Physical Foundations of Dental Materials Science

Introduction

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Important informations

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- Department of Biophysics and Radiation Biology, left elevators, 2nd floor
  Head: Prof. Miklós Kellermayer
- http://biofiz.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

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Lectures

1	Atomic interactions, bonds. Multiatomic systems, gases. Interpretation of temperature, Boltzmann-distribution. If you cannot be present at the lecture, follow it on zoom using this link. (Zsolt Mártonfalvi)	2020.09.07.
2	Fluids, solids, liquid crystals. (Zsolt Mártonfalvi)	2020.09.14.
3	Cohesion, adhesion, interfacial phenomena. Phase, phasediagram, phase transitions. (Zsolt Mártonfalvi)	2020.09.21.
4	Methods for structural examination (diffraction, microscopic, spectroscopic methods) (Zsolt Mártonfalvi)	2020.09.28.
5	Crystallisation. Metals, alloys, ceramics. (Zsolt Mártonfalvi)	2020.10.05.
6	Polymers, composites. (Zsolt Mártonfalvi) 3D printing in dentistry (Balázs Kiss)	2020.10.12.
7	Mechanical properties of materials 1. Elasticity. (Zsolt Mártonfalvi)	2020.10.19.
8	Mechanical properties of materials 2. Plasticity, fracture, hardness. (Zsolt Mártonfalvi)	2020.10.26.
9	Mechanical properties of materials 3. Rheological properties, viscoelasticity. (Zsolt Mártonfalvi)	2020.11.02.
10	Thermal and electrical properties of materials. (Zsolt Mártonfalvi)	2020.11.09.
11	Bases of biomechanics. Structure, mechanical and other properties of dental tissues. (Zsolt Mártonfalvi)	2020.11.16.
12	Optical properties of materials. Comparison of the properties of dental materials based on their structure. (Zsolt Mártonfalvi)	2020.11.23.
13	Physical bases of implantology. (Zsolt Mártonfalvi)	2020.11.30.
14	Physical bases of orthodontics. (Zsolt Mártonfalvi)	2020.12.07.

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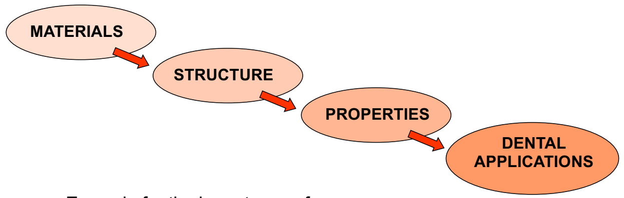
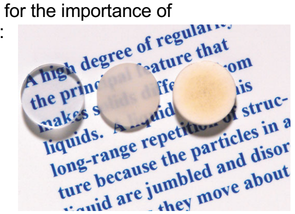
How to start? – How to proceed?

The way how the lectures proceed



Example for the importance of structure:



All are Al_2O_3 !

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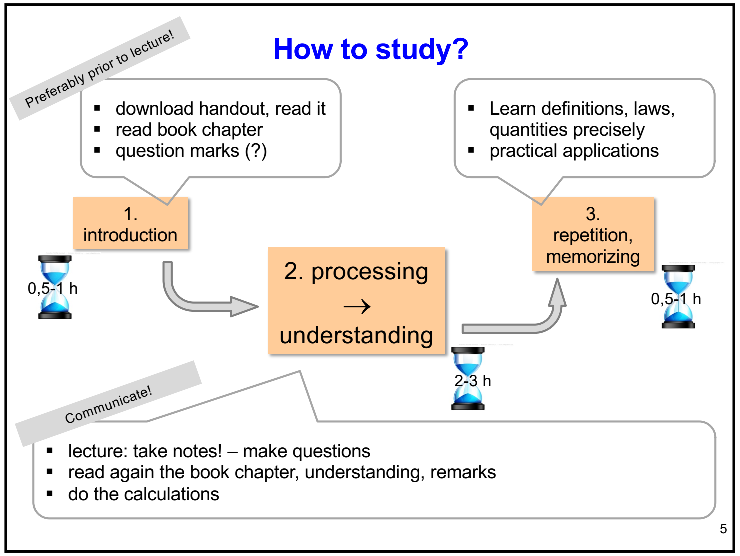
How to study?
Preferably prior to lecture!
download handout, read it
read book chapter
question marks (?)
1. introduction
0,5-1 h
2. processing → understanding
2-3 h
Learn definitions, laws, quantities precisely
practical applications
3. repetition, memorizing
0,5-1 h
Communicate!
lecture: take notes! – make questions
read again the book chapter, understanding, remarks
do the calculations
5

