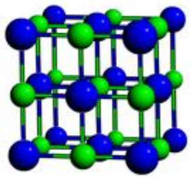
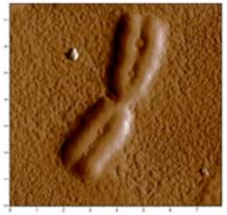


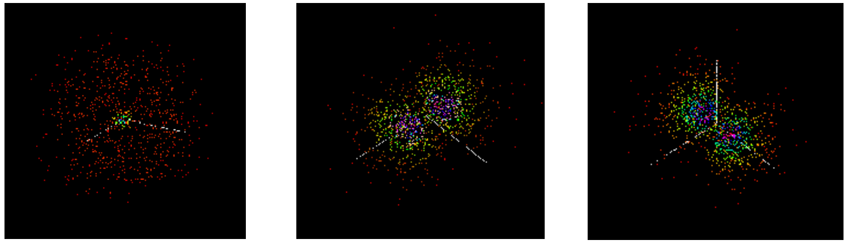


The microscopic world

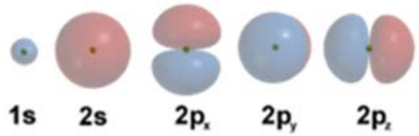
Multi-atomic systems

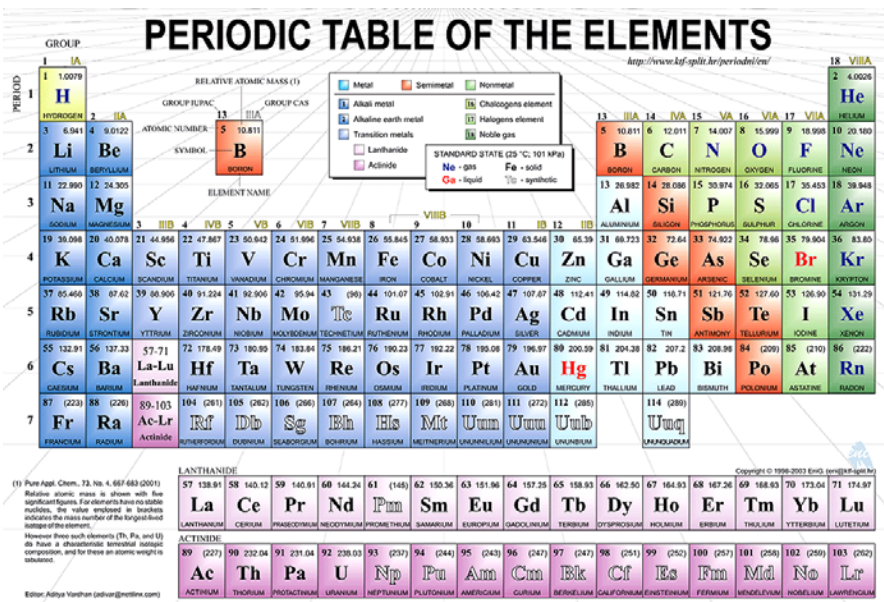
Irén Bárdos-Nagy

Electron clouds of the individual carbon atoms



$^{12}_{6}C$

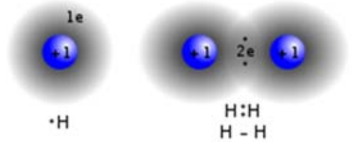


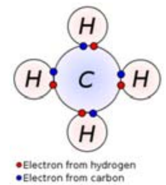


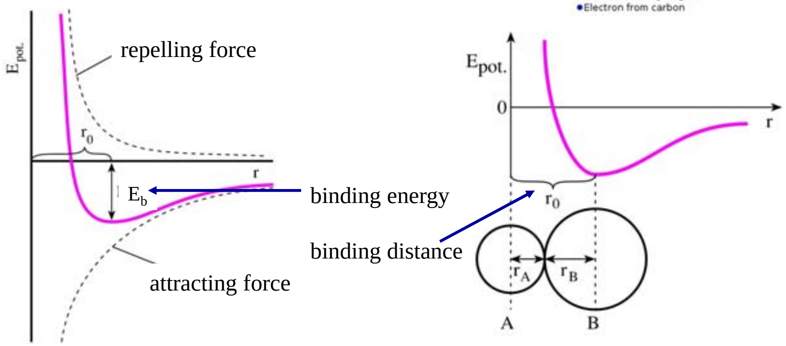
Interaction between the atoms → chemical binding

