Physical Foundations of Dental Materials Science

Introduction

1

1

Important informations

- **Tutor:** Zsolt Mártonfalvi, PhD (martonfalvi.zsolt@med.semmelweis-univ.hu)
- Department of Biophysics and Radiation Biology, left elevators, 2nd floor
  Head: Prof. Miklós Kellermayer
- http://itc.semmelweis.hu/
- Pdf format e -book (Physical bases of dental material science)
- Exam: written test composed of three sections:
  1) Definitions, 2) Calculations, 3)Theory

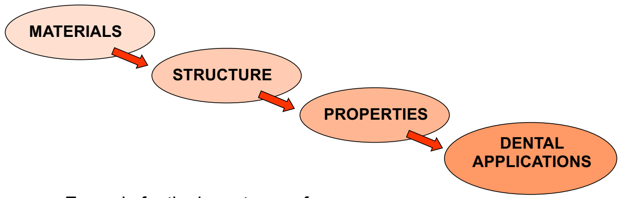
Further readings:

- 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, Szöllősi: *Medical Biophysics*, Medicina, Budapest, 2009

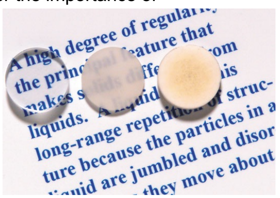
2

How to start? – How to proceed?

The way how the lectures proceed



Example for the importance of structure:



All are Al_2O_3 !

3

Physical Foundations of Dental Materials Science 1.

Structure of matter

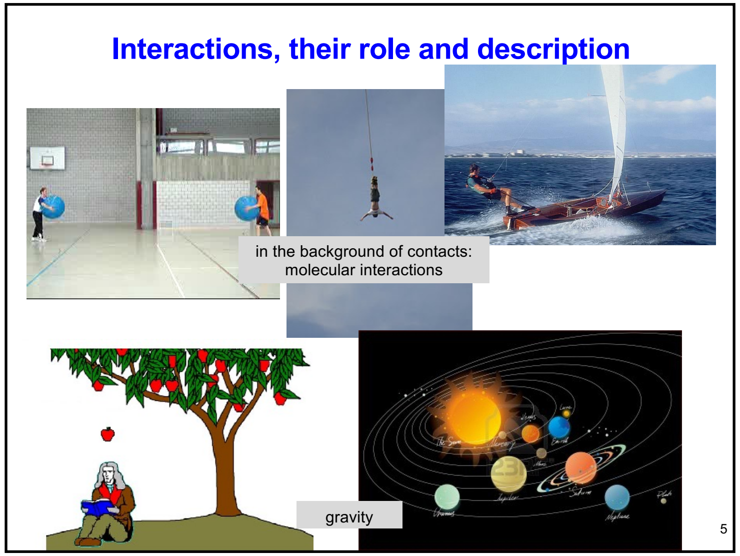
Atomic interaction, multiatomic system - gases

E-book chapters: 1, 2, 3

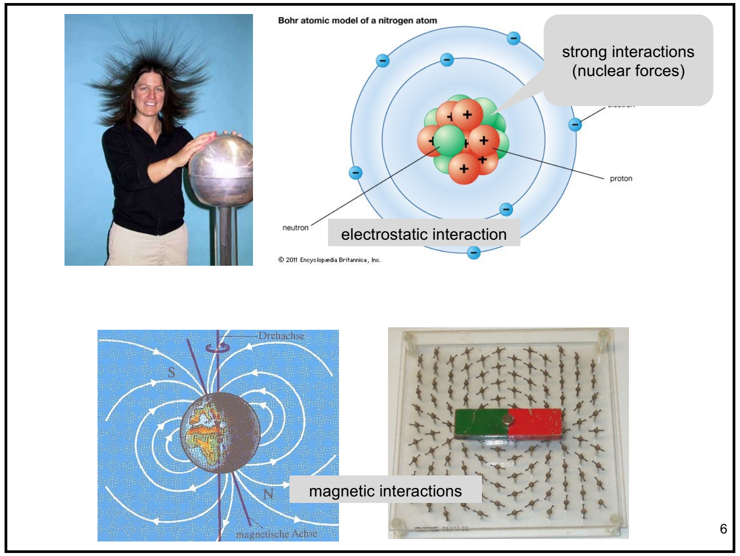
Highlights:
- ❖ Interactions
- ❖ Energy curve of atomic and molecular interactions
- ❖ Interpretation of temperature
- ❖ Boltzmann-distribution