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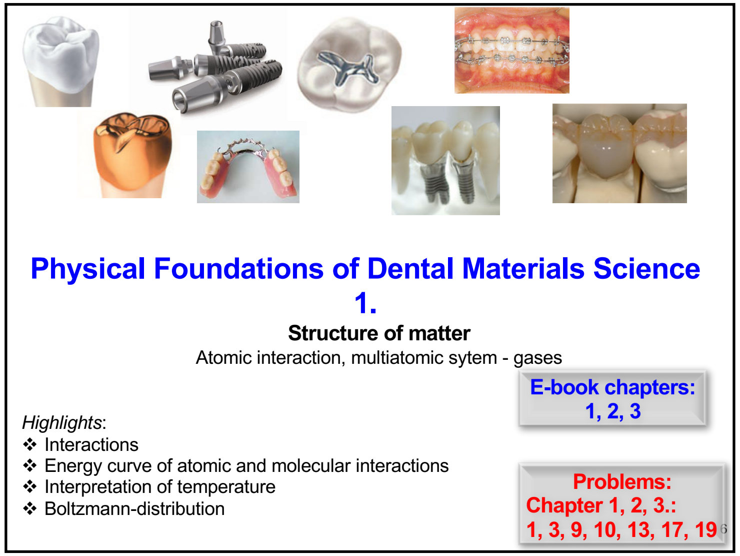
Physical Foundations of Dental Materials Science
1.
Structure of matter
Atomic interaction, multiatomic sytem - gases
E-book chapters: 1, 2, 3
Highlights:
❖ Interactions
❖ Energy curve of atomic and molecular interactions
❖ Interpretation of temperature
❖ Boltzmann-distribution
Problems: Chapter 1, 2, 3.: 1, 3, 9, 10, 13, 17, 19
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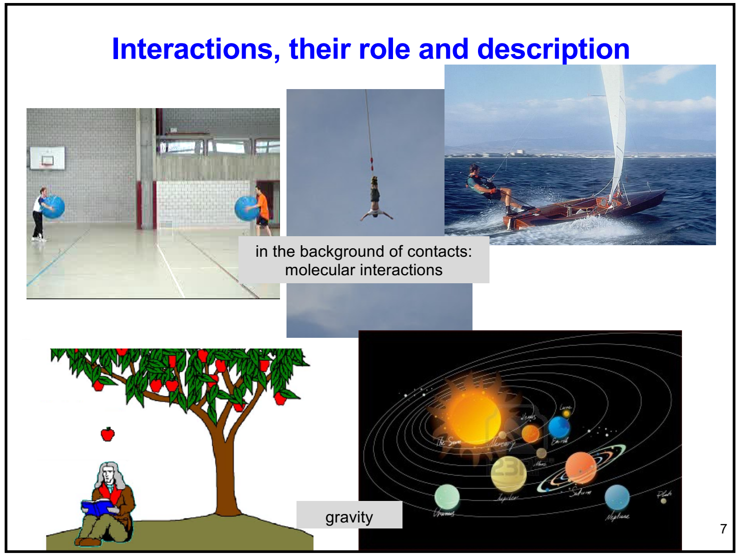
Interactions, their role and description
in the background of contacts: molecular interactions
gravity
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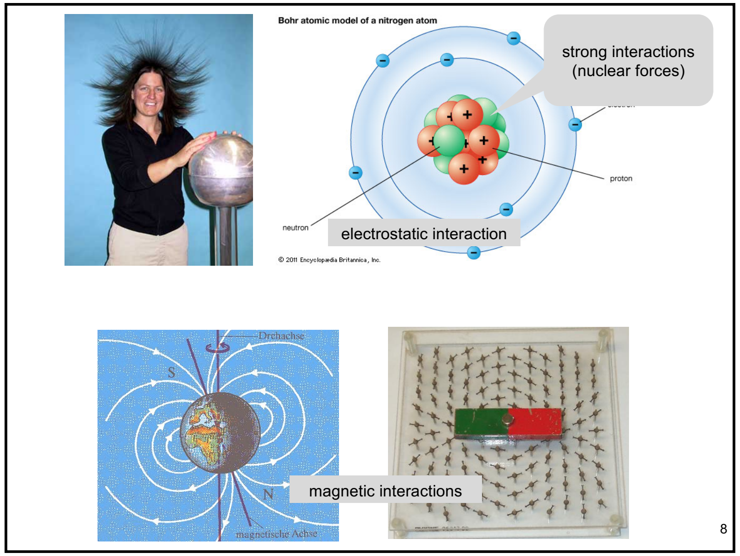
Bohr atomic model of a nitrogen atom
strong interactions (nuclear forces)
proton
neutron
electrostatic interaction
Drehachse
magnetische Achse
magnetic interactions
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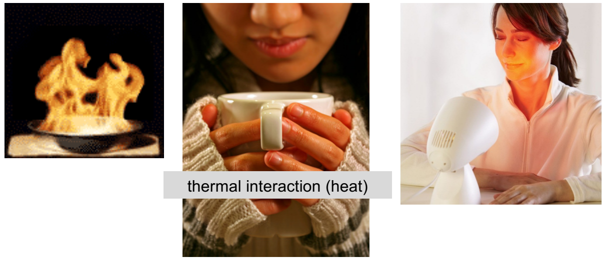
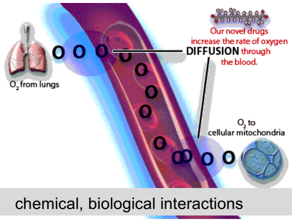


