CHAPTER 2
INTERATOMIC FORCES

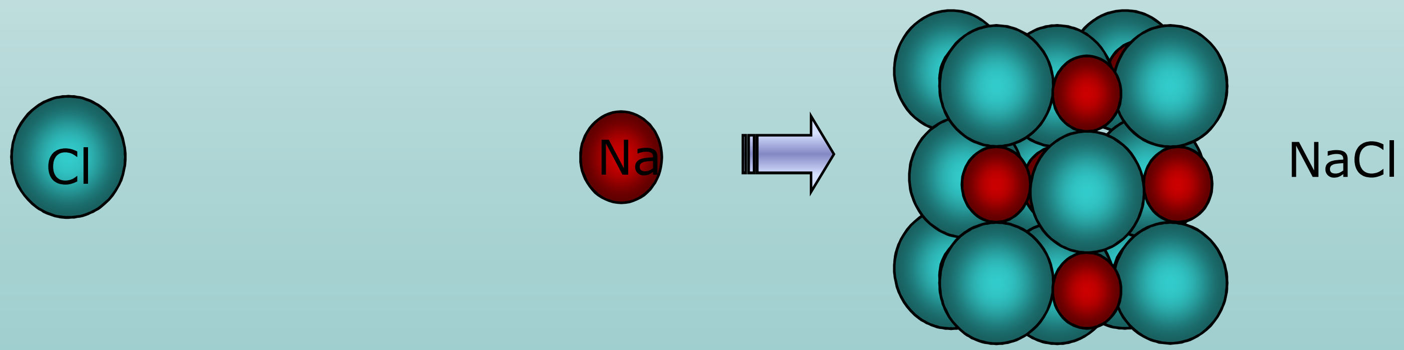
What kind of force holds the atoms together in a solid?

Interatomic Binding

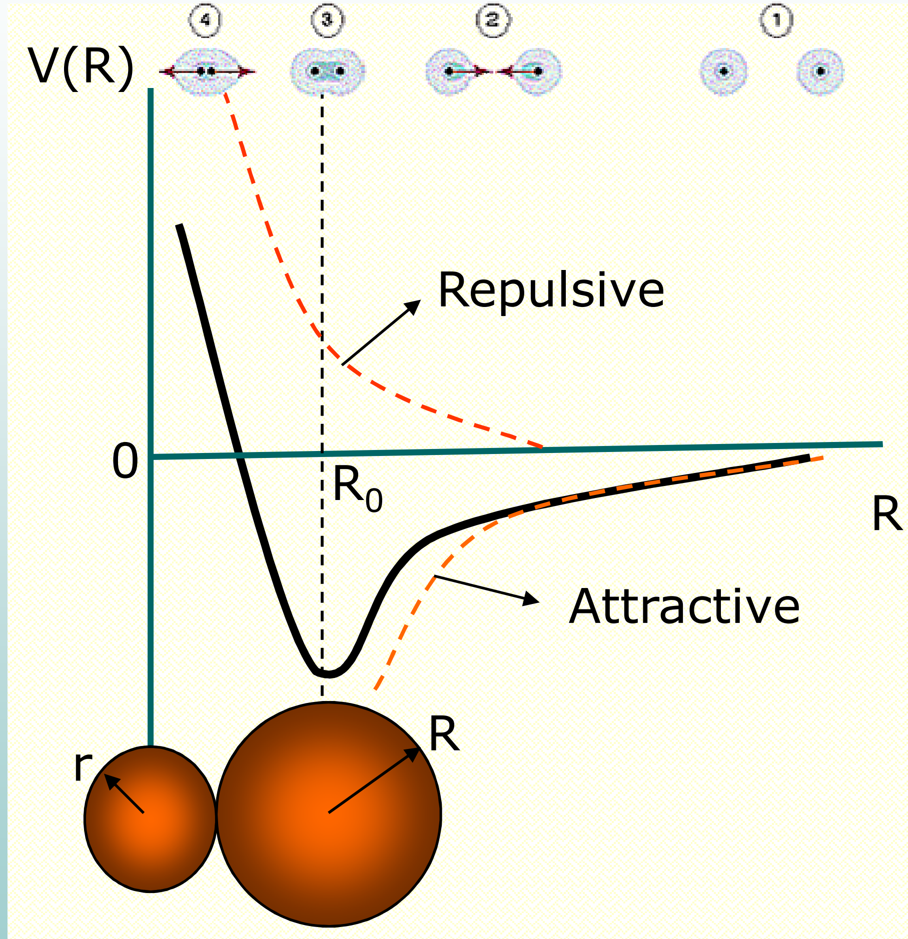
- All of the mechanisms which cause bonding between the atoms derive from electrostatic interaction between nuclei and electrons.
- The differing strengths and differing types of bond are determined by the particular electronic structures of the atoms involved.
- The existence of a stable bonding arrangement implies that the spatial configuration of positive ion cores and outer electrons has less total energy than any other configuration (including infinite separation of the respective atoms).
- The energy deficience of the configuration compared with isolated atoms is known as cohesive energy, and ranges in value from 0.1 eV/atom for solids which can muster only the weak van der Waals to 7ev/atom or more in some covalent and ionic compounds and some metals.

