Universidad
Carlos III de Madrid
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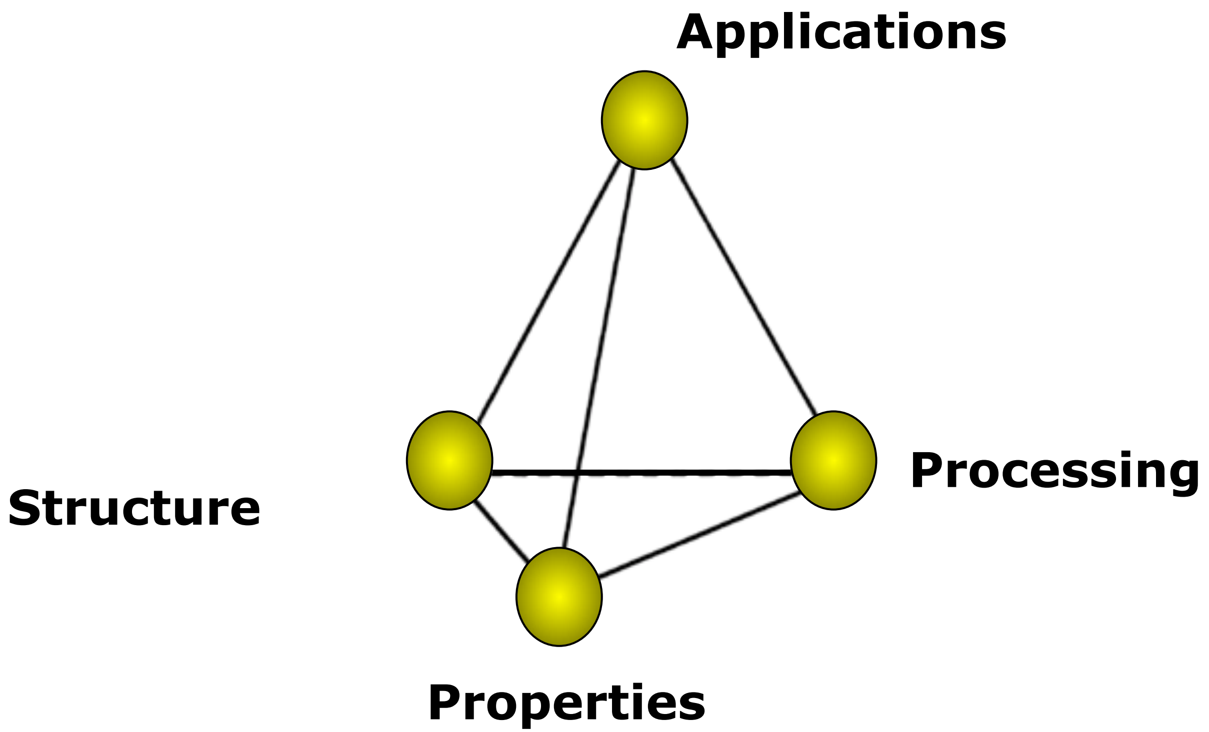
MATERIALS SCIENCE AND ENGINEERING

TOPIC 1.2. BONDING IN SOLIDS. RELATION BETWEEN BONDING, STRUCTURE AND PROPERTIES OF MATERIALS

- **Introduction**
- **Bonding in solids**
  - Ionic bond
  - Covalent bond
  - Metallic bond
  - Intermolecular forces

INTRODUCTION

Nature of bonding <> properties <> type of materials <> Processing and applications