thermal interaction (heat)



chemical, biological interactions

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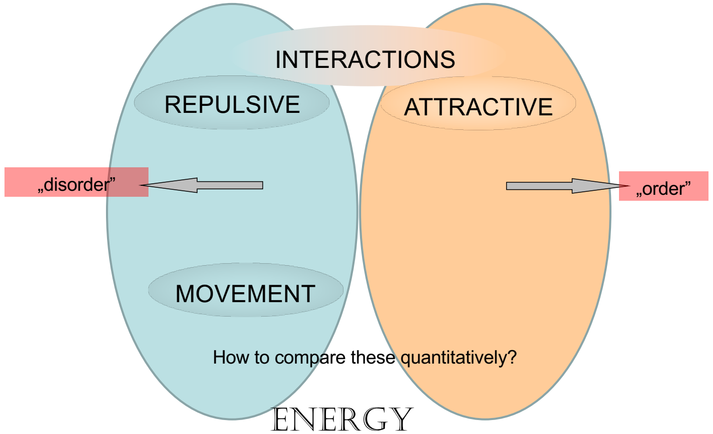
How bodies are formed in general:



ENERGY

Energy of an interaction (potential energy), kinetic energy

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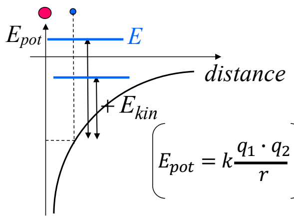
INTERACTIONS

MOVEMENT | REPULSIVE | ATTRACTIVE

$$E_{kin} = \frac{1}{2} m v^2$$



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

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

$E = E_{pot} + E_{kin} > 0$ ⟹ free e⁻

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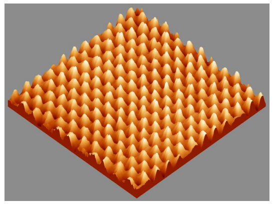
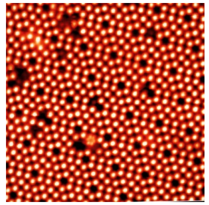
All matter is composed of atoms