Primer (strong) chemical bonds (binding energy 100 – 200 kJ/mol few eV/bond)

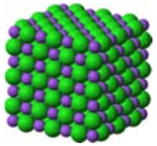
a./ the covalent bond

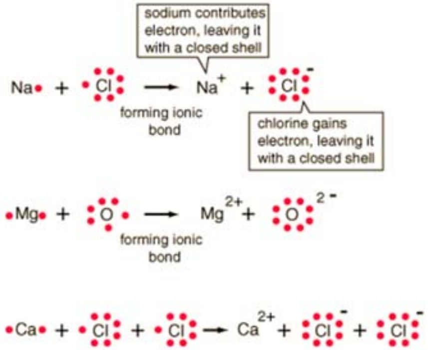




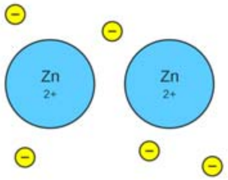


b./ the ionic bond



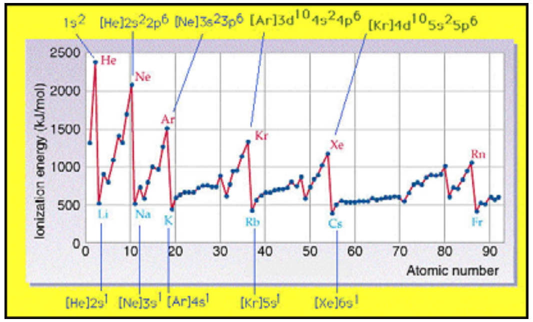


c./ the metallic bond

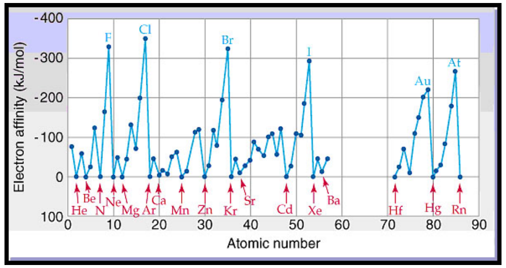


Ionization energy (I):

The minimum energy required to remove an electron bound in an atom in the gas phase (eV/atom; kJ/mol)



$1(eV/atom) = 96.485(kJ/mol) \cong 100(kJ/mol)$



Electronaffinity (E_{ea}):

The energy released when an electron attaches to an atom in the gas phase (eV/atom; kJ/mol)

Exothermic electron attachment: $E_{ea}>0$
-- incoming electron interacts strongly with the nucleus on its orbital
Endothermic electron attachment: $E_{ea}<0$
-- A^- has higher energy than A and e-

Electronegativity χ

is the measure of the power of an atom of an element to attract electrons when it is part of a compound

Mulliken's absolute definition: $\chi_M = \frac{1}{2}(I + E_{ea})$

arithmetical average of the ionization energy and electron affinity

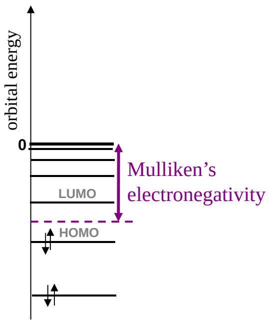
Pauling's relative scale:
characterizes the polar character of bonds