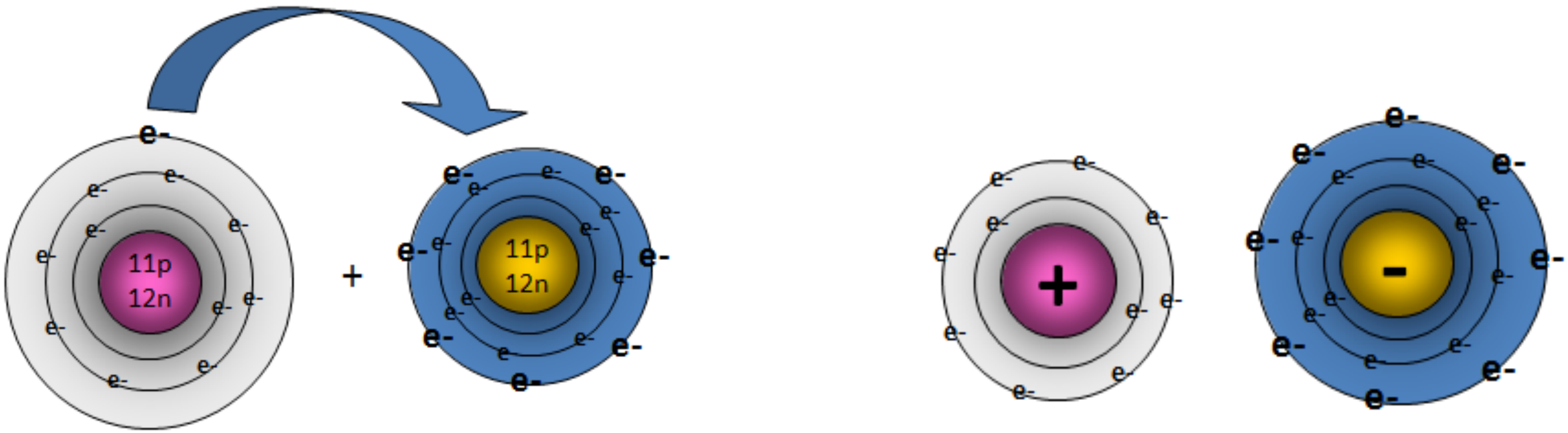
IONIC BOND

It forms between a metal and a non metal.

There is electron transfer from the less electronegative atom to the more electronegative .

Bonding forces $\Rightarrow$ F electrostatic attraction between opposite charged ions.

- Pure ionic bond: ideal.
- $\Rightarrow$ Always exists covalent participation

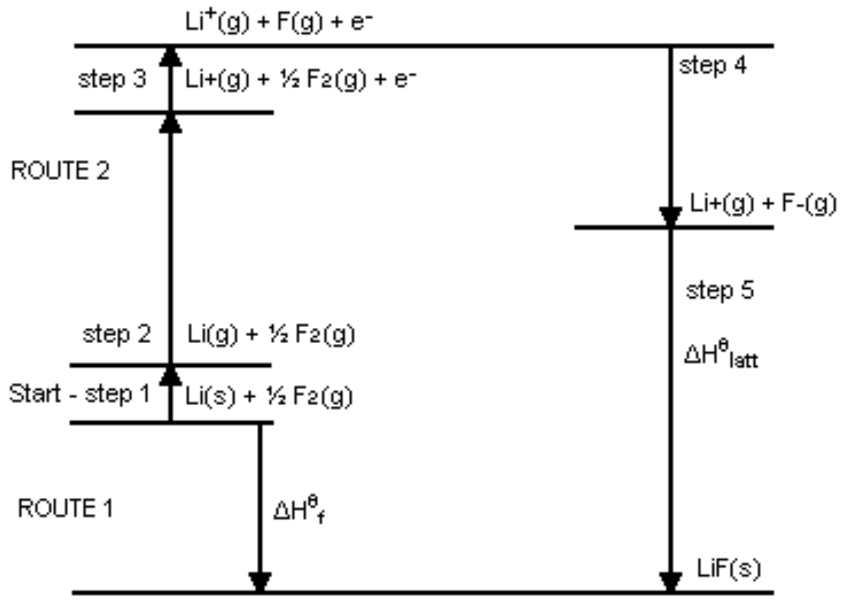


IONIC BOND

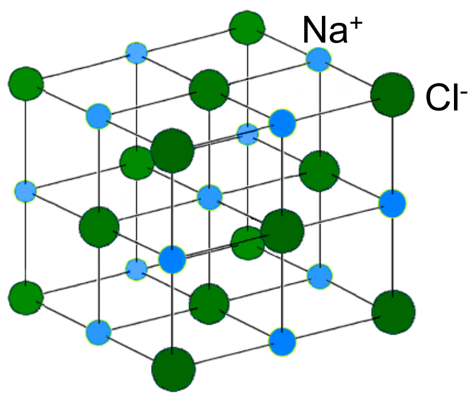
Ionic compounds are crystalline solids

It is a non directional bond formed by strong electrostatic interactions

LATTICE ENERGY:
Energy released when a mole of ionic solid is formed from its ions in the gas state.



