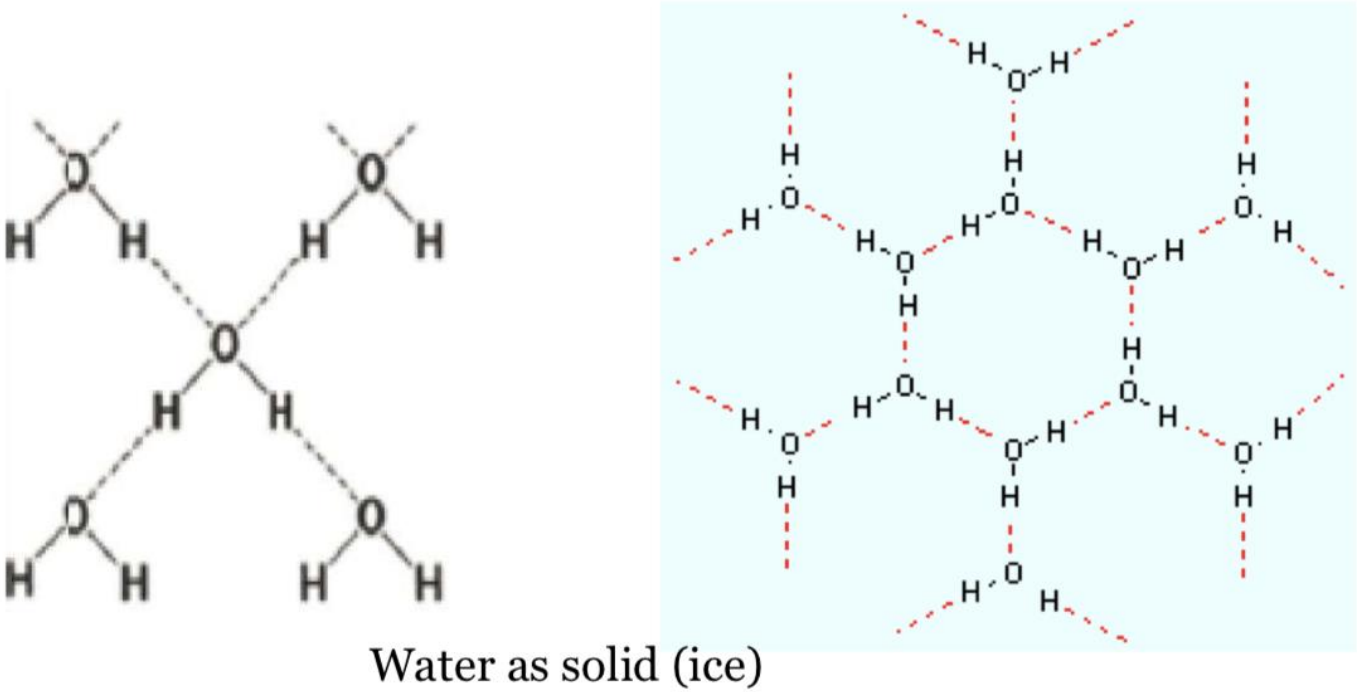
Hydrogen Bonding in water



Water as solid (ice)

About one sixth of the hydrogen bonds of ice are broken when ice convert to liquid state and all are destroyed when it vaporize

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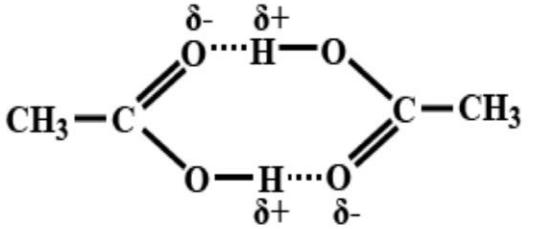
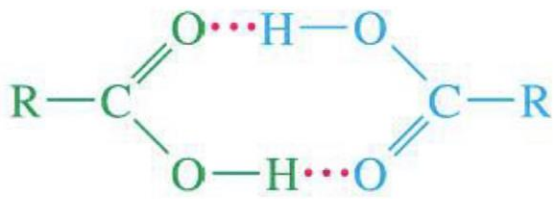
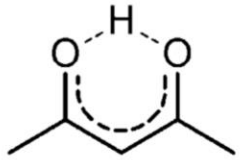
Examples on Hydrogen Bonding



