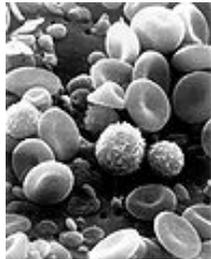


The microscopic world

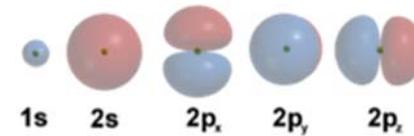
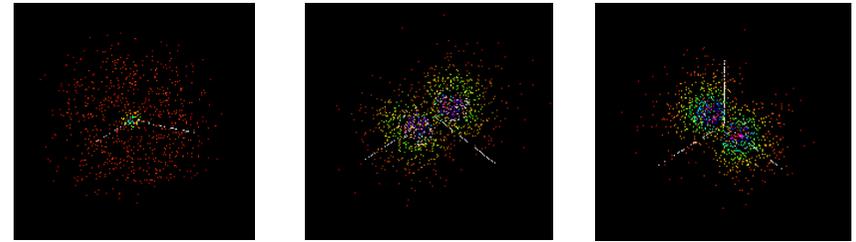
Multi-atomic systems



Irén Bárdos-Nagy



Electron clouds of the individual carbon atoms



PERIODIC TABLE OF THE ELEMENTS

http://www.kj-soft.hr/periodni/en/

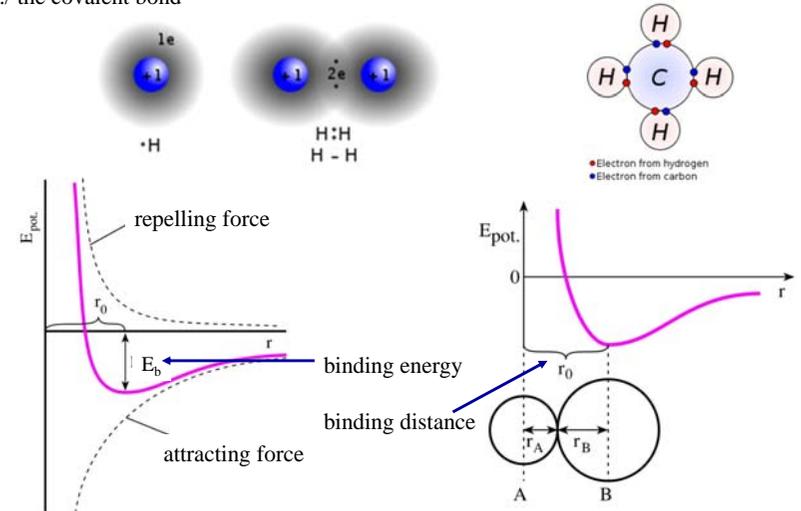
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18									
1 H 1.0079 HYDROGEN	2 He 4.0026 HELIUM											3 Li 6.941 LITHIUM	4 Be 9.0122 BERYLLIUM	5 B 10.811 BORON	6 C 12.011 CARBON	7 N 14.007 NITROGEN	8 O 15.999 OXYGEN	9 F 18.998 FLUORINE	10 Ne 20.180 NEON							
3 Na 22.990 SODIUM	4 Mg 24.305 MAGNESIUM											13 Al 26.982 ALUMINUM	14 Si 28.086 SILICON	15 P 30.974 PHOSPHORUS	16 S 32.065 SULFUR	17 Cl 35.453 CHLORINE	18 Ar 39.948 ARGON									
19 K 39.098 POTASSIUM	20 Ca 40.078 CALCIUM	21 Sc 44.956 SCANDIUM	22 Ti 47.867 TITANIUM	23 V 50.942 VANADIUM	24 Cr 51.996 CHROMIUM	25 Mn 54.938 MANGANESE	26 Fe 55.845 IRON	27 Co 58.933 COBALT	28 Ni 58.693 NICKEL	29 Cu 63.546 COPPER	30 Zn 65.39 ZINC	31 Ga 69.723 GALLIUM	32 Ge 72.64 GERMANIUM	33 As 74.922 ARSENIC	34 Se 78.96 SELENIUM	35 Br 79.904 BROMINE	36 Kr 83.80 KRYPTON									
37 Rb 85.460 RUBIDIUM	38 Sr 87.62 STRONTIUM	39 Y 88.906 YTRBIUM	40 Zr 91.224 ZIRCONIUM	41 Nb 92.906 NIOBIUM	42 Mo 95.94 MOLYBDENUM	43 Tc 98 TECHNETIUM	44 Ru 101.07 RUTHENIUM	45 Rh 101.07 RHODIUM	46 Pd 106.42 PALLADIUM	47 Ag 107.87 SILVER	48 Cd 112.41 CADMIUM	49 In 114.82 INDIUM	50 Sn 118.71 TIN	51 Sb 121.76 ANTIMONY	52 Te 127.60 TELLURIUM	53 I 126.90 IODINE	54 Xe 131.29 XENON									
55 Cs 132.91 CAESIUM	56 Ba 137.33 BARIUM	Lanthanoids										74 Hf 178.49 HAFNIUM	75 Ta 180.95 TANTALUM	76 W 183.84 WOLYBDENUM	77 Re 186.21 RHENIUM	78 Os 190.23 OSMIUM	79 Ir 192.22 IRIDIUM	80 Pt 195.08 PLATINUM	81 Au 196.97 GOLD	82 Hg 200.59 MERCURY	83 Tl 204.38 THALLIUM	84 Pb 207.2 LEAD	85 Bi 208.98 BISMUTH	86 Po 209 POLONIUM	87 At 210 ASTATINE	88 Rn 222 RADON
87 Fr 223 FRANCIUM	88 Ra 226 RADIUM	Actinoids										104 Rf 261 RUFORDIUM	105 Db 262 DUBNIUM	106 Sg 266 SEABORGIUM	107 Bh 264 BOHRIUM	108 Hs 265 HASSIUM	109 Mt 268 MEITNERIUM	110 Uun 271 UNUNBIUM	111 Uuu 272 UNUNTRIUM	112 Uub 285 UNUNBIUM	113 Uut 284 UNUNTRIUM	114 Uuq 289 UNUNQUADIUM				
LANTHANOID		57 La 138.91 LANTHANUM	58 Ce 140.12 CERIUM	59 Pr 140.91 PRASEODYMIUM	60 Nd 144.24 NEODYMIUM	61 Pm 145 PROMETHIUM	62 Sm 150.36 SAMARIUM	63 Eu 151.96 EUROPIUM	64 Gd 157.25 GADOLINIUM	65 Tb 158.93 TERBIUM	66 Dy 162.50 DYSPROSIUM	67 Ho 164.93 HOLMIUM	68 Er 167.26 ERBIUM	69 Tm 168.93 THULIUM	70 Yb 173.04 YTERBIUM	71 Lu 174.97 LUTETIUM										
ACTINOID		89 Ac 227 ACTINIUM	90 Th 232.04 THORIUM	91 Pa 231.04 PROTACTINIUM	92 U 238.03 URANIUM	93 Np 237 NEPTUNIUM	94 Pu 244 PLUTONIUM	95 Am 243 AMERICIUM	96 Cm 247 CURIUM	97 Bk 247 BERKELIUM	98 Cf 251 CALIFORNIUM	99 Es 252 EINSTEINIUM	100 Fm 257 FERMIUM	101 Md 258 MENDELIUM	102 No 259 NOBELIUM	103 Lr 262 LAWRENCEIUM										