Born-Haber cycle for LiF.



Step	**ΔH(kJ/mol)**
Sublimation of Li	155.2
Dissociation of $F_{2\ (g)}$	150.6
Ionization of $Li_{(g)}$	520
Gain of e^- of $F_{(g)}$	-328
Formation of LiF from $Li_{(s)}$ and $½F_{2(g)}$	-594.1

IONIC BOND

LATTICE ENERGY:

Many properties are dependant on the lattice energy (melting point, hardness, thermal expansion coefficient)

Ionic Solids	Lattice Energies (kJ/mol)	Melting point (ºC)
LiCl	-829	613
NaCl	-766	801
KCl	-686	776
RbCl	-670	715
CsCl	-649	646
MgO	-3932	2800
CaO	-3583	2580
SrO	-3311	2430
BaO	-3127	1923

When the ion size ↑ ⇒ lattice energy ↓ and T_f ↓
Valence +1

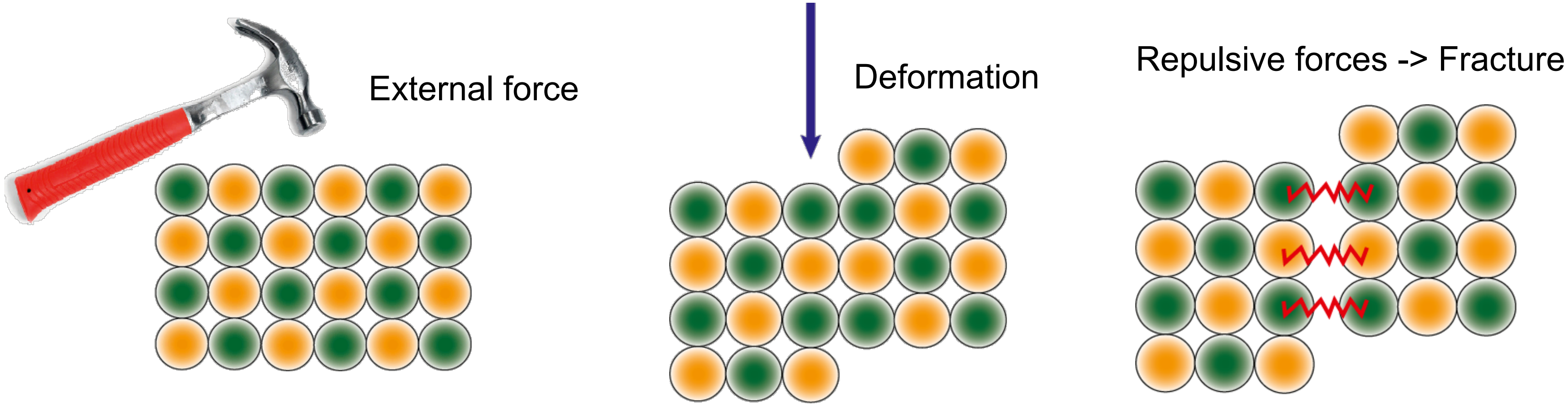
Valence +2

Valance number ↑ ⇒ lattice energy ↑ ⇒ T_f ↑

IONIC BOND

- General properties of ionic compounds

Strong electrostatic attraction → High melting and evaporation points
Hard and brittle solids at room temperature



They do not conduct electricity (except in molten state or when dissolved in water)