$\Delta = E_{bond,AB}(\exp.) - E_{bond,AB}(theor., non-polar)$

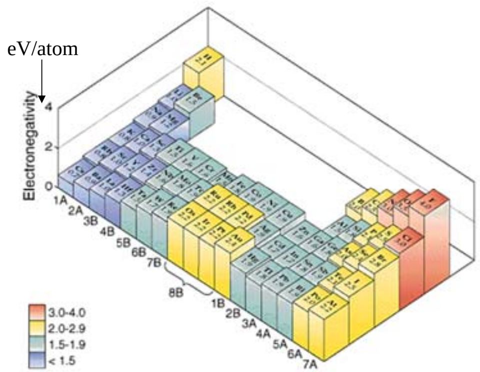
$E_{bond,AB}^{non-polar} = \frac{E_{bond}^{A-A} + E_{bond}^{B-B}}{2}$ ← if the bonds were purely covalent

$0.104 * \sqrt{\Delta} = |\chi_A - \chi_B|$

one of the electronegativities is empirically fixed – relative scale



Pauling-scale (relative):



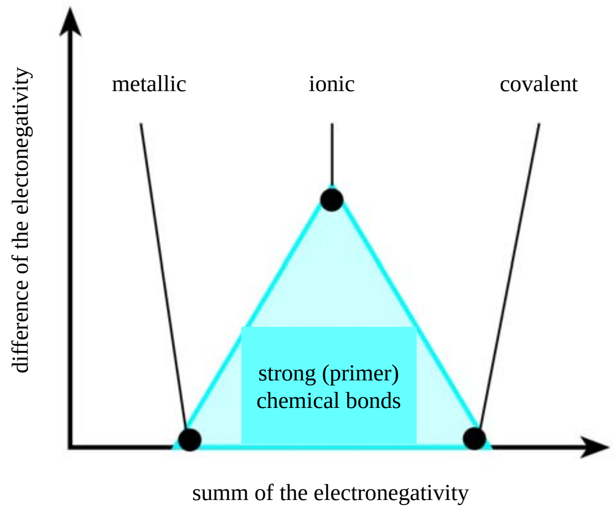
Practical use of electronegativity
(e.g. for molecule AB)

$|\chi_A - \chi_B|$

is related to the - electric dipole moment
- ionic character of the bond, given in %
- ionic-covalent resonance energy

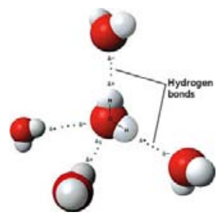
When a molecule is formed, the electrons flow towards the atoms of high electronegativity, the electronegativities of the atoms tend to equalize and acquire the same, uniform value

Influence of the electronegativity on the type of the chemical bond



secondary (week) chemical bonds (binding energy less than 20 kJ/mol few 0.2 eV/bond)

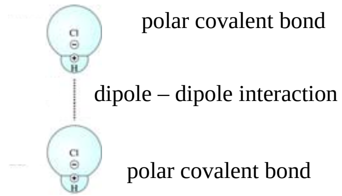
a./ the H – bond (~20 kJ/mol, 0.3 eV/bond) (water, HF)



b./ electrostatic interaction

ion – dipole (few kJ/mol, 0.05 eV/bond)

dipole – dipole (~ 2 kJ/mol, 0.01 eV/bond)

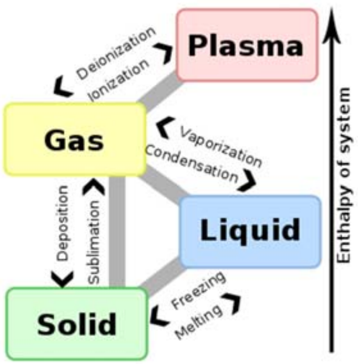


dispersion (~ 0.1 kJ/mol, 0. 001 eV/bond) (Noble gases, F_2, H_2, Cl_2 molecules)

The broad states of matter: gas
liquid
(liquid – crystal)
solid

General phase transitions

phase: physically and chemically homogeneuos part of the material



Macroscopic properties of different phases:

gas: no definite volume and shape (there is no (or very week) interaction between the particles