Energies of Interactions Between Atoms

- The energy of the crystal is lower than that of the free atoms by an amount equal to the energy required to pull the crystal apart into a set of free atoms. This is called the binding (cohesive) energy of the crystal.
  - NaCl is more stable than a collection of free Na and Cl.
  - Ge crystal is more stable than a collection of free Ge.



- This typical curve has a minimum at equilibrium distance R_0
- $R > R_0$;
  - the potential increases gradually, approaching 0 as $R \rightarrow \infty$
  - the force is attractive
- $R < R_0$;
  - the potential increases very rapidly, approaching ∞ at small separation.
  - the force is repulsive



- Force between the atoms is the negative of the slope of this curve. At equlibrium, repulsive force becomes equals to the attractive part.

The potential energy of either atom will be given by:

V= decrease in potential energy+increase in potential energy
(due to attraction) **(due to repulsion)**

or simply:

$$V(r) = \frac{-a}{r^m} + \frac{b}{r^n}$$

V(r): the net potential energy of interaction as function of r

r : the distance between atoms, ions, or molecules

a,b: proportionality constant of attraction and repulsion, respectively

m, n: constant characteristics of each type of bond and type of structure

Types of Bonding Mechanisms

It is conventional to classify the bonds between atoms into different types as

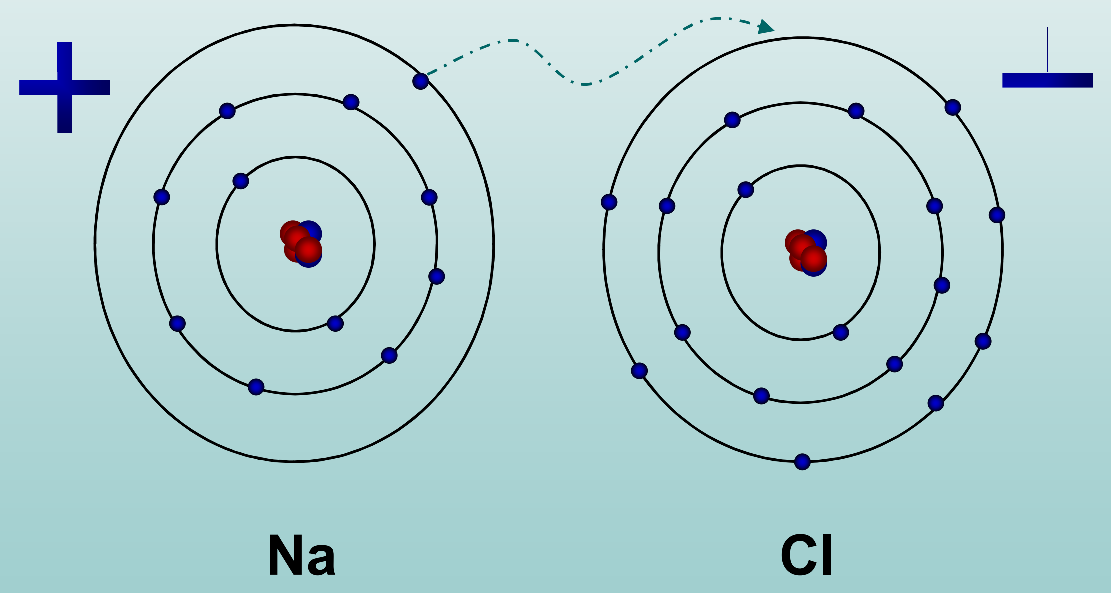
- Ionic,
- Covalent,
- Metallic,
- Van der Waals,
- Hydrogen.

All bonding is a consequence of the electrostatic interaction between nuclei and electrons obeying Schrödinger’s equation.