- 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

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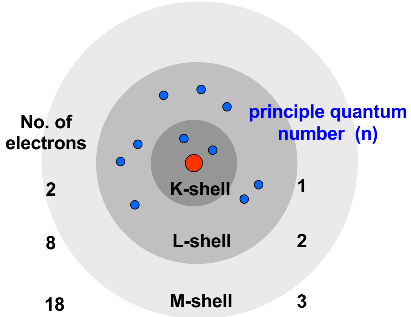
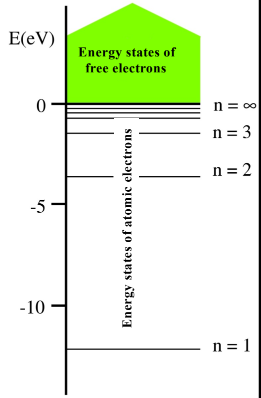
Structure of the atom

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

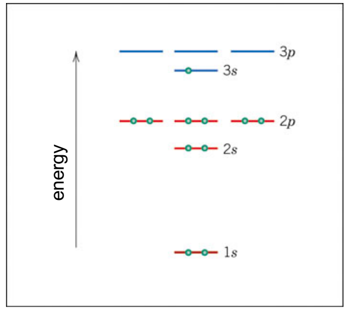




Energy unit:
elektronvolt (eV),
1 eV = $1,6 \cdot 10^{-19}$ J

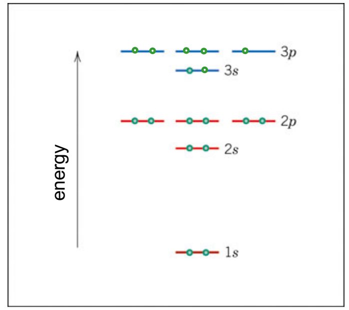
Electron configuration:

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



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

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

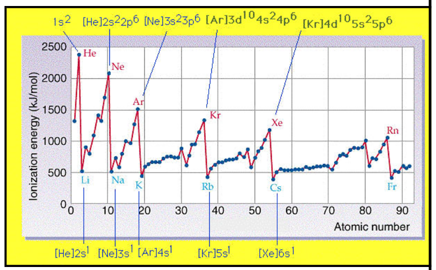


$1s^2 2s^2 2p^6 3s^2 3p^5$

Electronegativity

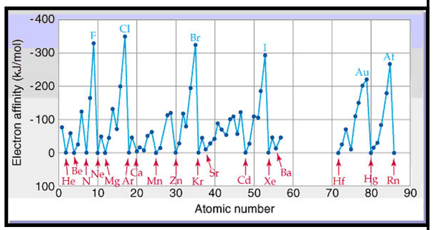
Ionization energy(*I*):

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



Electronaffinity (*A*):

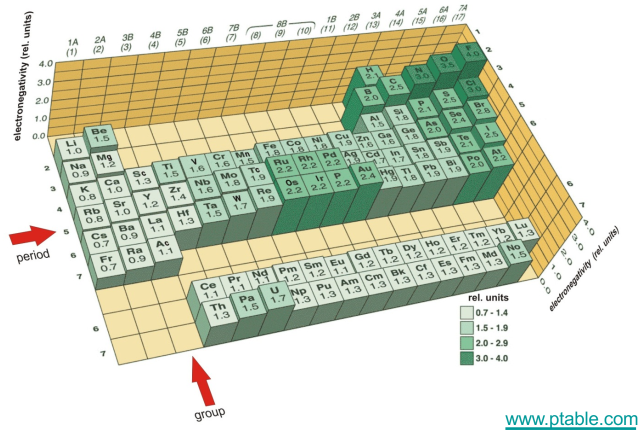
The amount of energy released when an electron is added to an atom **(eV/atom; kJ/mol)**



Electronegativity (EN):