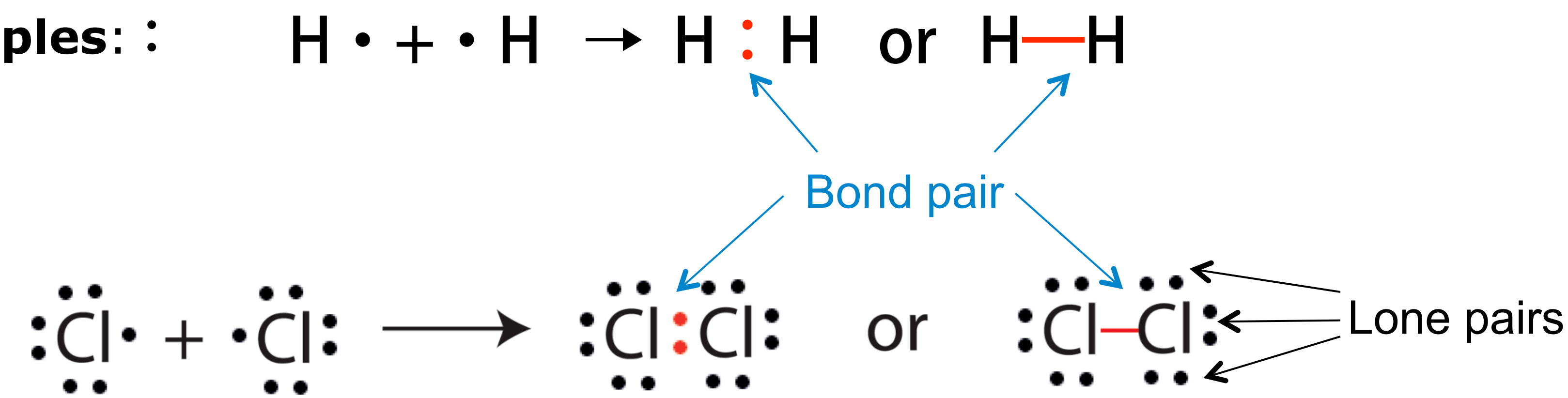
Water soluble.

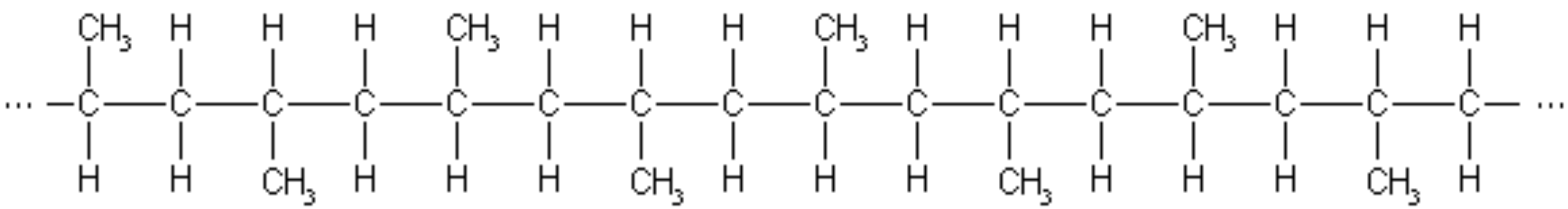
COVALENT BOND

Generally it forms between the non metallic elements of the periodic table

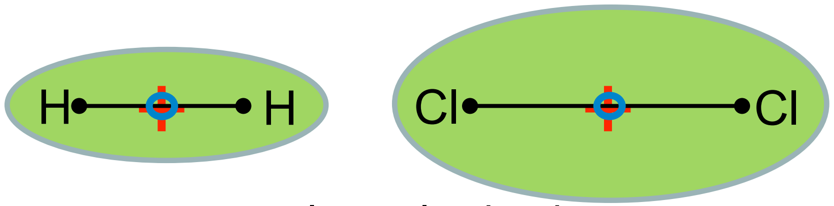
It forms by electron sharing

Examples:

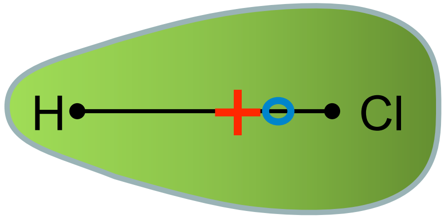




POLAR COVALENT BOND

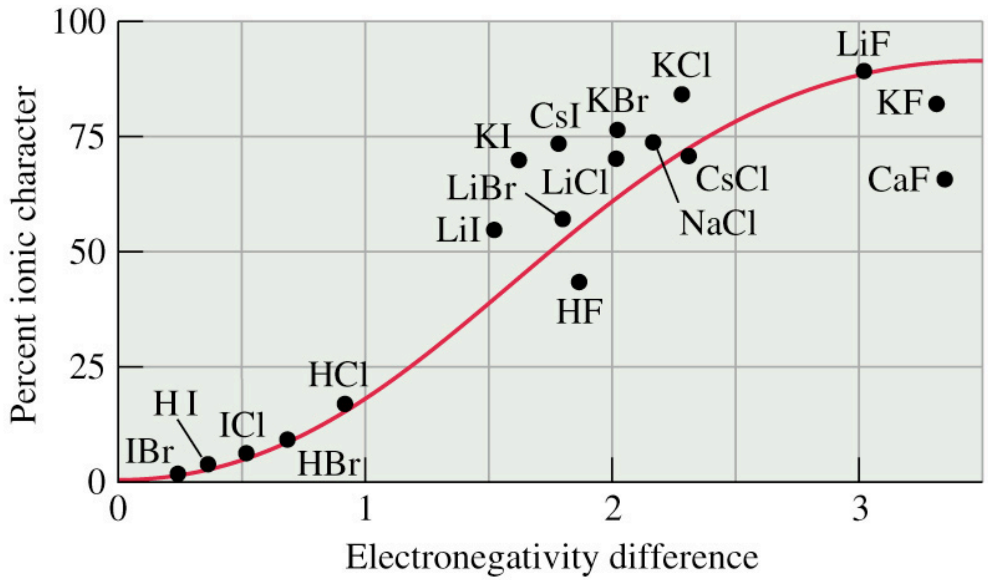


Non-polar covalent bond



Polar covalent bond

• = Atomic nucleus
+ = center of + ve charge
o = center of -ve charge



General Chemistry Principles and modern applications, 8th ed., RF Petrucci, WS Harwood, G Herring

Dipole moment

μ = Q x r

r = Distance between atoms;
Q =charge

Units: Debye, D; 1 D = 3.33 10^{-30} C·m

$$\%\,\text{ionic character} = \left(1 - e^{-0.25(X_A - X_B)^2}\right) \times 100\%$$

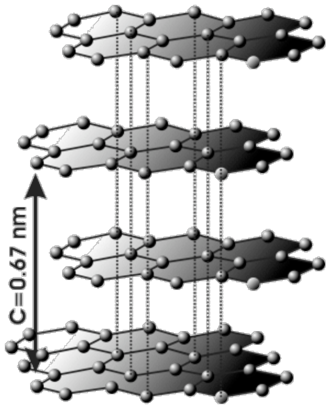
X_i : electronegativity of element i

COVALENT BOND

- Properties of the compounds with covalent bonds

  ✓ Covalent Solids

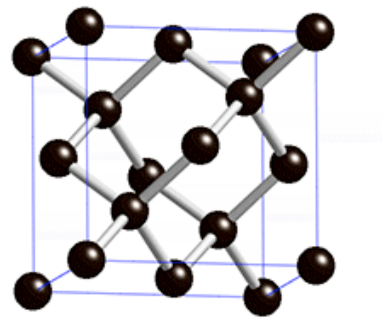
Formed by a system of continuous covalent bonds
Non conductive LATTICES both in the solid and in the molten state
Diamond, boron nitride, quartz (SiO_2), silicon carbide (SiC)



graphite

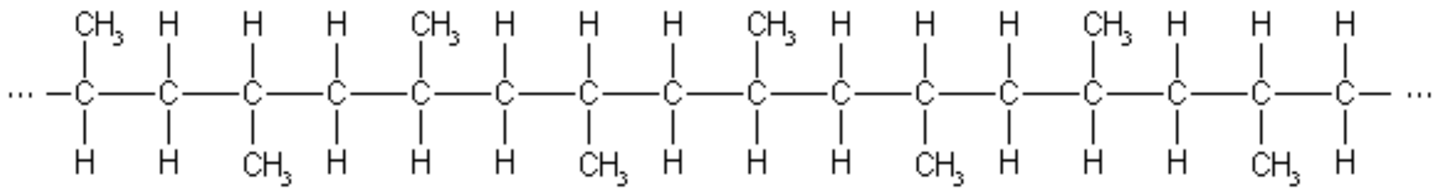
http://commons.wikimedia.org/wiki/File:Graphit_gitter.png