1 - IONIC BONDING

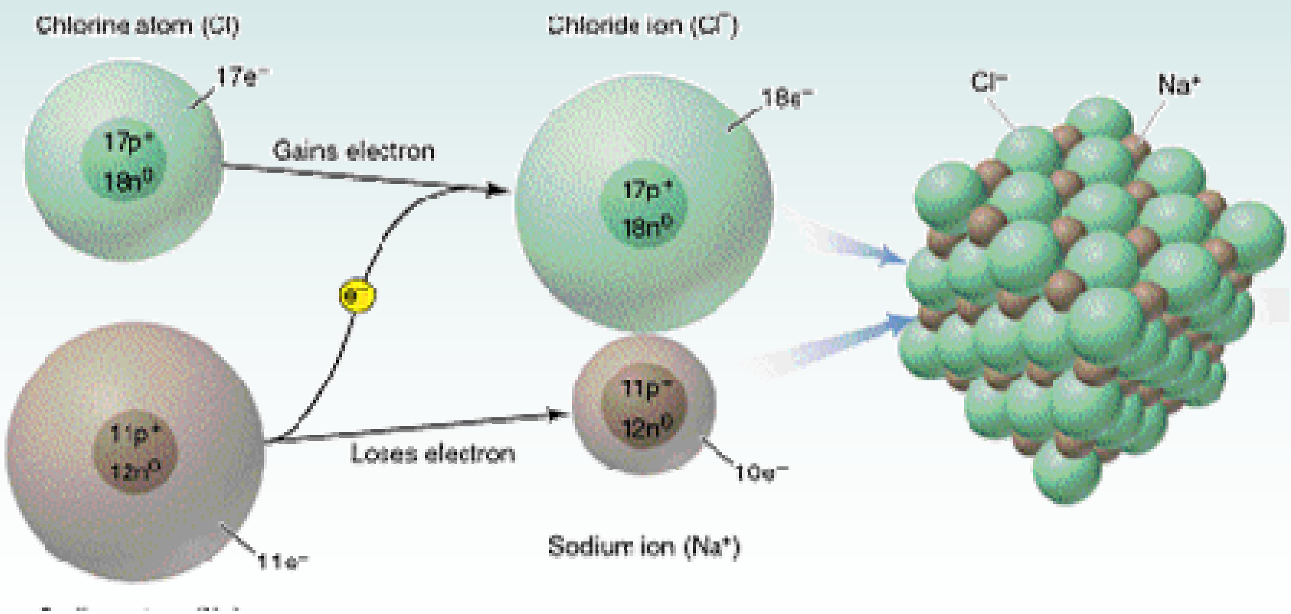
- Ionic bonding is the electrostatic force of attraction between positively and negatively charged ions (between non-metals and metals).
- These ions have been produced as a result of a transfer of electrons between two atoms with a large difference in electro negativities.
- All ionic compounds are crystalline solids at room temperature.
- NaCl is a typical example of ionic bonding.

- The metallic elements have only up to the valence electrons in their outer shell will lose their electrons and become positive ions, whereas electronegative elements tend to acquire additional electrons to complete their octed and become negative ions, or anions.

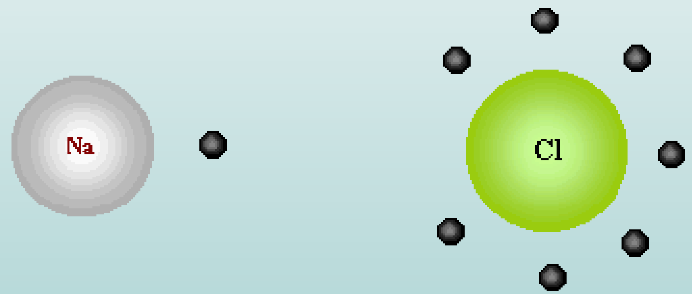


NaCl

- Notice that when sodium loses its one valence electron it gets smaller in size, while chlorine grows larger when it gains an additional valance electron. After the reaction takes place, the charged Na+ and Cl- ions are held together by electrostatic forces, thus forming an ionic bond.



- When the Na^+ and Cl^- ions approach each other closely enough so that the orbits of the electron in the ions begin the overlap each other, then the electron begins to repel each other by virtue of the repulsive electrostatic coulomb force. Of course the closer together the ions are, the grater the repulsive force.

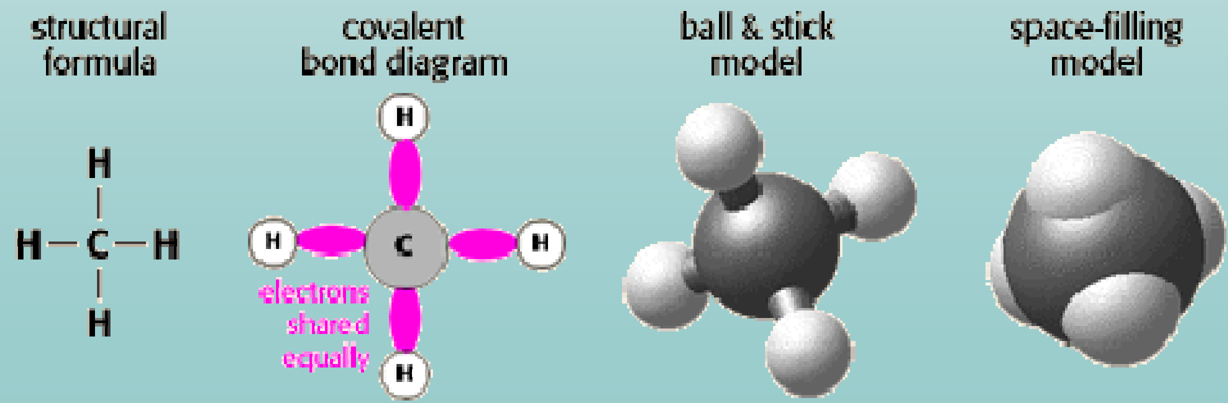


- Pauli exclusion principle has an important role in repulsive force. To prevent a violation of the exclusion principle, the potential energy of the system increases very rapidly.