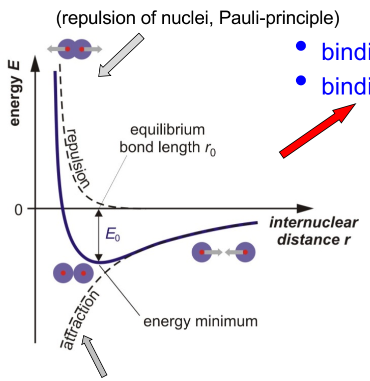
$$EN = I + |A|$$

Pauling-scale:

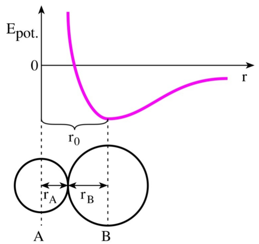


www.ptable.com

Atomic interactions



- 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)

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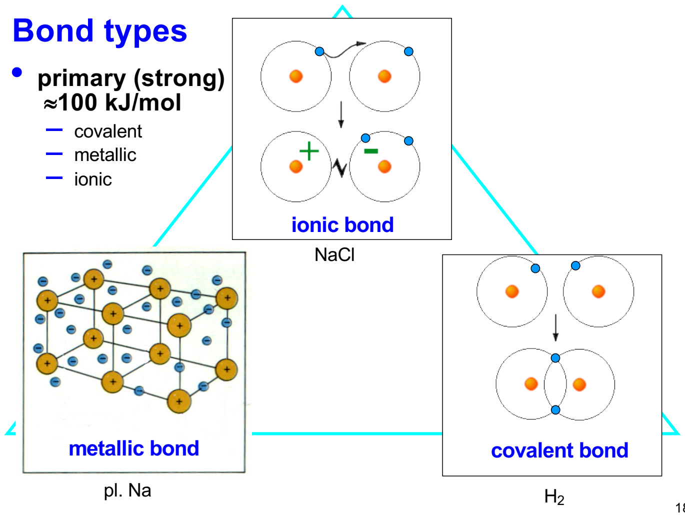
Bond types

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



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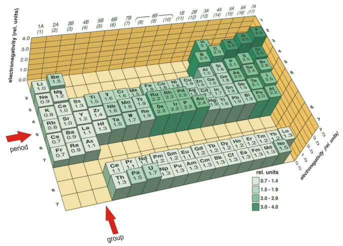

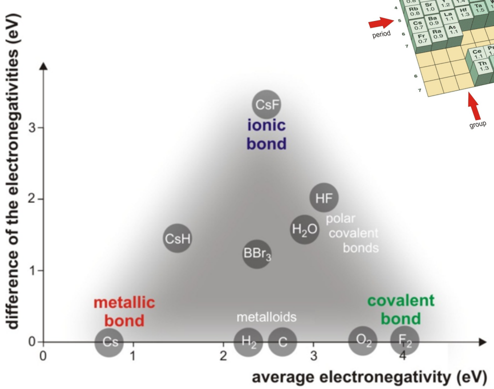

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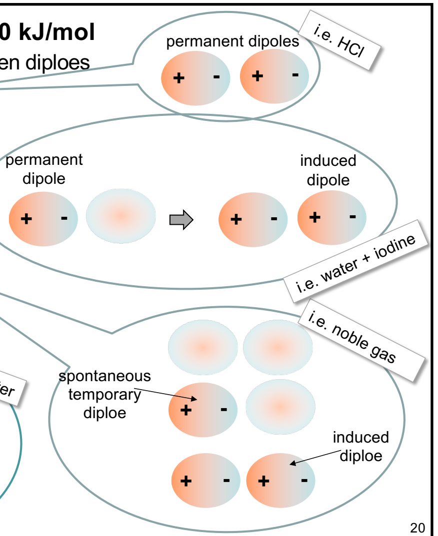
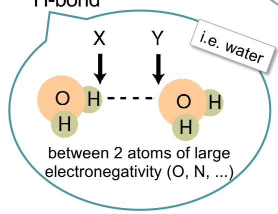
- **secondary (weak) ≈ 10 kJ/mol**
  - van der Waals - between diploes
    - orientation
    - induction
    - dispersion
  - H-bond