✓ Hard and incompressible
✓ T_f high, non volatile
✓ insoluble



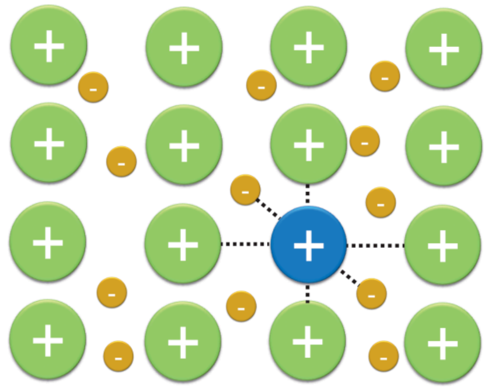
Diamond

✓ Substances with covalent bonds

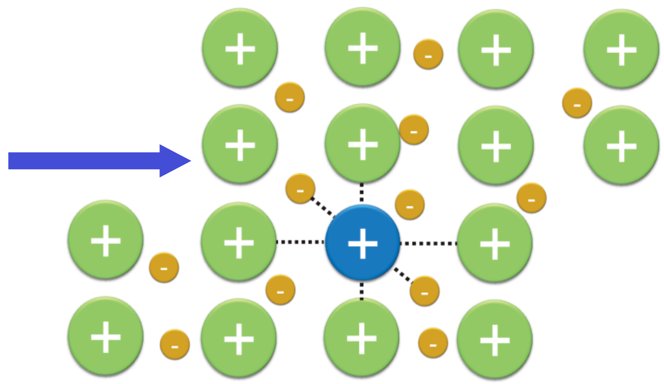


METALLIC BONDS

- Model of a sea of electrons
  - Atomic nucleus surrounded from a sea of e^-.
  - Metallic shine .
  - Workability.

