

# Physical bases of dental material science

Irén Bárdos-Nagy



Materials Science – Dentistry

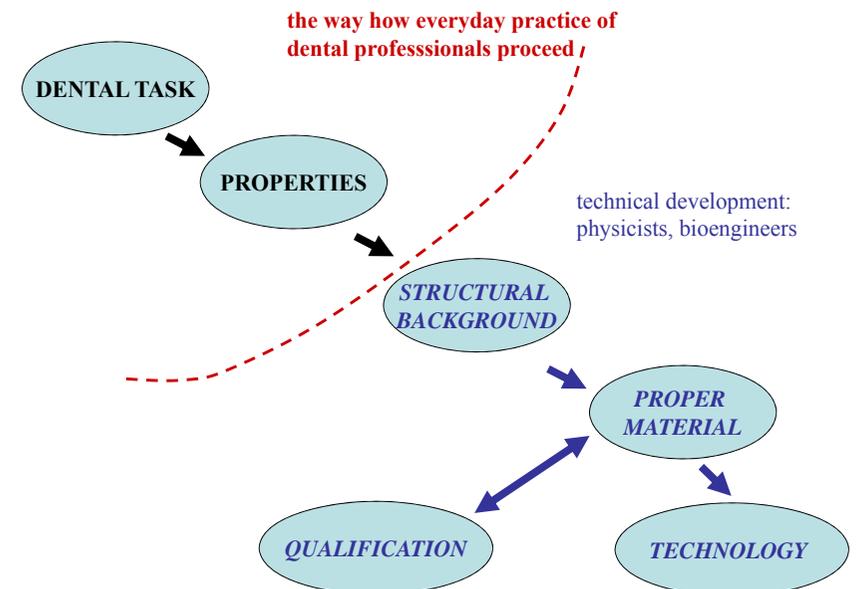


## Important informations

- **Tutor:** Károly Módos, PhD, Assistant Professor ([karoly.modos@med.semmelweis-univ.hu](mailto:karoly.modos@med.semmelweis-univ.hu))
- Biofizikai és Sugárbiológiai Intézet – Department of Biophysics and Radiation Biology, EOK left, 2nd floor, Director: Prof. Miklós Kellermayer
- max 3 absencies
- <http://biofiz.semmelweis.hu>
- e book (Physical bases of dental material science)
- W.D. Callister: *Materials Science and Engineering*. An Introduction (7th ed.), Wiley&Sons, 2007
- K.J. Anusavice: Phillips' *Science of Dental Materials* (11th ed.), Saunders, 2003
- Damjanovich, Fidy, Szöllösi: *Medical Biophysics*, Medicina, Budapest, 2009
- Exam: written test, completed by an oral exam for results higher then the passing mark



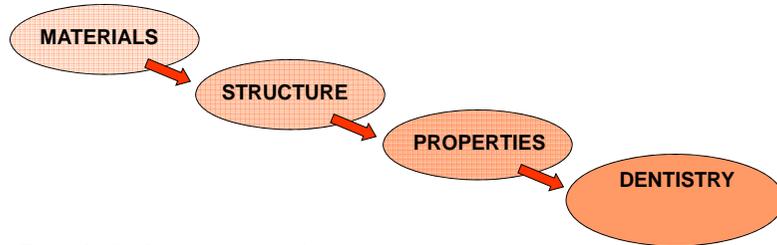
Good luck!



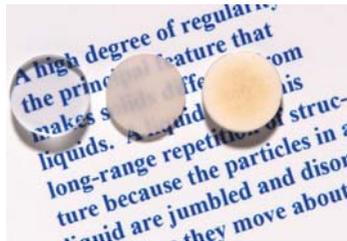


How to start? – How to proceed?

The way how the lectures proceed



Example for the importance of structure



All are Al<sub>2</sub>O<sub>3</sub> !