Editor: Aditya Varshney (advarsh@rediffmail.com)

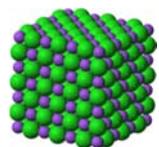
Interaction between the atoms → chemical binding

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

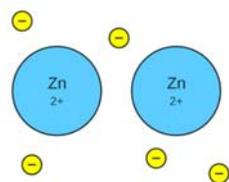
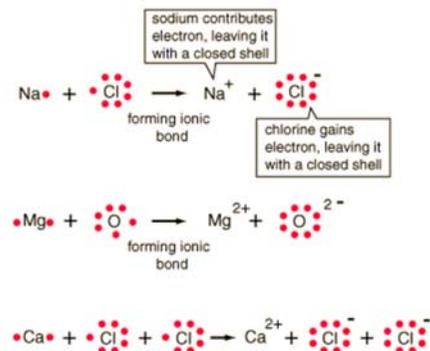
a./ the covalent bond



b./ the ionic bond

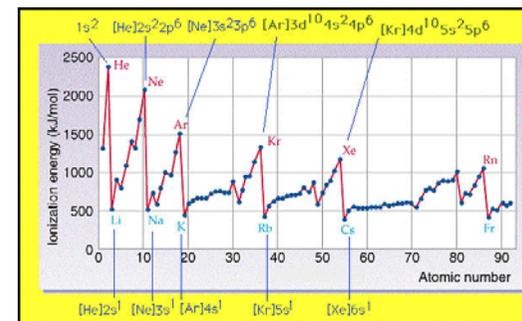


c./ the metallic bond

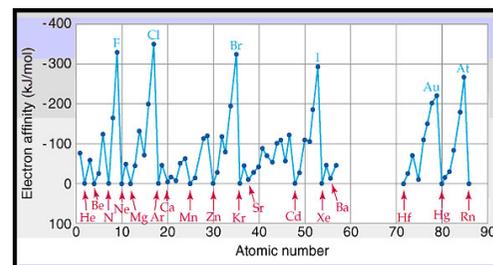


Ionization energy (I):