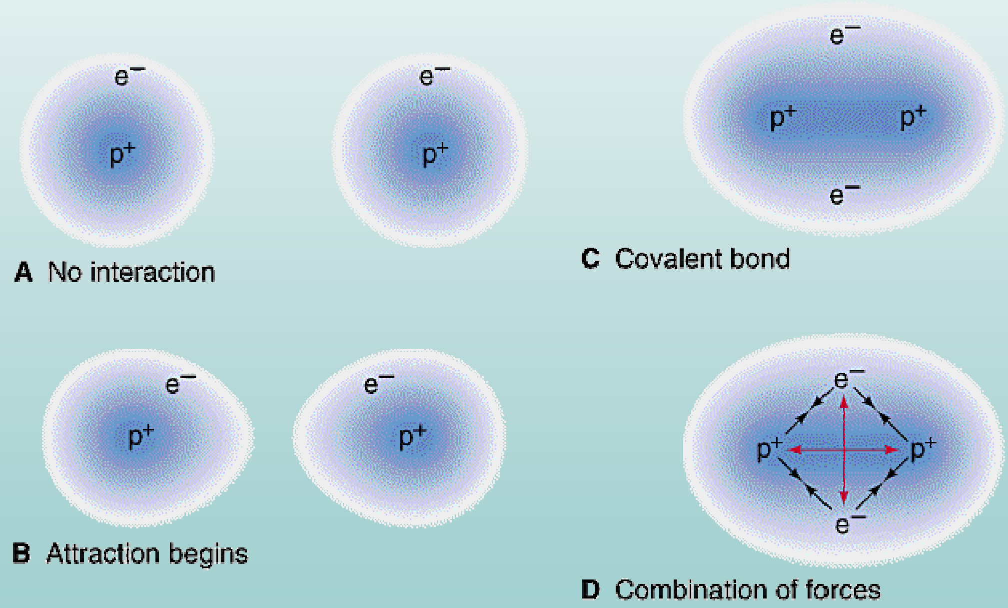
Property	Explanation
Melting point and boiling point	The melting and boiling points of ionic compounds are high because a large amount of thermal energy is required to separate the ions which are bound by strong electrical forces.
Electrical conductivity	Solid ionic compounds do not conduct electricity when a potential is applied because there are no mobile charged particles. No free electrons causes the ions to be firmly bound and cannot carry charge by moving.
Hardness	Most ionic compounds are hard; the surfaces of their crystals are not easily scratches. This is because the ions are bound strongly to the lattice and aren't easily displaced.
Brittleness	Most ionic compounds are brittle; a crystal will shatter if we try to distort it. This happens because distortion cause ions of like charges to come close together then sharply repel.

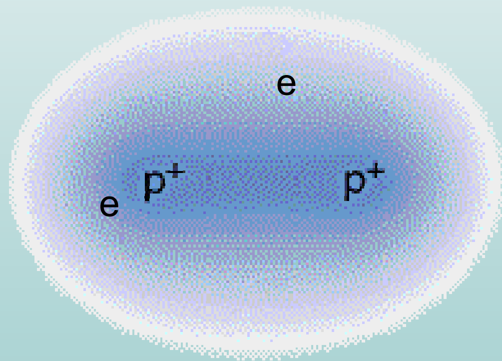
2 - COVALENT BONDING

- Covalent bonding takes place between atoms with small differences in electronegativity which are close to each other in periodic table (*between non-metals and non-metals*).
- The covalent bonding is formed by sharing of outer shell electrons (i.e., s and p electrons) between atoms rather than by electron transfer.
- This bonding can be attained if the two atoms each share one of the other's electrons.
- So the noble gas electron configuration can be attained.



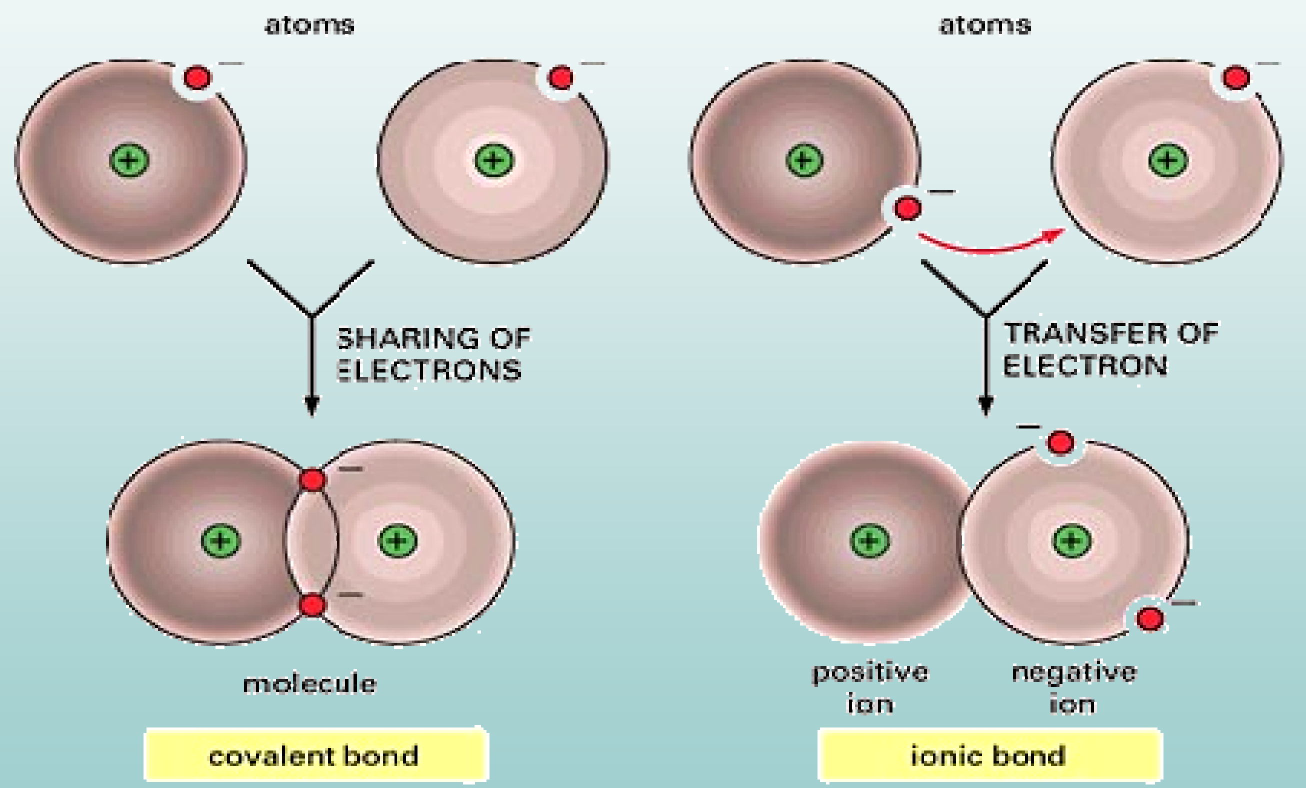
- Each electron in a shared pair is attracted to both nuclei involved in the bond. The approach, electron overlap, and attraction can be visualized as shown in the following figure representing the nuclei and electrons in a hydrogen molecule.





