

Biophysics I

5. Structure of matter Atoms, molecules, crystals

Liliom, Károly

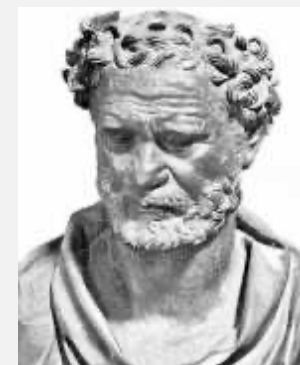
07. 10. 2022.

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karoly.liliom.mta@gmail.com

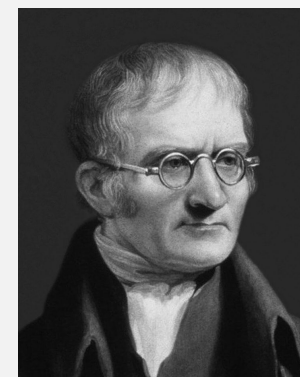
Development of the atom concept

Democritus (460–370 BC): everything is composed of "atoms," which are physically, but not geometrically, indivisible; that between atoms, there lies empty space; that atoms are indestructible, and have always been and always will be in motion.

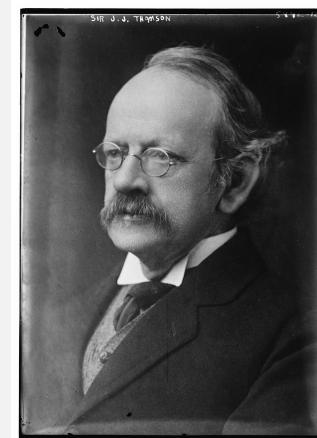
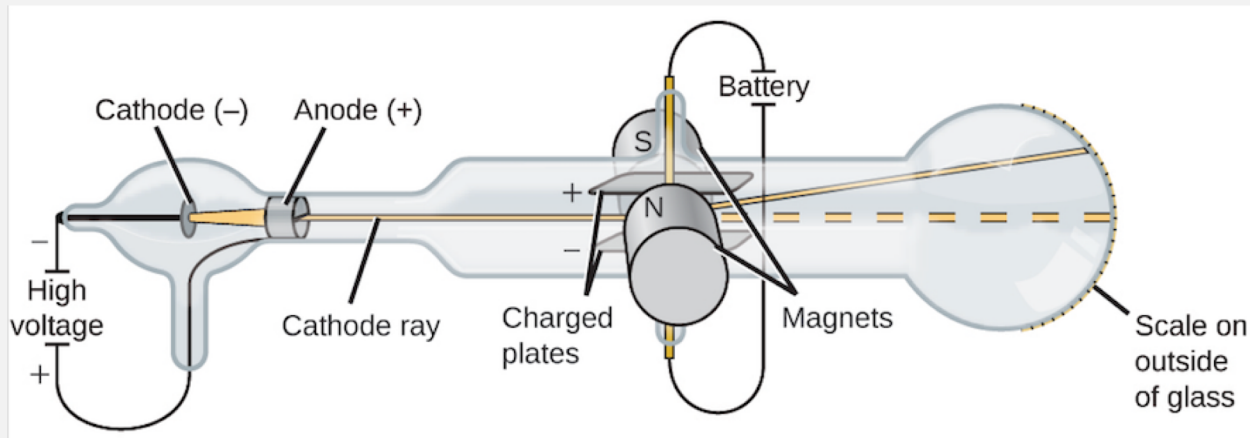
(greek *atomos* means uncuttable)



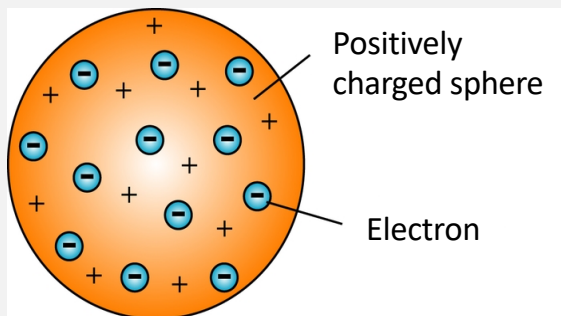
John Dalton (1803-1811) the law of multiple proportions: if the same two elements can be combined to form a number of different compounds, then the ratios of the masses of the two elements in their various compounds will be represented by small whole numbers – so elements react in multiples of some basic indivisible unit of mass.