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



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



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

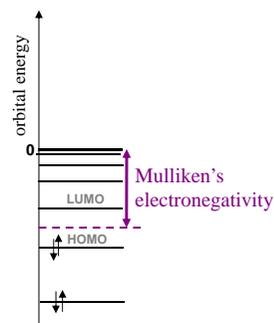
Pauling's relative scale: characterizes the polar character of bonds

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

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

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

one of the electronegativities is empirically fixed – relative scale



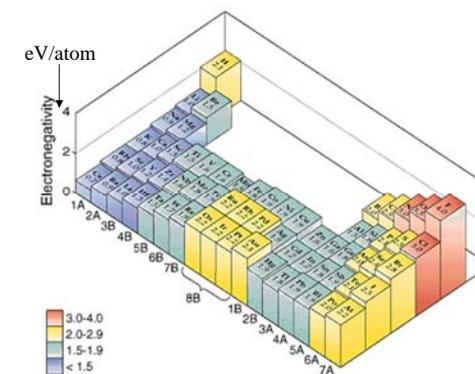
Pauling-scale (relative):

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

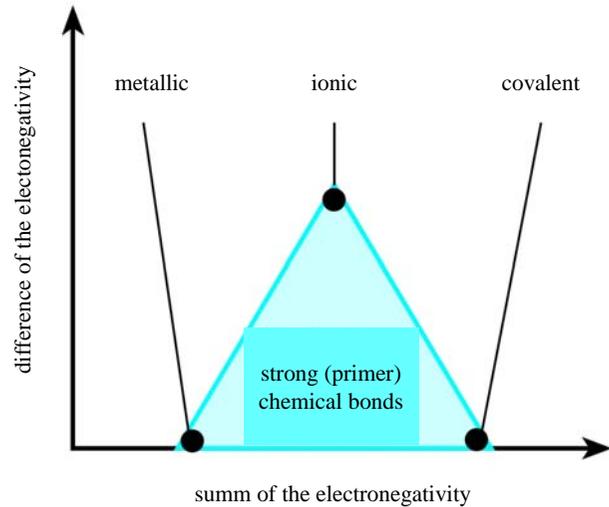
$$|\chi_A - \chi_B|$$

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

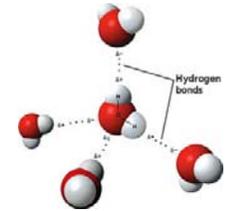


Influence of the electronegativity on the type of the chemical bond



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)

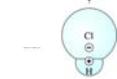


polar covalent bond

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



dipole – dipole interaction



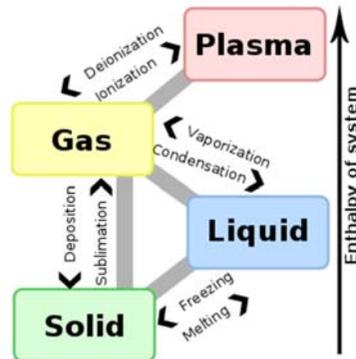
polar covalent bond

dispersion (~ 0.1 kJ/mol, 0.001 eV/bond) (Noble gases, F₂, H₂, Cl₂ molecules)

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

General phase transitions

phase: physically and chemically homogeneus 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)

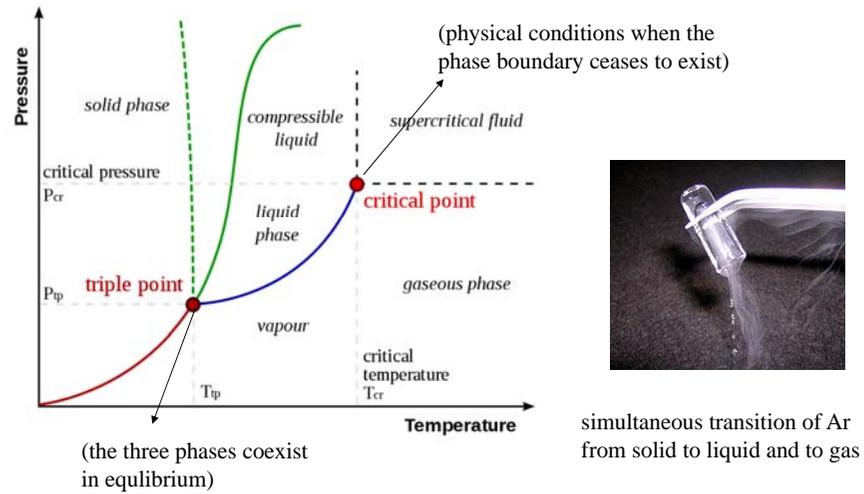
liquid: the volume is definite, the shape is changing, short range order (secondary interactions between the molecules)