Problems: Chapter 1, 2, 3.: 1, 3, 9, 10, 13, 17, 19

4


Interactions, their role and description
in the background of contacts:
molecular interactions
gravity
5

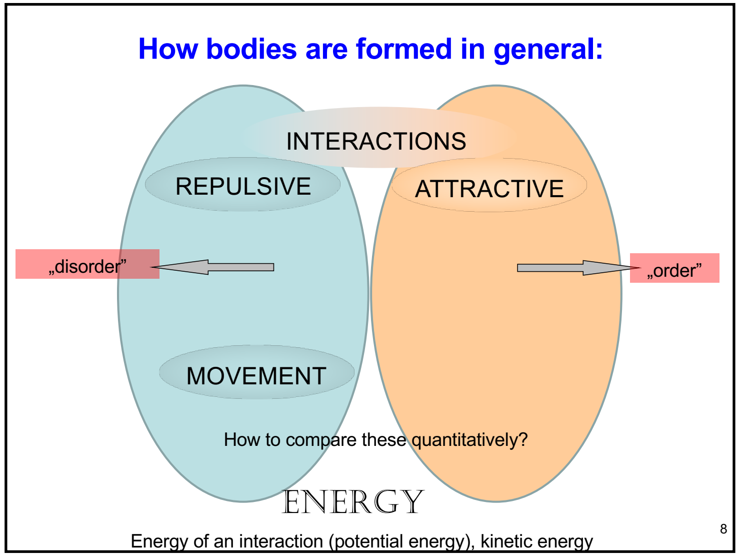
5


Bohr atomic model of a nitrogen atom
strong interactions
(nuclear forces)
proton
neutron
electrostatic interaction
© 2011 Encyclopædia Britannica, Inc.
Drehachse
S
N
magnetische Achse
magnetic interactions
6

6


thermal interaction (heat)
Our novel drugs
increase the rate of oxygen
DIFFUSION through
the blood.
O_2 from lungs
O_2 to
cellular mitochondria
chemical, biological interactions
7

7


How bodies are formed in general:
INTERACTIONS
REPULSIVE
ATTRACTIVE
„disorder"
„order"
MOVEMENT
How to compare these quantitatively?
ENERGY
Energy of an interaction (potential energy), kinetic energy
8

8

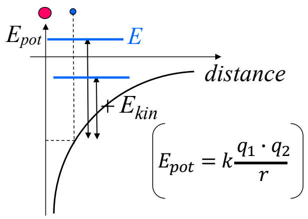
INTERACTIONS

MOVEMENT

REPULSIVE

ATTRACTIVE

$$E_{kin} = \frac{1}{2}mv^2$$



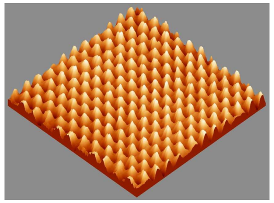
$$E_{pot} = k\frac{q_1 \cdot q_2}{r}$$

$E = E_{pot} + E_{kin} < 0$ ⟹ bound e^-

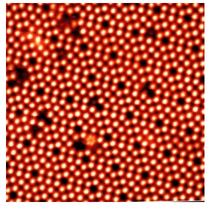
$E = E_{pot} + E_{kin} > 0$ ⟹ free e^-

All matter is composed of atoms

- Democritus B.C. 5th century
- Dalton's atomic theory 1803
- Rutherford 1911
- Bohr 1913



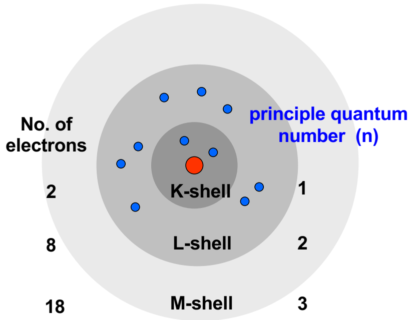
C atoms in crystal lattice
no vacancies

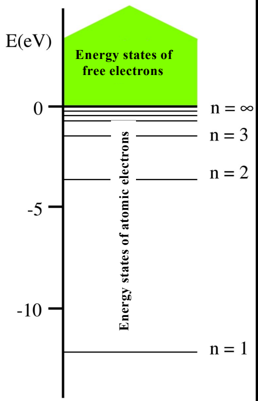


Si crystal with
vacancies

Structure of the atom

- Rutherford experiment, Spectroscopy (Bohr)
- Discrete energy levels
- Energy minimum
- Pauli-principle