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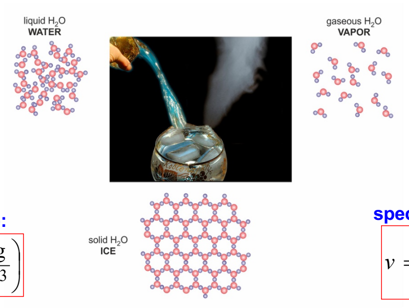
States of matter - Phases

T →

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



density (ρ):

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

specific volume (v):

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

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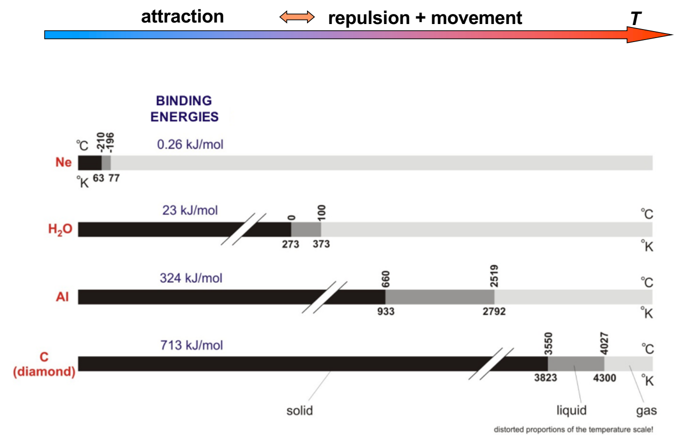

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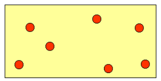
Gases



Macroscopic description:

- No definite volume or shape
- isotropic

p, V, n, T

$$pV = nRT$$

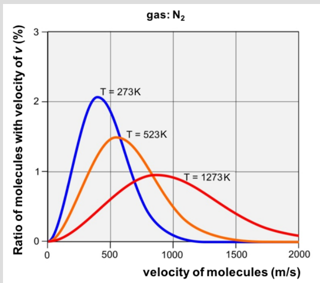
(ideal gas)

Microscopic description:

- random
- movement in many degrees of freedom

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

Maxwell-Boltzmann- distribution



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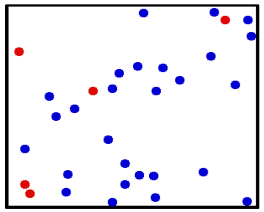
Temperature

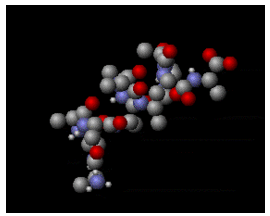
Temperature is a parameter proportional to the average kinetic energy available for each degree of freedom.

$$T(K) = t(°C) + 273$$

hot and cold gas particles



macromolecule



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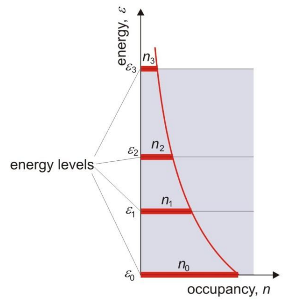
Boltzmann-distribution

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, n_0 —— ε_0, $\}\,\Delta\varepsilon$

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



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

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

$$R = k \cdot N_A$$

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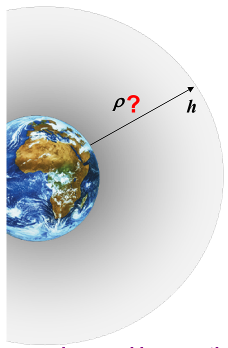
Gas in a force field – gravitation

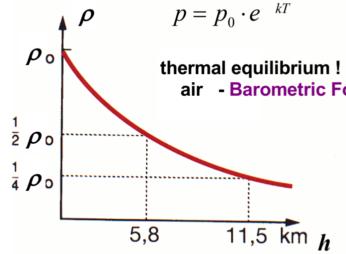
Example: density (ρ) of air ***changes*** in function of the potential energy

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

$$p = const * \rho$$

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





thermal equilibrium !
air - Barometric Formula

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

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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
- ...

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