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

phase diagram: graphical presentation of stable phases as a function of different parameters

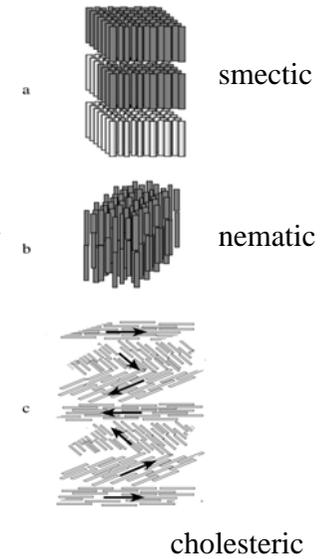
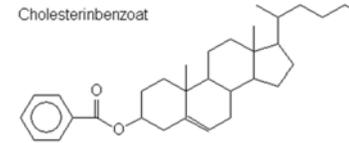


Liquid crystals: a mesomorphous state of matter

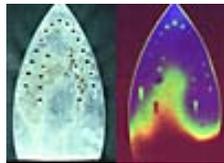
Thermotropic - liotropic

General properties

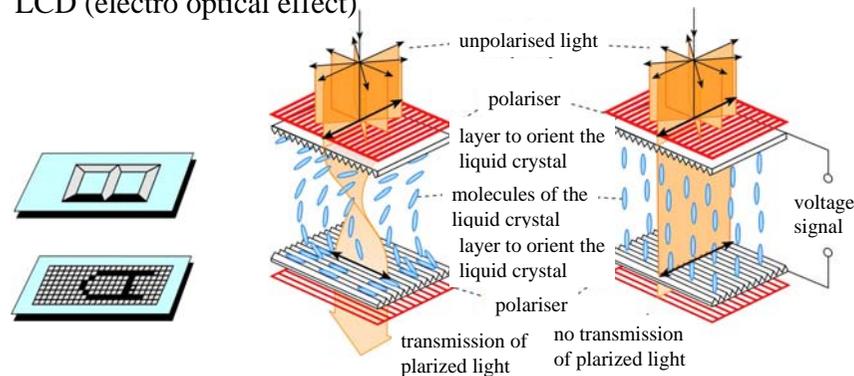
- elongated shape of molecules
- relatively long range order stabilized by secondary bonds
- fluidity, deformability
- anisotropy in fluid state



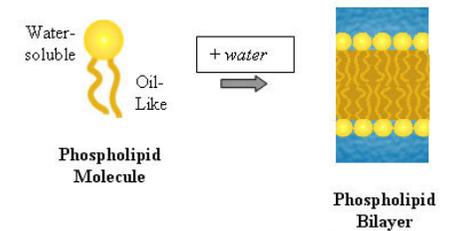
Use of thermotropic liquid crystals



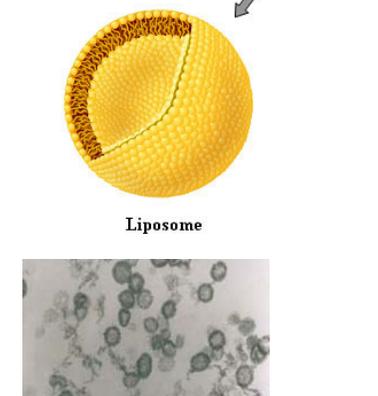
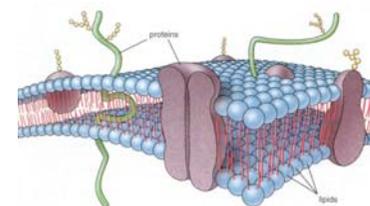
LCD (electro optical effect)