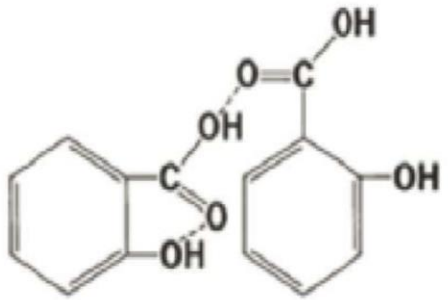


hydrogen-bonded acid dimer

- Hydrogen bonding between two carboxylic molecules
- The hydrogen bonds of formic acid and acetic acid are sufficiently strong to yield dimers **(two molecules attached together)**, which can exist even in the vapor state.



- Intramolecular hydrogen bonding within one carboxylic molecule
- It is noticed that intra- as well as intermolecular hydrogen bonds may occur



(as in salicylic acid)

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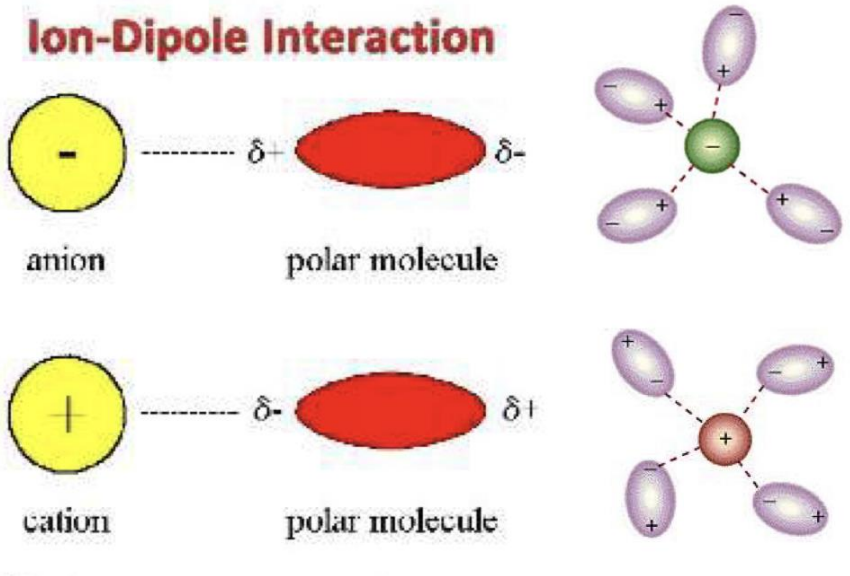
Intermolecular Forces: ion - dipole force

- A dipole that is close to a positive or negative ion will orient itself so that the end whose partial charge is opposite to the ion charge will point toward the ion.
- This kind of interaction is very important in aqueous solutions of ionic substances.
- **Energy of attraction: 1-7 Kcal/mole**



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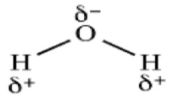
Intermolecular Forces: ion - dipole force

- **Example:Solubility of NaCl in water.**



- In a solution of sodium chloride, **H2O** is a highly polar molecule, and **NaCl** breaks up to Na+ and Cl- because the ion dipole with water is stronger than the attraction of **Na+ to Cl-.**

- The **Na+** ions will be enveloped by a shell of water molecules with their oxygen-ends pointing toward these ions, while H2O molecules surrounding the **Cl–** ions will have their hydrogen ends directed inward.