## Classes of materials - structural basis

### The structure of atoms



**Demokritos (5th century BC)**: materials are constructed of an infinite number of indivisible units, **atoms**

**Dalton (~ 1800)**: materials are constructed of **elements** characterized by **specific atoms**

**J.J.Thomson (1897)**: discovery of the **electron**  
identical constituents in the specific atoms of each elements

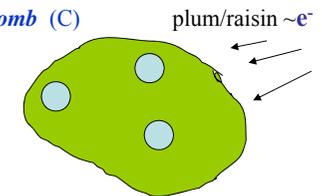
*electron is a particle of*

mass  $\ll$  lightest atom, H  $m_e = 9.11 \cdot 10^{-31}$  kg  
 $\sim 2 \cdot 10^3$ -times smaller

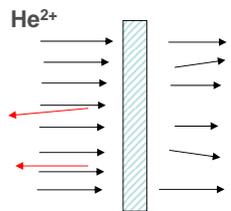
charge: **negative**,  $q_e = -1.6 \cdot 10^{-19}$  Coulomb (C)

**atom = plummy pudding**

structure of the atom  
was not known



**Ernest Rutherford (1909-11)** : scattering of He-ions ( $\alpha$  particles ) on a thin metal foil



Only a few particles were influenced in their path, some slightly deviated, and very few got reflected/repelled



- the mass of the atoms is concentrated in very small region
- this small region carry positive charges
- Rutherford's model: atom is like Sun and its orbiting planets
- most part of the volume of materials is „empty“

Structure of atoms: **atomic nucleus** (small, carries the mass, positive charge)  
**electron**, with negative charge

**Results and models concerning the electronic structure of atoms**

**Niels Bohr (1913)**  $\rightarrow$  model

**James Franck, Gustav L. Hertz (1914)**  $\rightarrow$  verification by experiment

$$hf = h \frac{c}{\lambda}$$

$$h = 6.62 \cdot 10^{-34} \text{ Js}$$

$$c = 2.998 \cdot 10^8 \text{ m/s}$$

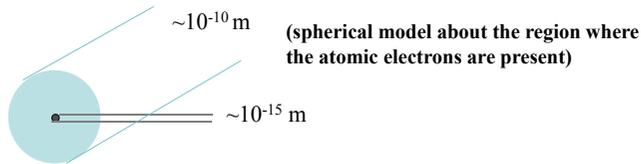
**Atomic electrons are bound on atomic orbitals of discrete energies**

**Results of quantum physics and supporting experimental results**

**Albert Einstein, Max Planck, Johannes de Haas, Otto Stern, Walther Gerlach**

**Present understanding of the atomic structure**

## Dimensions of the atomic structure



„diameter” of a H-atom ~ 10<sup>-10</sup>m

10<sup>-3</sup> milli-    10<sup>-6</sup> micro-    10<sup>-9</sup> nano-    10<sup>-12</sup> pico-    10<sup>-15</sup> femto-

The atoms interact with each other by their electronic „clouds”/orbitals. The physical/chemical properties of materials derive from the properties of electronic orbitals.

## The atomic mass

It is based on the **atomic nucleus** composed of **protons (p)** and **neutrons (n)**

### Proton (+)

Electric charge = (-1)\* charge of the electron = 1.6\*10<sup>-19</sup> C  
 Mass  $m_p \sim 1.66 \cdot 10^{-27}$  kg, (~1840\* $m_e$ )  
 Number of protons in a nucleus: **Z**

### Neutron

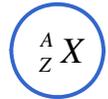
Electrically neutral  
 Mass  $m_n \sim 1.67 \cdot 10^{-27}$  kg, slightly larger than  $m_p$   
 Number of neutrons in a nucleus: **N**

nucleons

The atoms are electrically neutral

**Atomic number**

Number of protons = number of bound electrons = **Z**



**Mass number**  $A = N + Z$  (the total number of nucleons)

Symbol of an element X „nuclide”

The absolute value of the atomic mass is based on the „unified atomic mass unit” (u)  
 $u = 1.660\,538\,782 \times 10^{-27}$  kg (one-twelfth of the mass of the nucleus of a <sup>12</sup>C atom)  
 $1\,u \sim m_p \sim m_n$