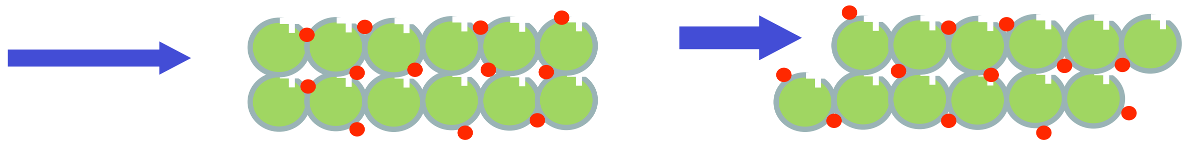


Applied force



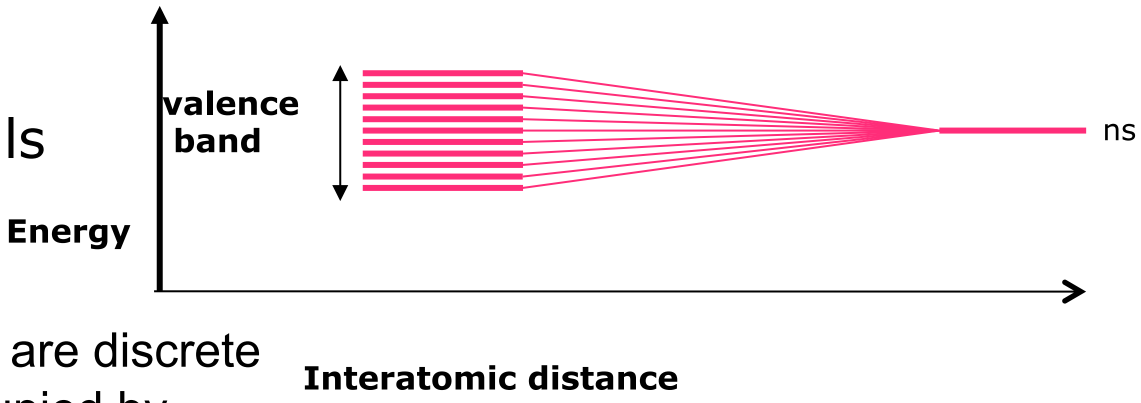
Applied force

Deformation

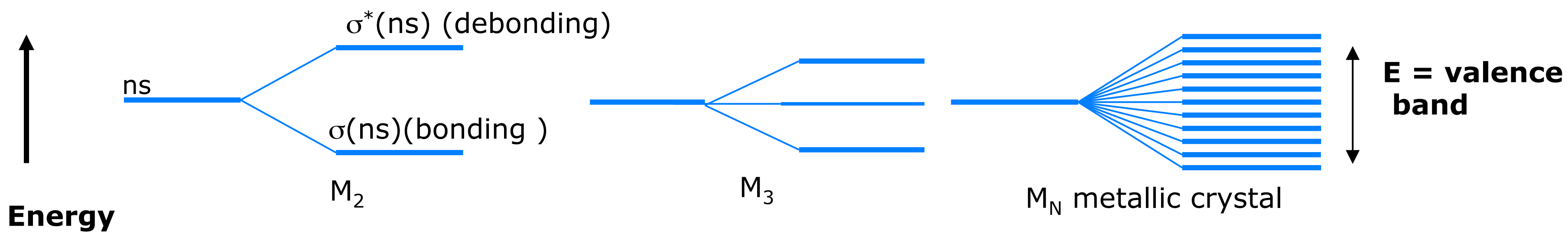


METALLIC BOND

- Band theory
  - Alkaline metals
  - Alkaline earth metals



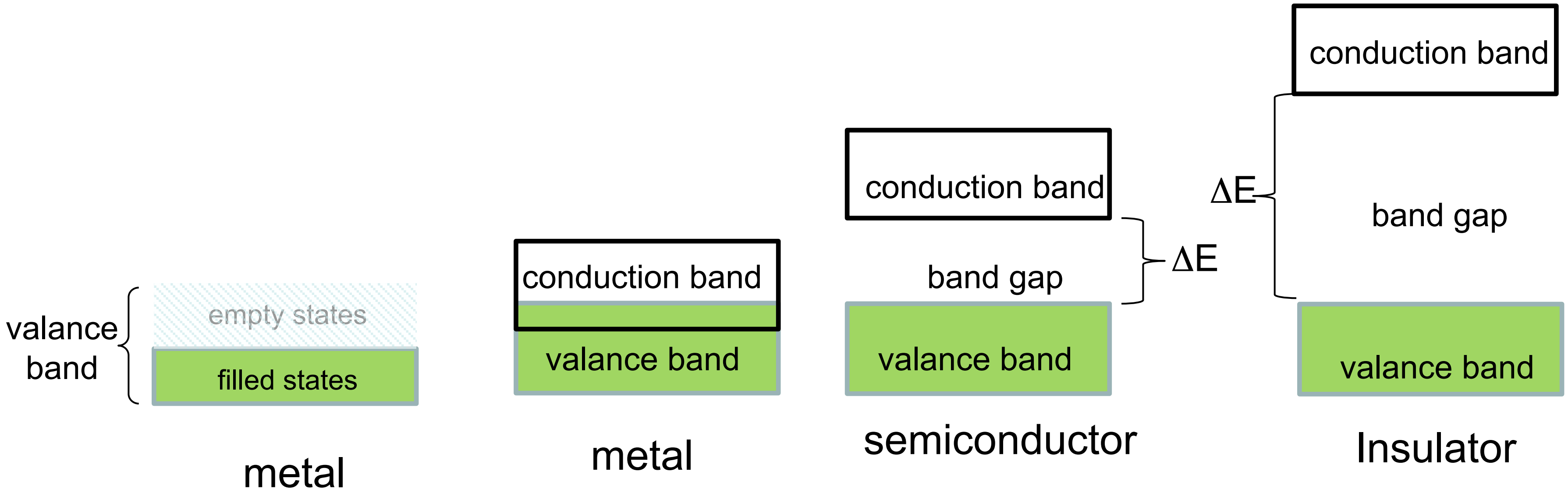
For each individual atom there are discrete energy levels that may be occupied by electrons



As atoms come within close proximity, electrons are acted upon by the electrons and nuclei of adjacent atoms. This causes each distinct atomic state to split into a series of closely spaced electron states in the solid, to form what is termed an **electron energy band.**

METALLIC BOND

The number of electrons available for electrical conduction in a particular material is related to the arrangement of electron states with respect to energy, and then the manner in which these states are occupied by electrons.