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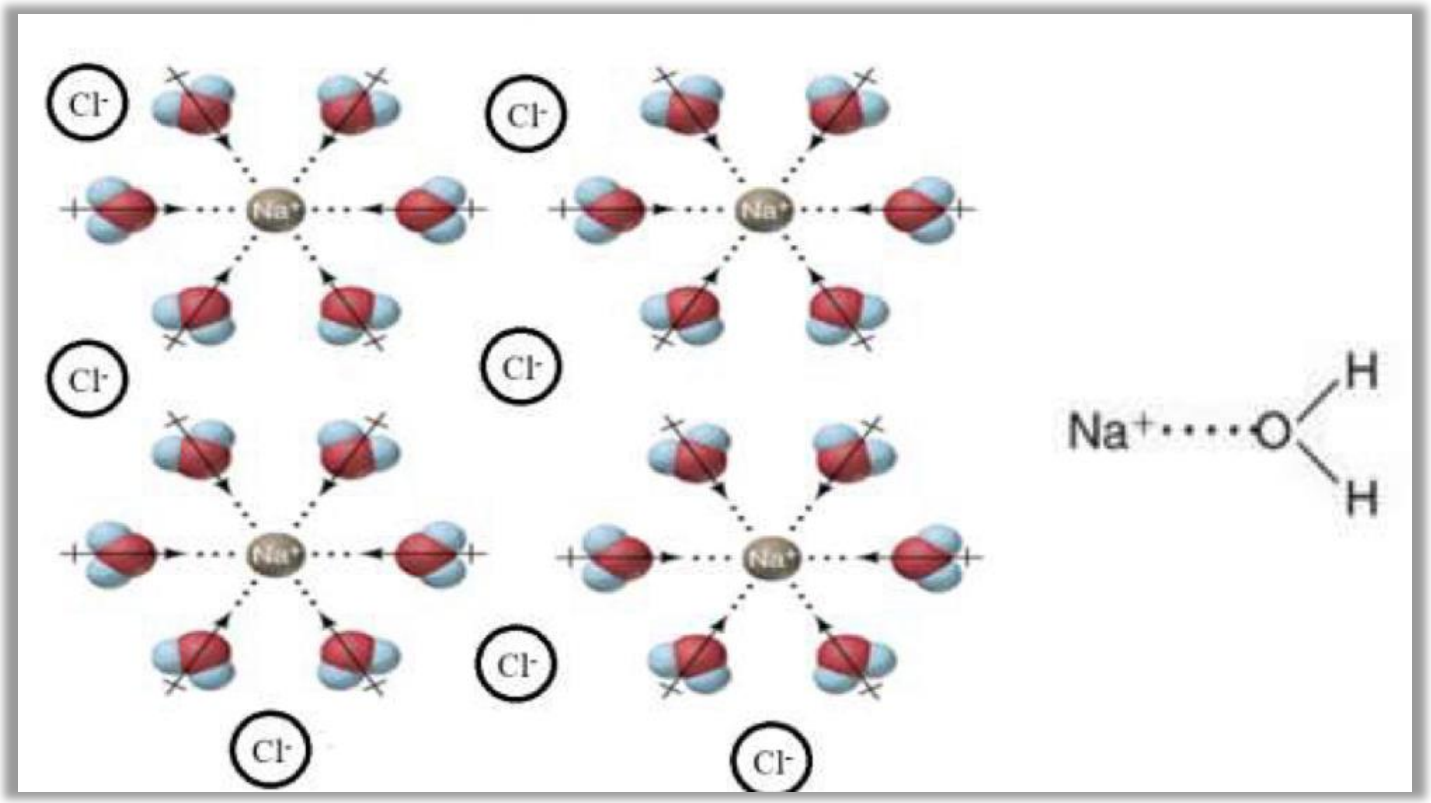
Intermolecular Forces: ion - dipole force



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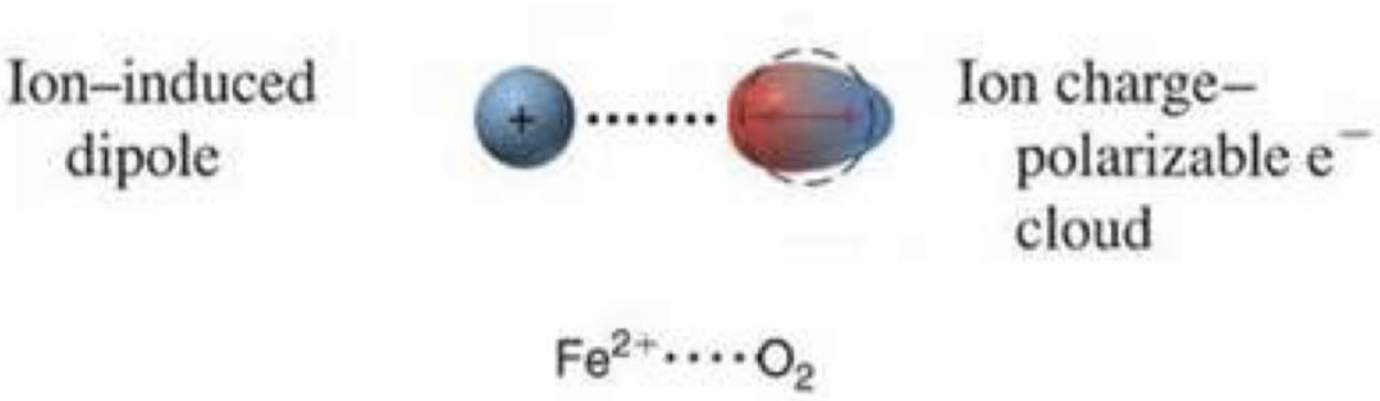
Intermolecular Forces: ion – Induced dipole force