Property	Explanation
Melting point and boiling point	Very high melting points because each atom is bound by strong covalent bonds. Many covalent bonds must be broken if the solid is to be melted and a large amount of thermal energy is required for this.
Electrical conductivity	Poor conductors because electrons are held either on the atoms or within covalent bonds. They cannot move through the lattice.
Hardness	They are hard because the atoms are strongly bound in the lattice, and are not easily displaced.
Brittleness	Covalent network substances are brittle.If sufficient force is applied to a crystal, covalent bond are broken as the lattice is distorted. Shattering occurs rather than deformation of a shape.

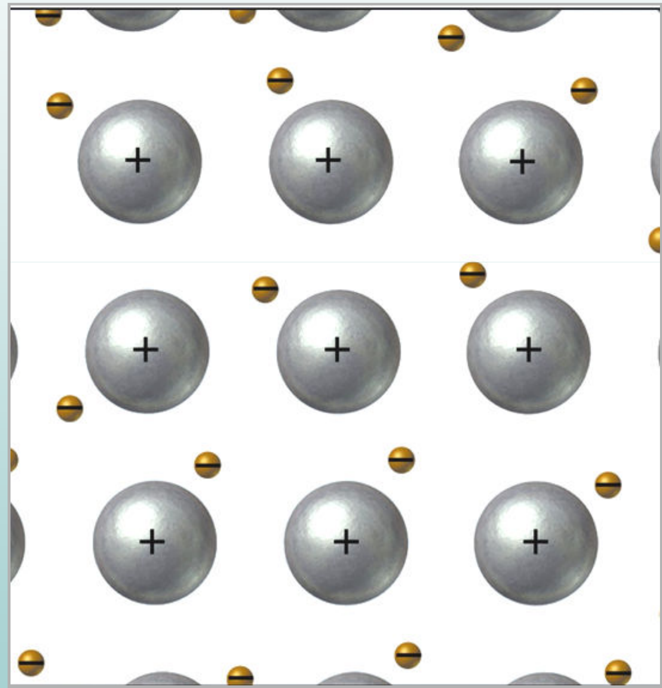
Comparison of Ionic and Covalent Bonding



3 - METALLIC BONDING

- Metallic bonding is the type of bonding found in metal elements. This is the electrostatic force of attraction between positively charged ions and delocalized outer electrons.

- The metallic bond is weaker than the ionic and the covalent bonds.



METALLIC BONDING

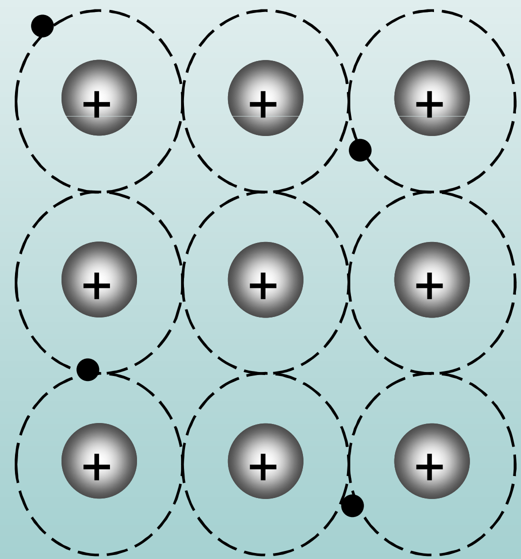
- Metallic structures are typically rather empty (having large internuclear spacings) and prefer lattice arrangements in which each atom has many nearest neighbors.

- The weakness of the individual bonding actions in a metal is due to the enlargement of the internuclear spacing.