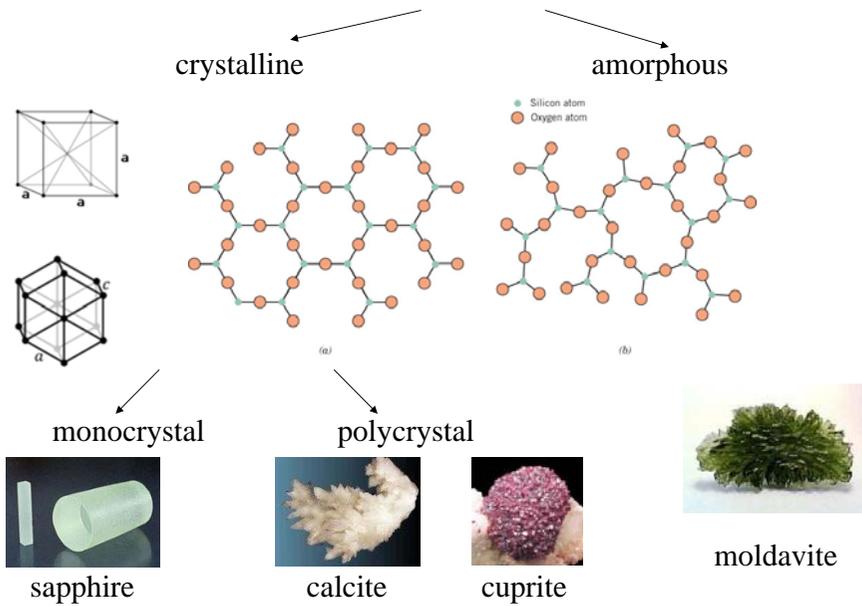
Liotropic liquid crystals



Cellular bi-layer membranes

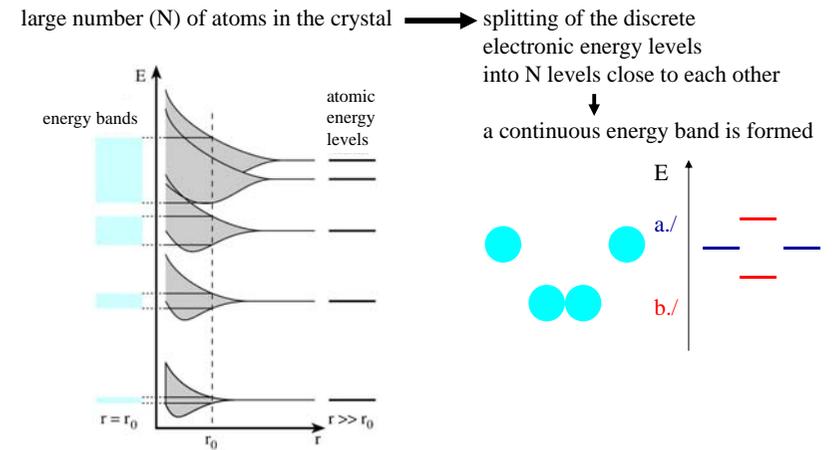


Classification of solid materials

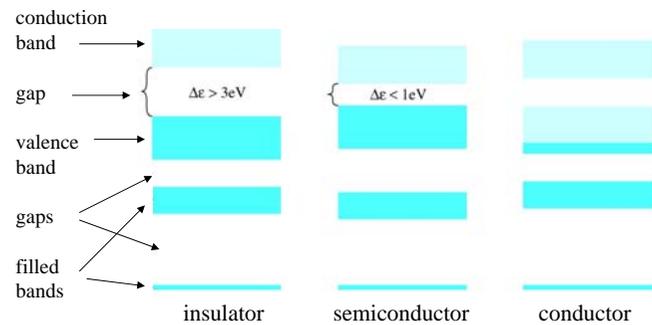


The electron states of atoms structured in crystalline order

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

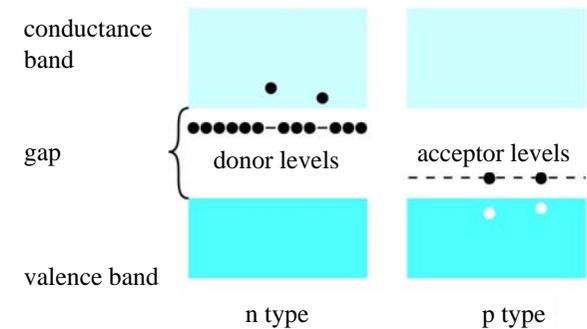


Classification of solid state materials based on their band structure



Doped semiconductors:

semiconductors (Si, Ge) + electron acceptor (B, Al) p type conductance
+ electron donor (As, In) n type conductance
(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