- An ion-induced dipole attraction is a weak attraction that results when the approach of an ion induces a dipole in an atom or in a non-polar molecule by disturbing the arrangement of electrons in the non polar species.

- **Energy of attraction: 6 Kcal/mole**



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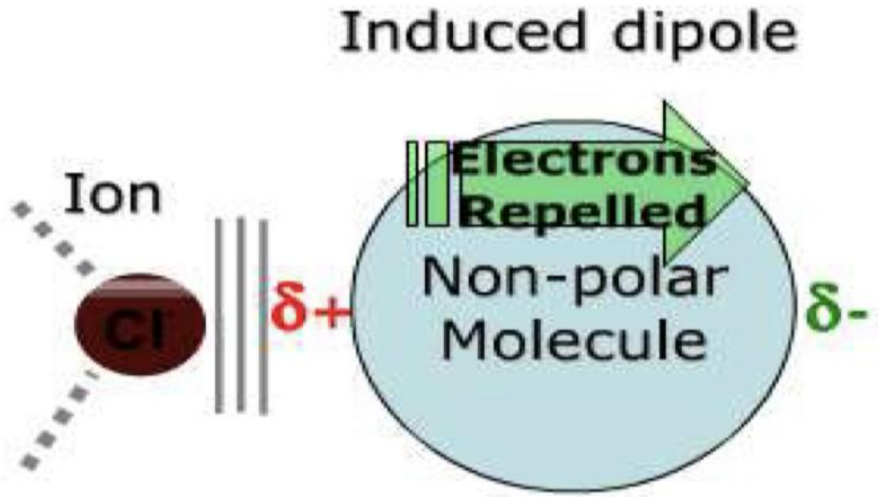
Intermolecular Forces: ion – Induced dipole force



Example:
NaCl & Hexane

$$KI + I_2 + \longrightarrow KI_3$$

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Various Forces and Bonding

Bond energies serve as a measure of the strength of bonds

Class		Unit 1	Unit 2	Energy (Kcal/mole)	bonding
Van der Waals forces	Keesom forces	Dipole	Dipole	1~7	Physical bonding (intermolecular interaction)
	Debye forces	Dipole	Induced dipole	1~3	
	London forces	Induced dipole	Induced dipole	0.5~1	
Ion-dipoles forces		Ion	Dipole	1~7	
Ion-induced dipole forces		Ion	Induced dipole	-	
Hydrogen bond		H atom	O, N, F	2~8	
Ionic bond		Ion	Ion	100~200	Chemical bonding (atomic bonding)
Covalent bond		Polar atom	Polar atom	50~150	

Special type of dipole-dipole interaction

Bond strength

The strength between intermolecular bonds is a lot weaker than the strength of intramolecular bonds and the weakest form of intermolecular bond is a bond that uses Van der Waals forces or an instantaneous induced-dipole bond.

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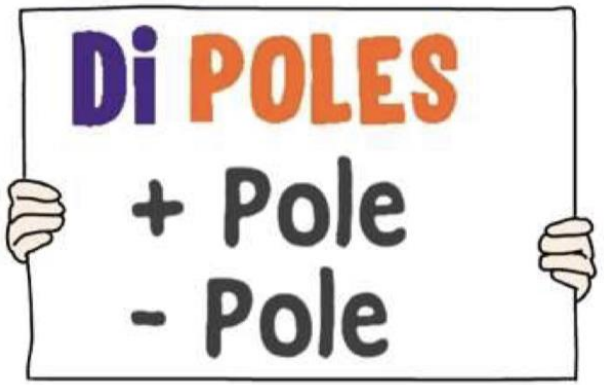
Supplementary information: what is a dipole

- Dipole is a body or system **(in our case a molecule)** having a pair of equal and opposite electric charges separated by a small distance.