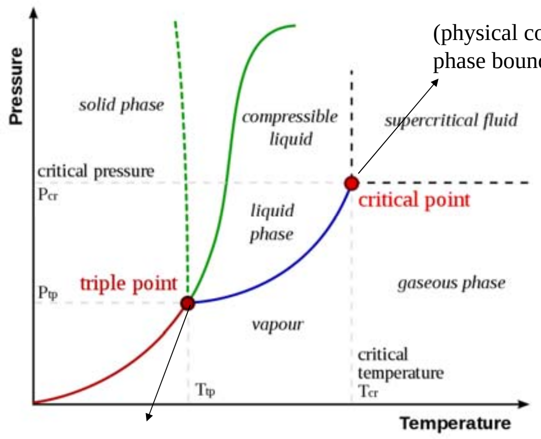
liquid: the volume is definite, the shape is changing, short range order (secondary interactions between the molecules)

liquid – crystal: special shape of individual molecules, relatively long range of order, anisotropy (intermediate phase between liquids and crystals)

solid: definite shape and volume (strong (primer) bonds between the particles)
macroscopic range order (crystals)
periodic crystal structure, symmetry, frequent anisotropy
low degree of translational motion

A typical phase diagram

<u>phase diagram:</u> graphical presentation of stable phases as a function of different parameters



(physical conditions when the phase boundary ceases to exist)

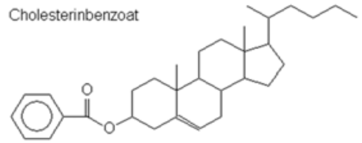
(the three phases coexist in equlibrium)

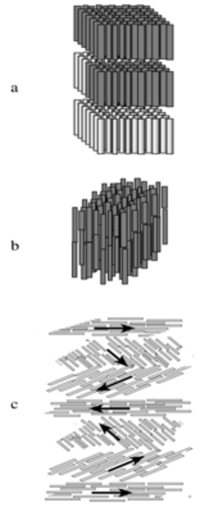
simultaneous transition of Ar from solid to liquid and to gas

Liquid crystals: a mesomorphous state of matter

Thermotropic - liotropic

General properties
- elongated shape of molecules
- relativly long range order stabilized by secondary bonds
- fluidity, deformability
- anisotropy in fluid state



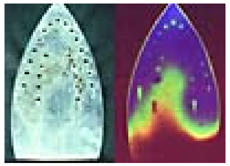


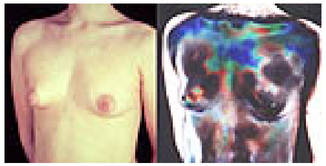
smectic

nematic

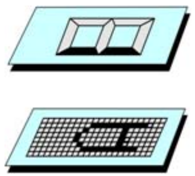
cholesteric

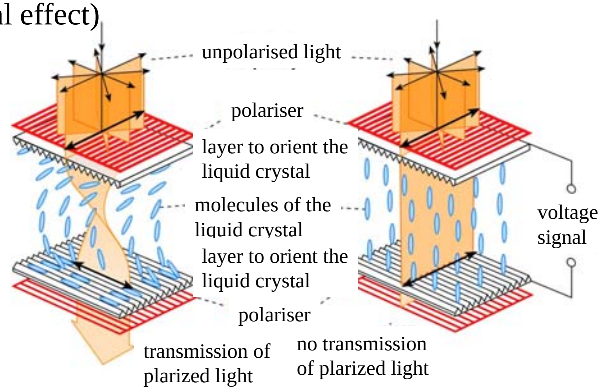
Use of thermotropic liquid crystals



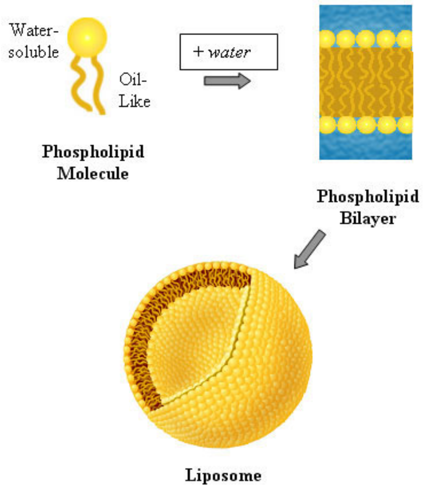


LCD (electro optical effect)