### PERIODIC TABLE OF THE ELEMENTS

<http://www.kjf-split.hr/periodni/en/>

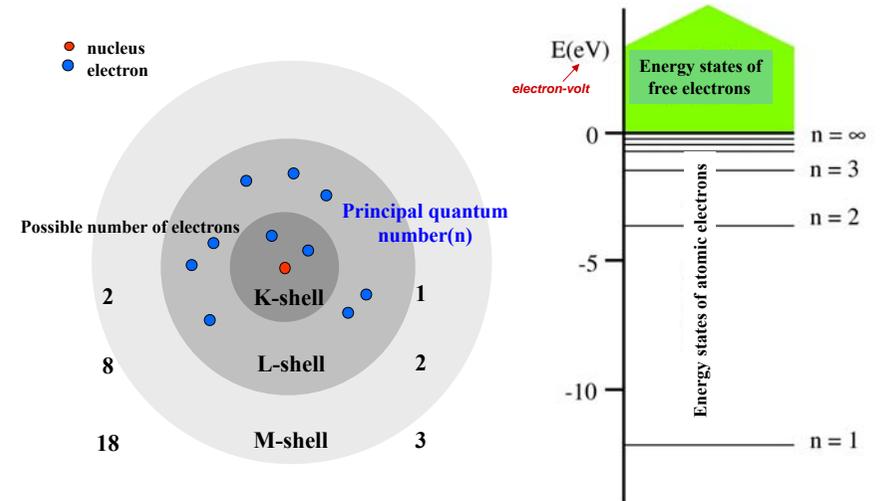
Legend:

- Metal (blue), Nonmetal (green), Metalloid (yellow)
- Alkali metal (1), Alkaline earth metal (2), Transition metals (d-block), Lanthanide (f-block), Actinide (f-block)
- Chalcogens element (16), Halogens element (17), Noble gas (18)

Standard State (25 °C, 101 kPa):  
 Na - gas, Fe - solid, Hg - liquid, Tc - synthetic

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## The structure and energetics of atomic electrons

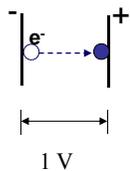


Electronic energy and momenta are quantized properties in the bound state.

**Quantum numbers:** principal-, angular momentum-, magnetic-, spin-

**Pauli's principle:** the bound electrons can not have identical quantum numbers

### The „electron-volt” as an energy unit



1 eV energy = the kinetic energy of one electron after it got accelerated by a voltage of 1 V

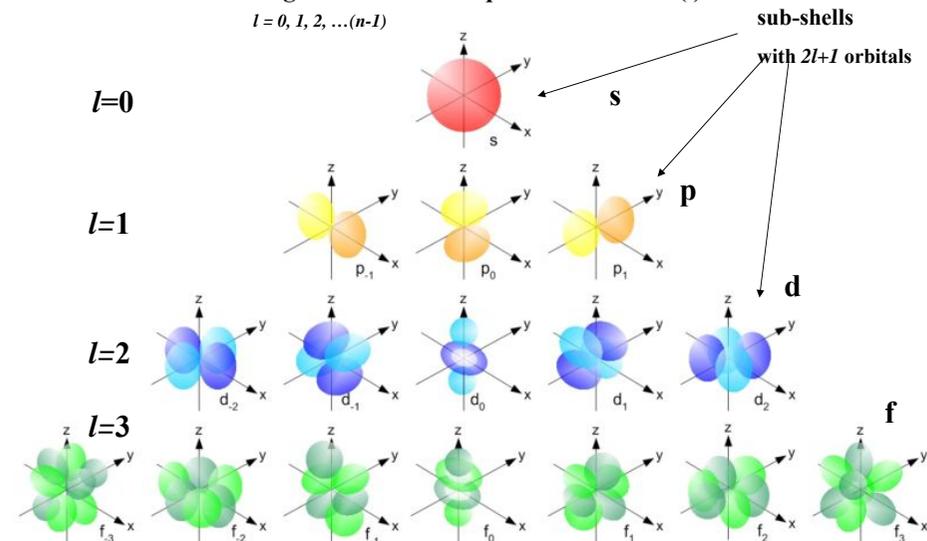
$$1eV = q * U = 1.6 * 10^{-19} C * 1V = 1.6 * 10^{-19} \text{ Joule}$$

charge      voltage

The electron-volt unit is widely used in the field of spectroscopy, and radiations like light and ionizing radiations (X-rays,  $\gamma$ ,  $\beta$ ,  $\alpha$ , etc.)