Development of the atom concept

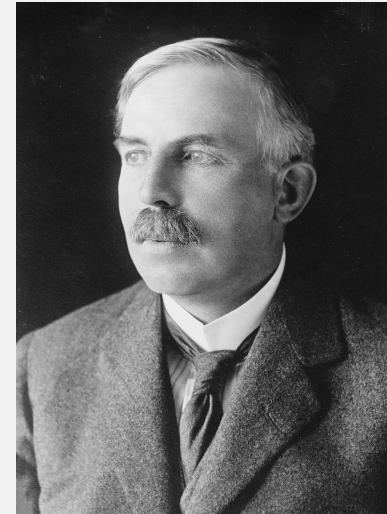
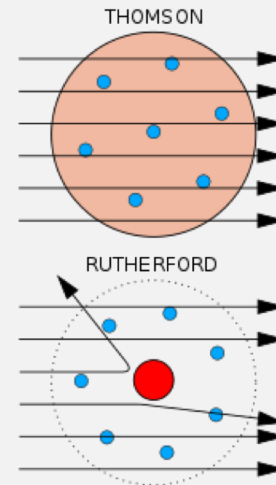
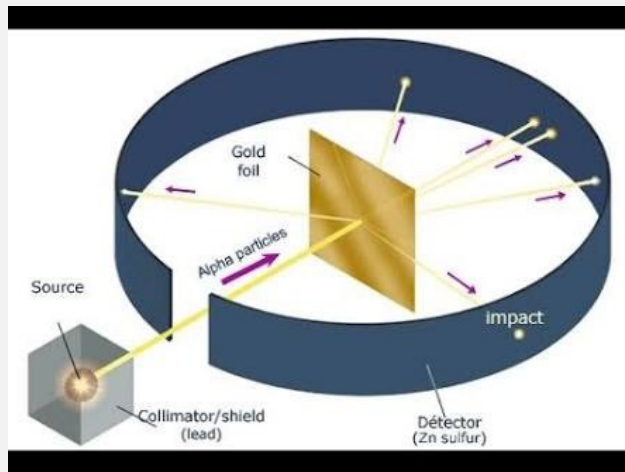


Joseph John Thomson (1897): Discovery of electrons by studying the cathode rays - identical particles with a mass $\sim 1/2000^{\text{th}}$ the mass of a H atom, independent of the cathode material – it must be the same constituent in all atoms.



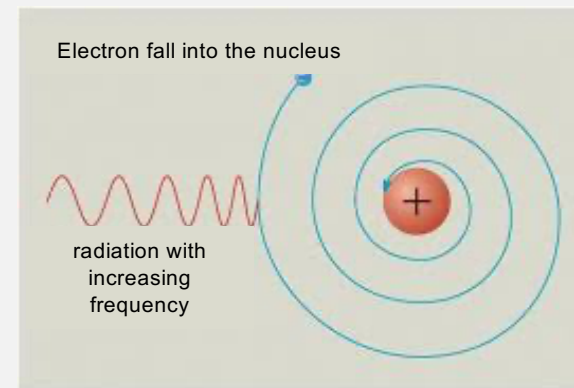
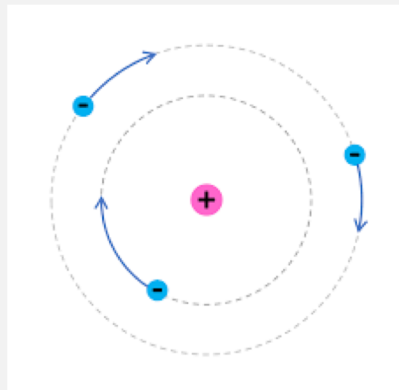
Joseph John Thomson "plum-pudding model" (1904): the positively charged main mass is distributed evenly in the atom, whereas the negatively charged small electrons are moving in it.