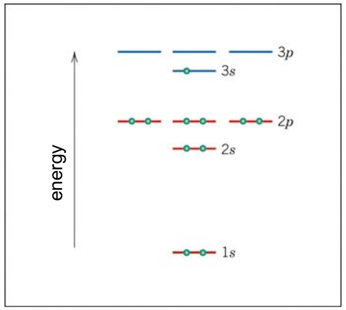




Energy unit:
elektronvolt (eV),
1 eV = 1,6·10^{-19} J

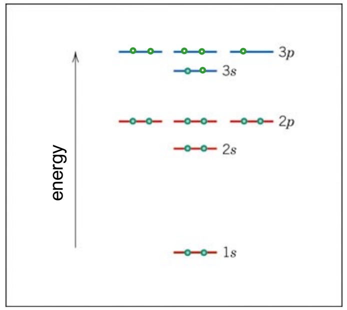
Electron configuration:

i.e. $_{11}$Na atom



$1s^2 2s^2 2p^6 3s^1$

i.e. $_{17}$Cl atom

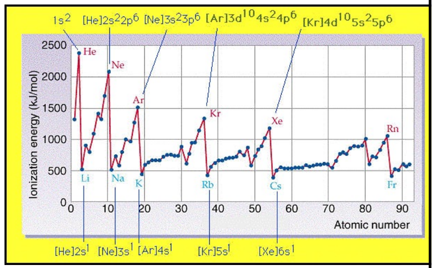


$1s^2 2s^2 2p^6 3s^2 3p^5$

Electronegativity

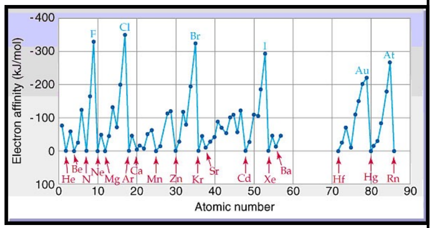
Ionization energy(*I*):

The amount of energy that is necessary to remove the most loosely bound electron from an atom **(eV/atom; kJ/mol)**



Electronaffinity (*A*):

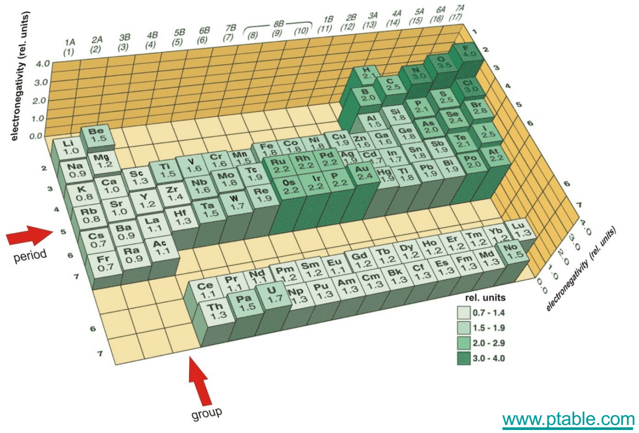
The amount of energy released when an electron is added to an atom **(eV/atom; kJ/mol)**



Electronegativity (EN):

$$EN = I + |A|$$

Pauling-scale:

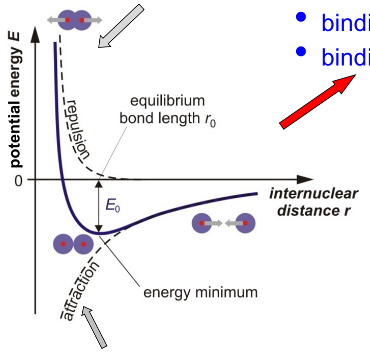


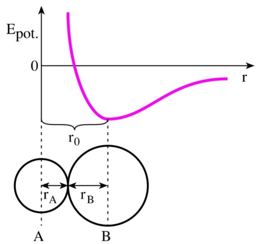
www.ptable.com

Atomic interactions

(repulsion of nuclei, Pauli-principle)