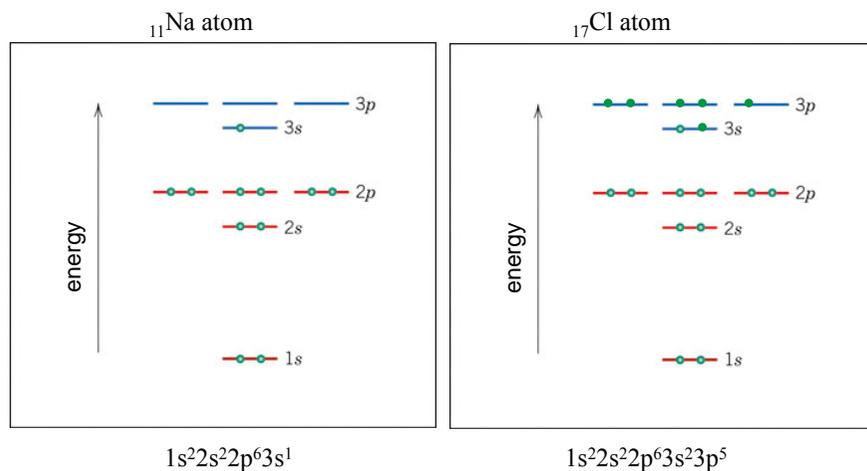
### Role of the orbital angular momentum quantum number ( $l$ )

$$l = 0, 1, 2, \dots, (n-1)$$



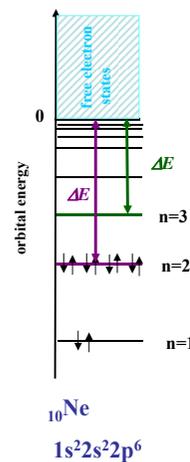
### Examples for the population of electronic orbitals

subshells may lead to a fine structure of the energy levels



### Population of electronic orbitals – relation to the state of free electrons

Simplified sketch of the electronic energy levels in an atom (subshells are not shown separately)



the energy states affected the most in chemical reactions, atomic bond formation, etc.

LUMO Lowest Unoccupied Molecular Orbital

HOMO Highest Occupied Molecular Orbital

$$\Delta E \sim \text{Ionization energy} - I \text{ (eV/atom or kJ/mol)}$$

$$\Delta E \sim \text{Electron affinity} - E_{ea} \text{ (eV/atom or kJ/mol)}$$

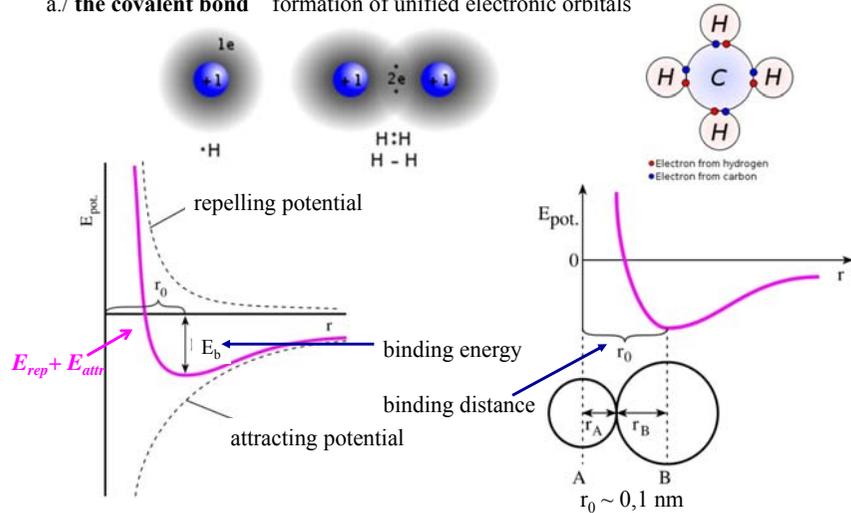
Interaction between the atoms → chemical binding