- Valance electrons are relatively bound to the nucleus and therefore they move freely through the metal and they are spread out among the atoms in the form of a low-density electron cloud.

- A metallic bond result from the sharing of a variable number of electrons by a variable number of atoms. A metal may be described as a cloud of free electrons.

- Therefore, metals have high electrical and thermal conductivity.



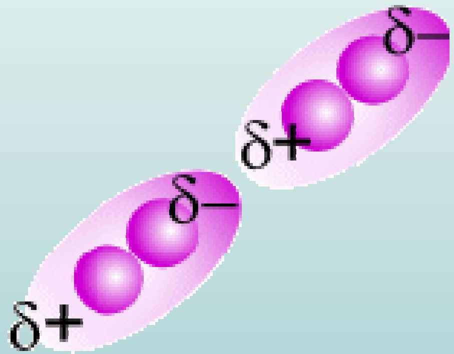
- All valence electrons in a metal combine to form a “sea” of electrons that move freely between the atom cores. The more electrons, the stronger the attraction. This means the melting and boiling points are higher, and the metal is stronger and harder.
- The positively charged cores are held together by these negatively charged electrons.
- The free electrons act as the bond (or as a “glue”) between the positively charged ions.
- This type of bonding is nondirectional and is rather insensitive to structure.
- As a result we have a high ductility of metals - the “bonds” do not “break” when atoms are rearranged – metals can experience a significant degree of plastic deformation.

4 - VAN DER WAALS BONDING

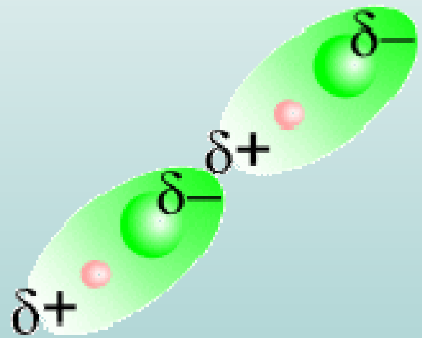
- It is a weak bond, with a typical strength of 0.2 eV/atom.
- It occurs between neutral atoms and molecules.
- The explanation of these weak forces of attraction is that there are natural fluctuation in the electron density of all molecules and these cause small temporary dipoles within the molecules. It is these temporary dipoles that attract one molecule to another. They are called van der Waals' forces.

- The bigger a molecule is, the easier it is to polarise (to form a dipole), and so the van der Waal's forces get stronger, so bigger molecules exist as liquids or solids rather than gases.

- The **shape** of a molecule influences its ability to form temporary dipoles. Long thin molecules can pack closer to each other than molecules that are more spherical. The bigger the 'surface area' of a molecule, the greater the van der Waal's forces will be and the higher the melting and boiling points of the compound will be.
- Van der Waal's forces are of the order of 1% of the strength of a covalent bond.

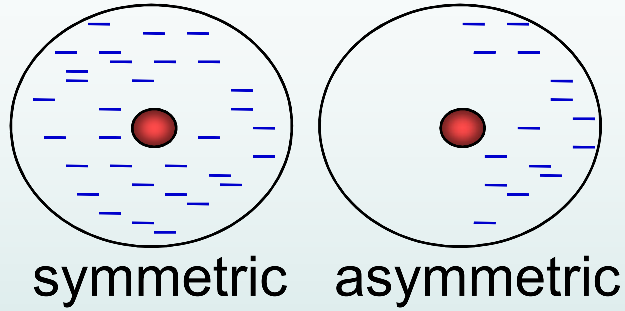


Homonuclear molecules, such as iodine, develop temporary dipoles due to natural fluctuations of electron density within the molecule