- This is caused by the location of a few more electrons on one side of the nucleus more than on the other (i.e., it is formed as a result of unbalanced distribution of electrons in asymmetrical molecules).

- In chemistry, dipole usually refers to the separation of charges within a molecule between two covalently bonded atoms or atoms that share an ionic bond.

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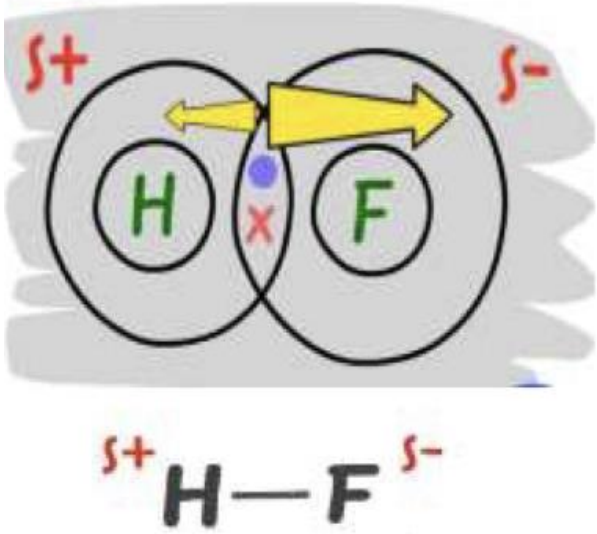
Supplementary information: what is a dipole

- **Example: Hydrogen Flourid**

- Flourine is more electronegative than hydrogenElectrons are predominantly around the F atom, which creates a permanent negative charge.

- Also, the H is electron deficient, so it has a permanent positive charge, which is separated by the bond length.



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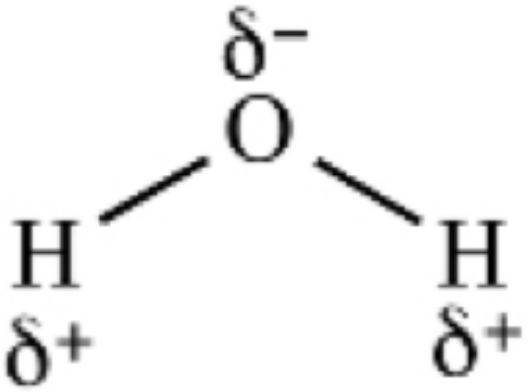
Supplementary information: what is a dipole

- **Water molecule (H2O) is a dipole.**

- The oxygen side of the molecule carries a net negative charge, while the side with the two hydrogen atoms has a net positive electrical charge.



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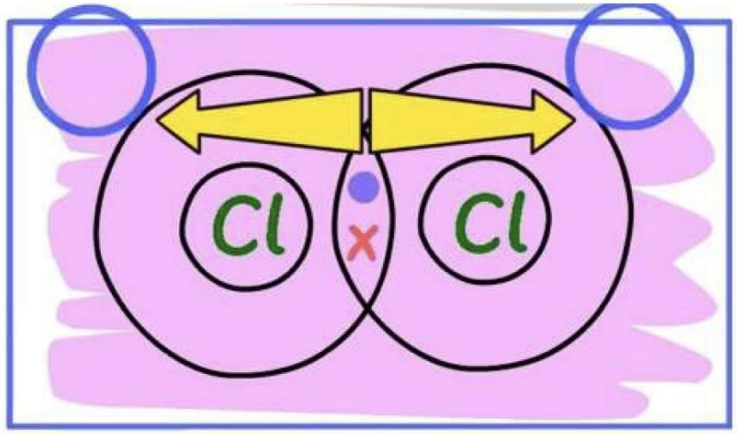
BEWARE

NOT A DIPOLE

ELECTRONIC CLOUD in Between

symmetrical molecules such as Cl_2



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Thank You !

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