**General concept of the formation of atomic bonds: minimizing the potential energy**

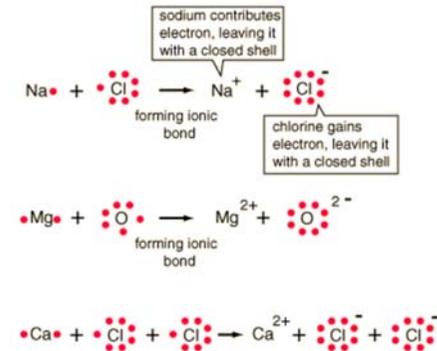
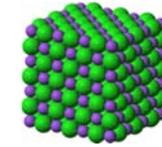
**Primer (strong) chemical bonds** (binding energy 100 – 500 kJ/mol few eV/bond)

a./ **the covalent bond** formation of unified electronic orbitals

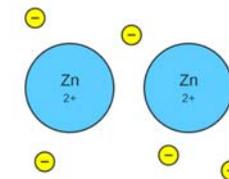
(1eV/bond ~ 100 kJ/mol)



b./ **the ionic bond**

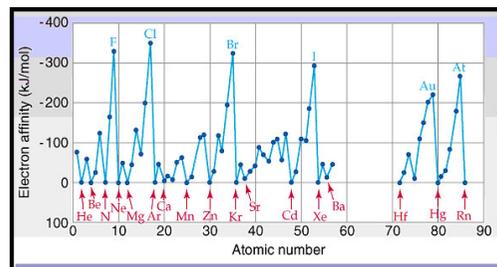
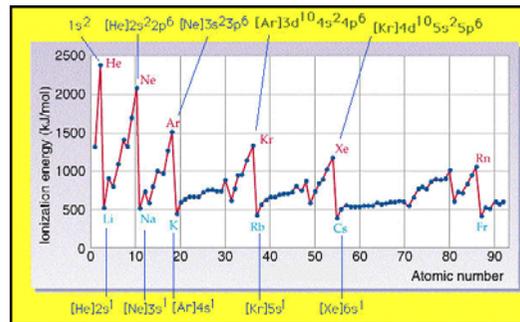


c./ **the metallic bond**



**Ionization energy (I):**

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



**Electronaffinity (E<sub>ea</sub>):**

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

Exothermic electron attachment: E<sub>ea</sub> > 0  
-- incoming electron interacts strongly with the nucleus on its orbital  
Endothermic electron attachment: E<sub>ea</sub> < 0  
-- A<sup>-</sup> has higher energy than A and e<sup>-</sup>

**Electronegativity**  $\chi$

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:

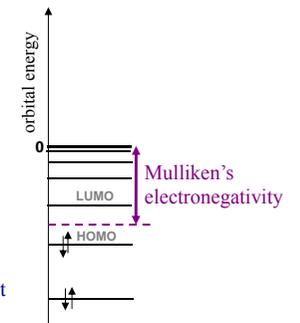
characterizes the polar character of bonds

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

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

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

one of the electronegativities is empirically fixed – relative scale



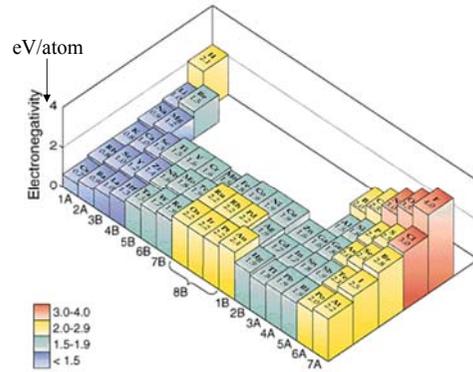
Pauling-scale (relative):