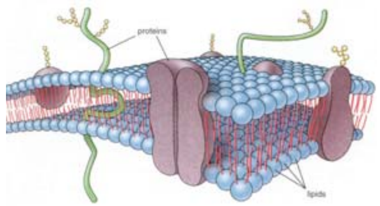


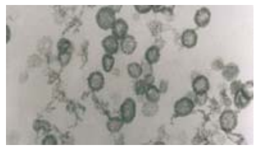


Liotropic liquid crystals



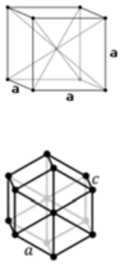
Cellular bi-layer membranes

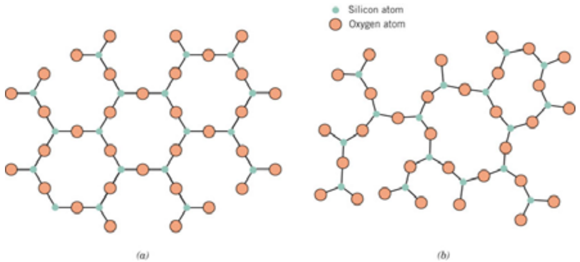




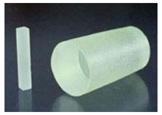
Classification of solid materials

crystalline amorphous





monocrystal polycrystal



sapphire

calcite

cuprite

moldavite

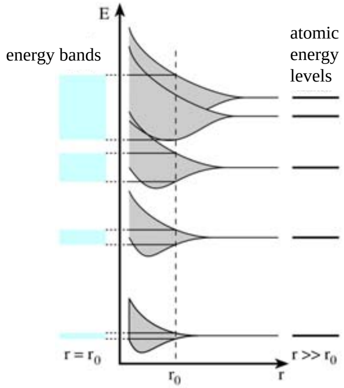
The electron states of atoms structured in crystalline order

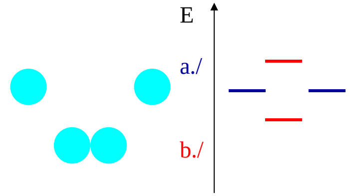
basic rules: energy minimum concept
number of electrons on a given orbital
Pauli principle

large number (N) of atoms in the crystal → splitting of the discrete electronic energy levels into N levels close to each other

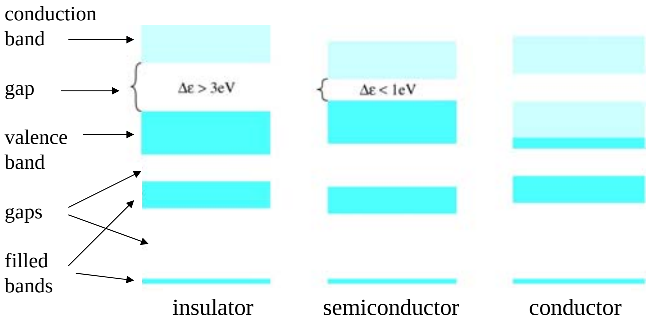
↓

a continuous energy band is formed



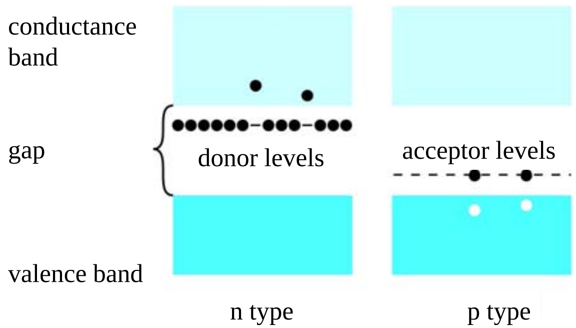


Classification of solid state materials based on their band structure



Doped semiconductores:

semiconductores (Si, Ge) + electron acceptor (B, Al) p type conductance
+ electron donor (As, In) n type conductanc
(the concentration of doping material is very small)



Chapters in the text book (Medical biophysics)

- I/2. atomic interactions
- I/3.2.1. gases
- I/3.3. solid materials
- I/3.4. liquids, liquid crystals
- I/4.1.2. the H-bond