- binding distance (r_0) ≈ 0,1 nm (1Å)
- binding energy (E_0) ≈ 2-1000 kJ/mol

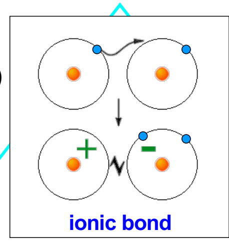




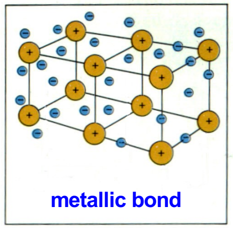
- shared electron orbitals
- electrostatic interactions (ion-ion, ion-dipole, dipole-dipole)

Bond types

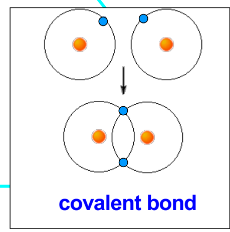
- **primary (strong) ≈100 kJ/mol**
  - covalent
  - metallic
  - ionic



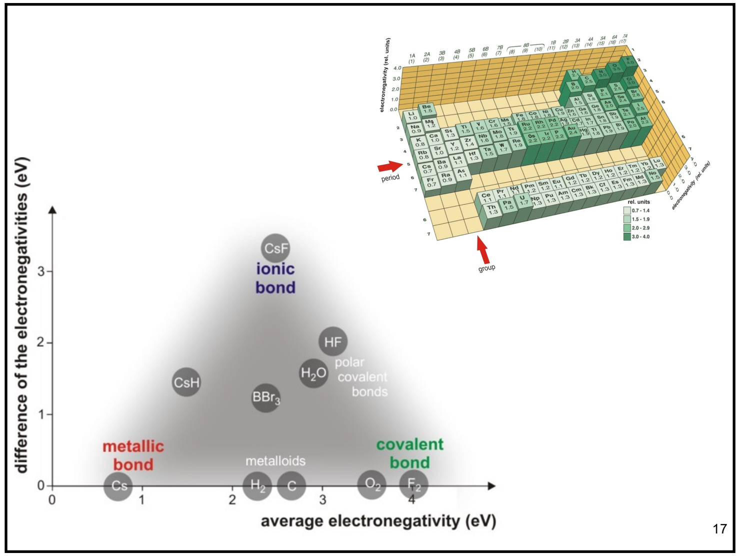
NaCl



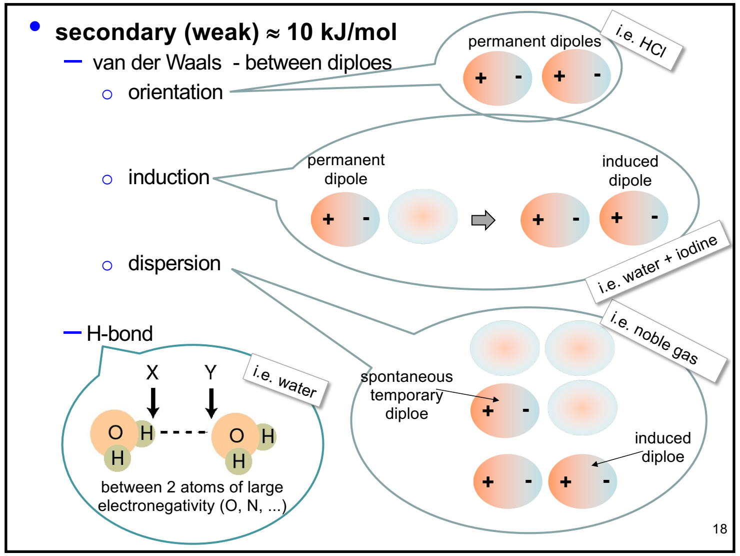
pl. Na



H_2



17

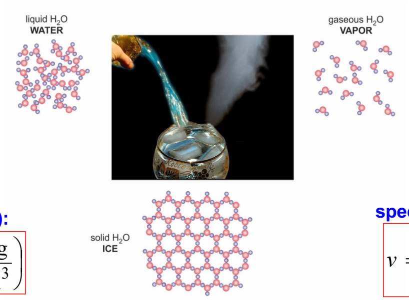


18

States of matter - Phases

T

	solid	liquid	gas
definite volume	+	+	-
stable shape	+	-	-



density (ρ):