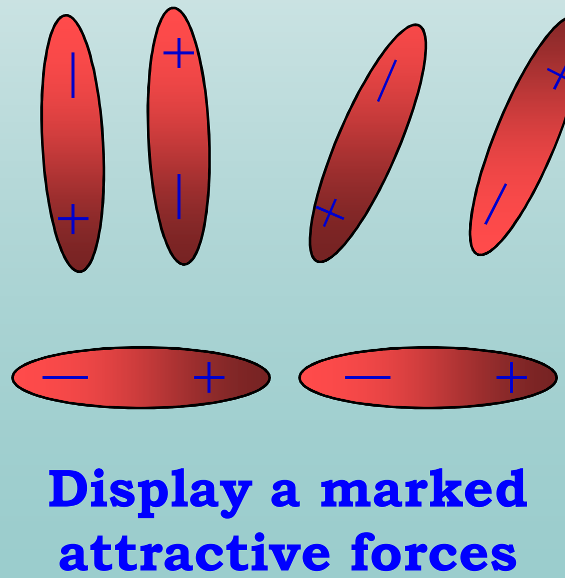


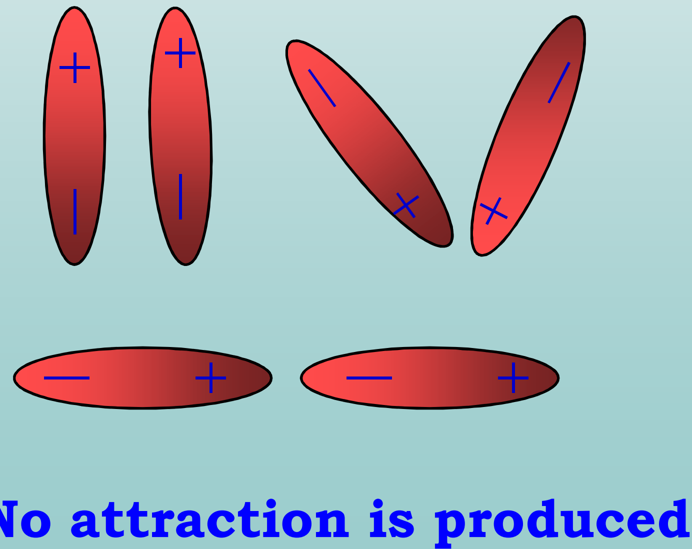
Heteronuclear molecules, such as H-Cl have permanent dipoles that attract the opposite pole in other molecules.

The dipoles can be formed as a result of unbalanced distribution of electrons in asymettrical molecules. This is caused by the instantaneous location of a few more electrons on one side of the nucleus than on the other.

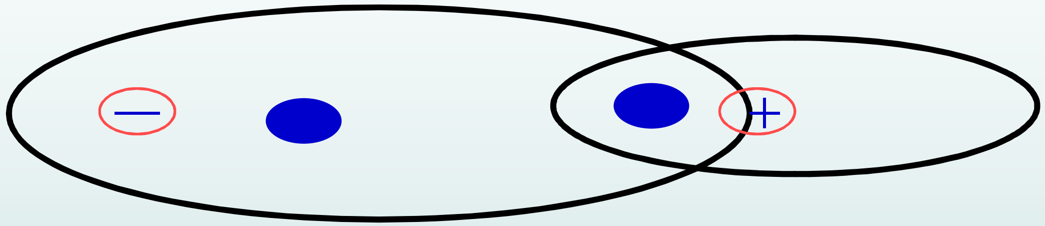


Therefore atoms or molecules containing dipoles are attracted to each other by electrostatic forces.

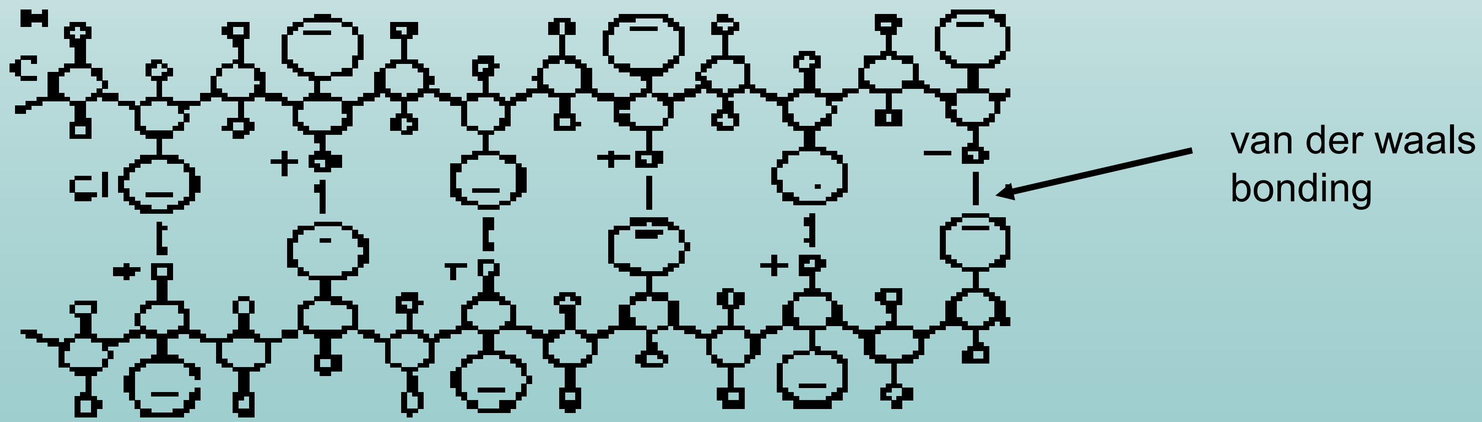




- These forces are due to the electrostatic attraction between the nucleus of one atom and the electrons of the other.