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

$$|\chi_A - \chi_B|$$

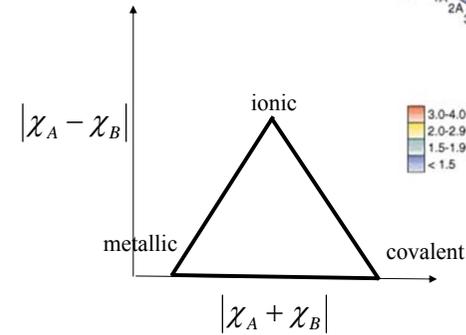
is related to the - electric dipole moment  
 - ionic character of the bond, given in %  
 - ionic-covalent resonance energy

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



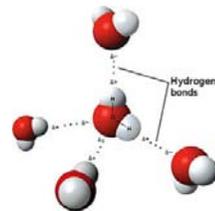
$$|\chi_A + \chi_B|$$

is related to the type of primary bond formed between A and B



**Secondary (weak) chemical bonds** (binding energy less than 50 kJ/mol few 0.1 eV/bond)

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



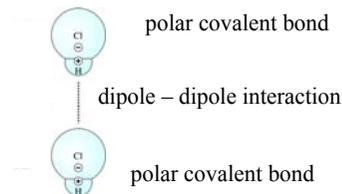
b./ **electrostatic interaction**

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

dipole – dipole (~ 2 kJ/mol, 0.02 eV/bond)

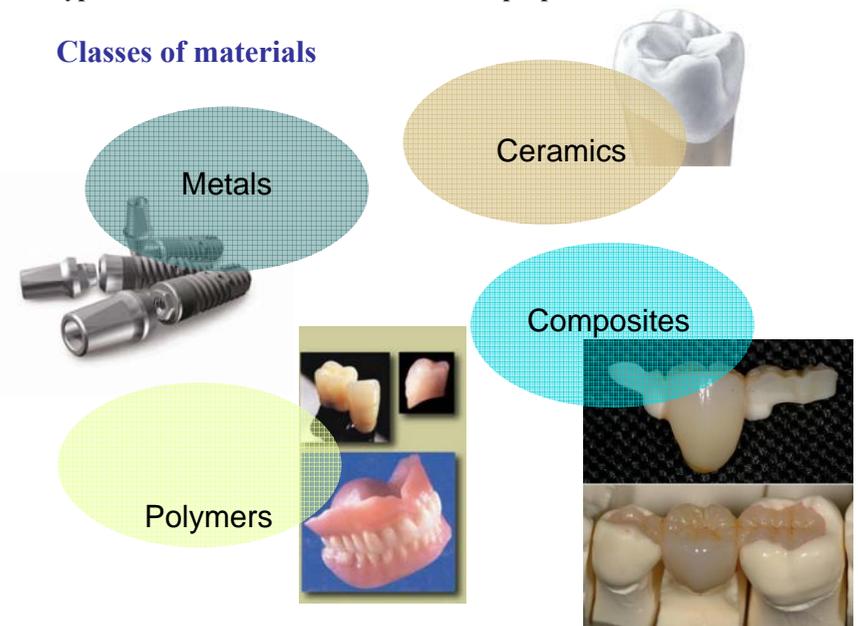
hydrophobic (~2 kJ/mol, 0,02 eV/bond)

van der Waals (dispersion) (~ 0.1 kJ/mol, 0. 001 eV/bond)  
 (Noble gases, F<sub>2</sub>, H<sub>2</sub>, Cl<sub>2</sub> molecules)



type of bonds → structure → properties

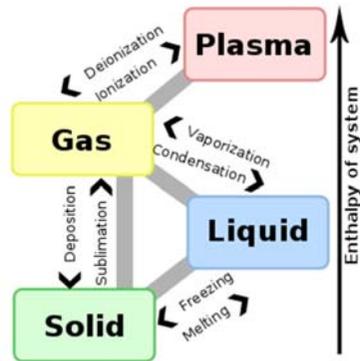
**Classes of materials**



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

### General phase transitions

phase: physically and chemically homogeneous part of the material



### General properties of different phases:

**gas**: no definite volume and shape (there is no (or very weak) interaction between the particles), isotropic

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

**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