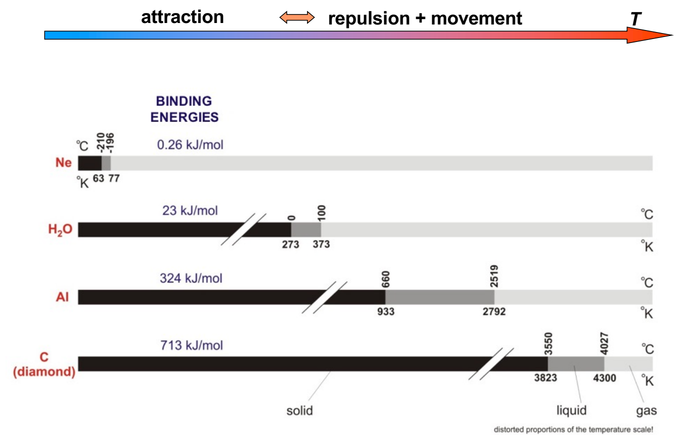
$$\rho = \frac{m}{V} \left(\frac{\text{kg}}{\text{m}^3}\right)$$

specific volume (v):

$$v = \frac{1}{\rho} \left(\frac{\text{m}^3}{\text{kg}}\right)$$

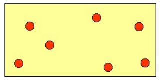
19

19



20

Gases



Macroscopic description:

- No definite volume or shape
- isotropic

p, V, n, T

$$pV = nRT$$

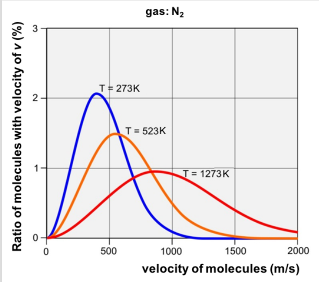
(ideal gas)

Microscopic description:

- random
- movement in many degrees of freedom

$$\frac{1}{2}m\overline{v^2} = \frac{3}{2}kT$$

Maxwell-Boltzmann- distribution



21

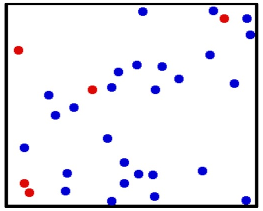
21

Temperature

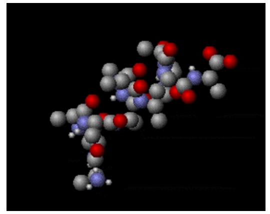
Temperature is a parameter proportional to the average kinetic energy available for each degree of freedom.

$$T(K) = t(°C) + 273$$

hot and cold gas particles



macromolecule



22

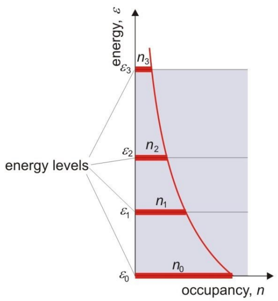
22

Boltzmann-distribution

The Boltzmann distribution describes the distribution of the particles between energy levels in a force field in case of thermal equilibrium.

n_i — ε_i } $\Delta\varepsilon$
n_0 — ε_0

$$n_i = n_0 \cdot e^{-\frac{\varepsilon_i - \varepsilon_0}{kT}}$$



$$n_i = n_0 \cdot e^{-\frac{\Delta\varepsilon}{kT}} = n_0 \cdot e^{-\frac{\Delta E}{RT}}$$

$$\Delta E = \Delta\varepsilon \cdot N_A$$

$$R = k \cdot N_A$$

23

23

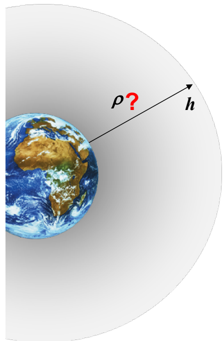
Gas in a force field – gravitation

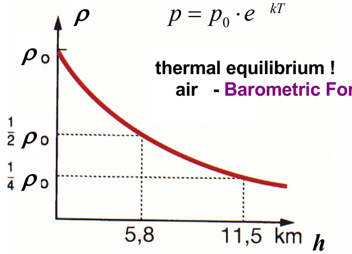
Example: density (ρ) of air ***changes*** in function of the potential energy

$$\rho = \rho_0 \cdot e^{-\frac{mgh}{kT}}$$

$$p = const * \rho$$

$$p = p_0 \cdot e^{-\frac{mgh}{kT}}$$





thermal equilibrium !

air - Barometric Formula

less and less particles are found (in the same volume) at higher potential energy (at higher altitudes)

24

Examples for Boltzmann-distribution:

- barometric formula
- thermal emission of electrons from metals
- Nernst-equation
- rate of chemical reactions
- conductivity of semiconductors
- number of vacancies in a metal
- ...

25

25

26

26