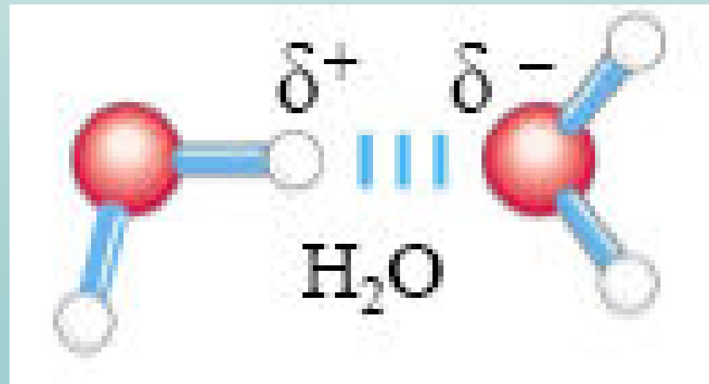


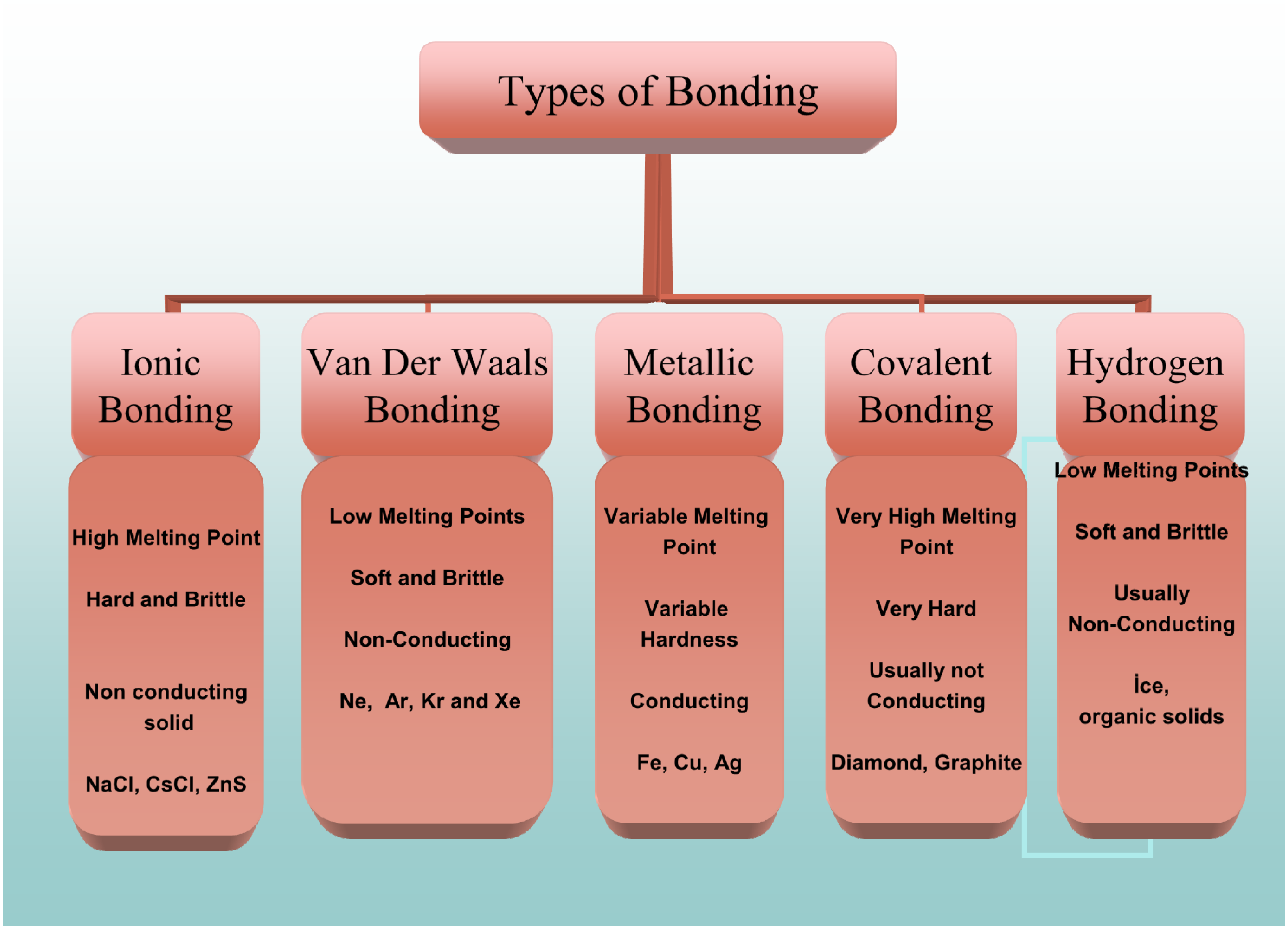
- Van der waals interaction occurs generally between atoms which have noble gas configuration.



5 – HYDROGEN BONDING

- A hydrogen atom, having one electron, can be covalently bonded to only one atom. However, the hydrogen atom can involve itself in an additional electrostatic bond with a second atom of highly electronegative character such as fluorine or oxygen. This second bond permits a ***hydrogen bond*** between two atoms or strucures.
- The strength of hydrogen bonding varies from 0.1 to 0.5 ev/atom.
  - Hydrogen bonds connect water molecules in ordinary ice. Hydrogen bonding is also very important in proteins and nucleic acids and therefore in life processes.




Types of Bonding
Ionic Bonding
High Melting Point
Hard and Brittle
Non conducting solid
NaCl, CsCl, ZnS
Van Der Waals Bonding
Low Melting Points
Soft and Brittle
Non-Conducting
Ne, Ar, Kr and Xe
Metallic Bonding
Variable Melting Point
Variable Hardness
Conducting
Fe, Cu, Ag
Covalent Bonding
Very High Melting Point
Very Hard
Usually not Conducting
Diamond, Graphite
Hydrogen Bonding
Low Melting Points
Soft and Brittle
Usually Non-Conducting
İce, organic solids