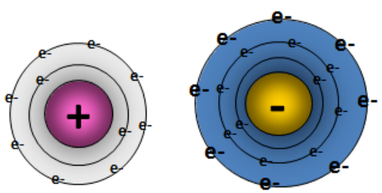
INTERMOLECULAR FORCES

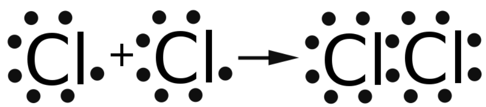
Primary bonds: (strong)

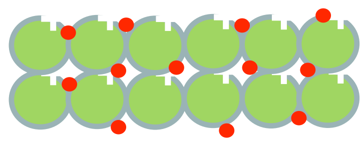
-Ionic bond: **(>150 kcal/mol)**
Transfer of e^- ⇒ cations and anions ⇒ $F_{coulomb}$ (non directional)

- Covalent bond: **(>50-150 kcal/mol)**
Sharing e^- (directional)

- Metallic bond: **(>20-120 kcal/mol)**
e- shared externally and very little tightened by the nucleus (non directional)





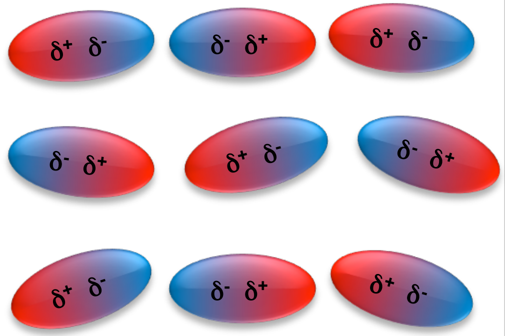


INTERMOLECULAR FORCES

Secondary bonds - weak (Van der Waals)

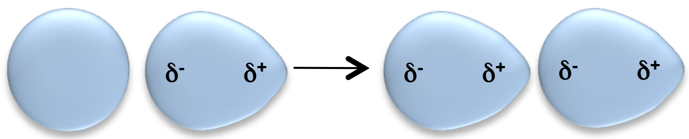
Permanent dipole 1-10 kcal/mol It forms between molecules:

- that present constant dipole moment μ
- made of atoms with different electronegativity that are united with covalent bonding.



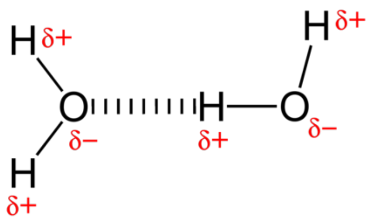
Fluctuating dipole: < 2 kcal/mol. It forms in non polar molecules in crystalline lattice

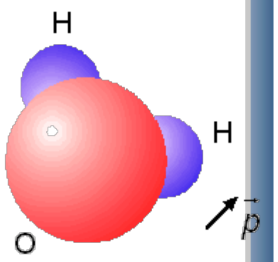
- Instantaneous fluctuations of electron charge distribution ⇒ *fluctuating dipoles*

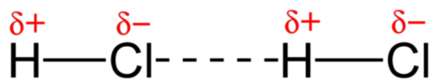


Hydrogen bond **7 kcal/mol in H_2O** (permanent dipole):

- In molecules with H and electronegative atoms (Polar covalent bond: O-H, N-H, F-H).
- Asymmetric distribution of charge ⇒ Permanent dipole







BONDING AND PROPERTIES

Bond	Type of substance	Melting and boiling points	Mechanical properties	Solubility
COVALENT	Molecular	Low	Soft in the solid state	Depends on the polarity of the molecules
COVALENT	Atomic, covalent or lattice	Very high	Very hard brittle	Insoluble in all solvents
IONIC	Ionic	High	Hard and brittle	Soluble in polar solvents
METALLIC	Metallic	High	Ductile and workable	Insoluble in all solvents

GENERAL PROPERTIES OF MATERIALS

Nature of bonding ↔ properties ↔ type of materials

Type of material	Character of bonding	Examples
Metal	Metallic	Fe, steels
Ceramic and glasses	Ionic/ covalent	Silica (SiO_2)
Polymers	Covalent and secondary	Polyethylene –(CH_2)-