Development of the atom concept

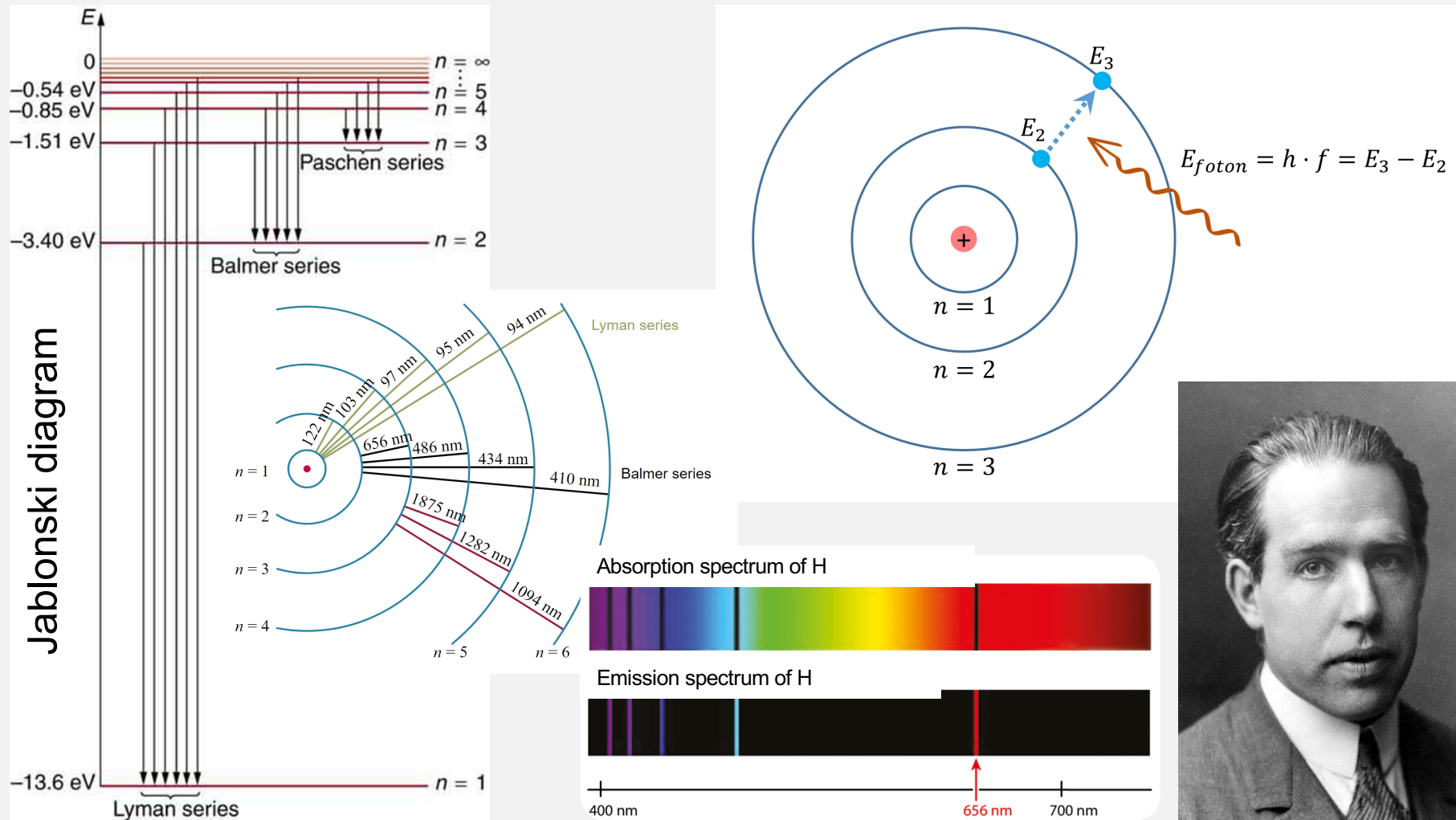


1909-1911: scattering of α -particles on gold

Ernest Rutherford (1911): the majority of mass of an atom is in a small central volume with positive charge (nucleus) and the electrons are orbiting around it in circles governed by the Coulomb interaction.

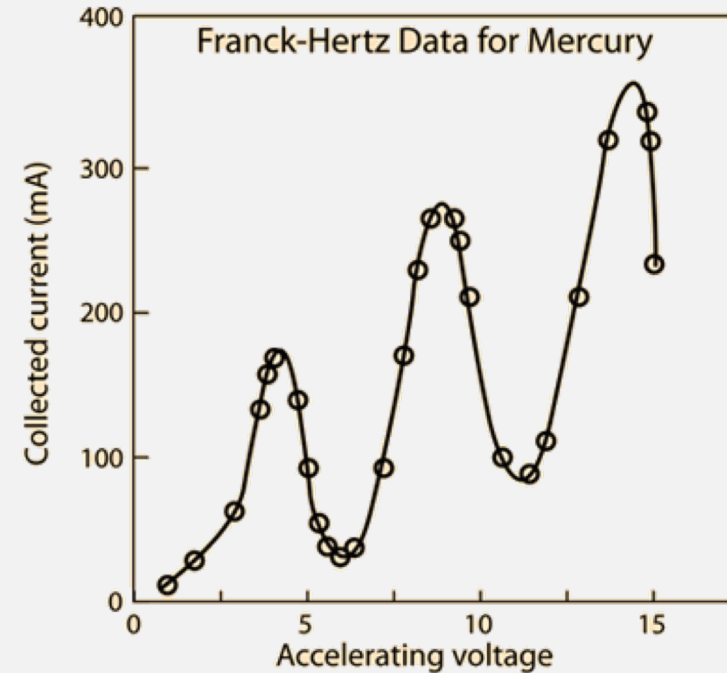
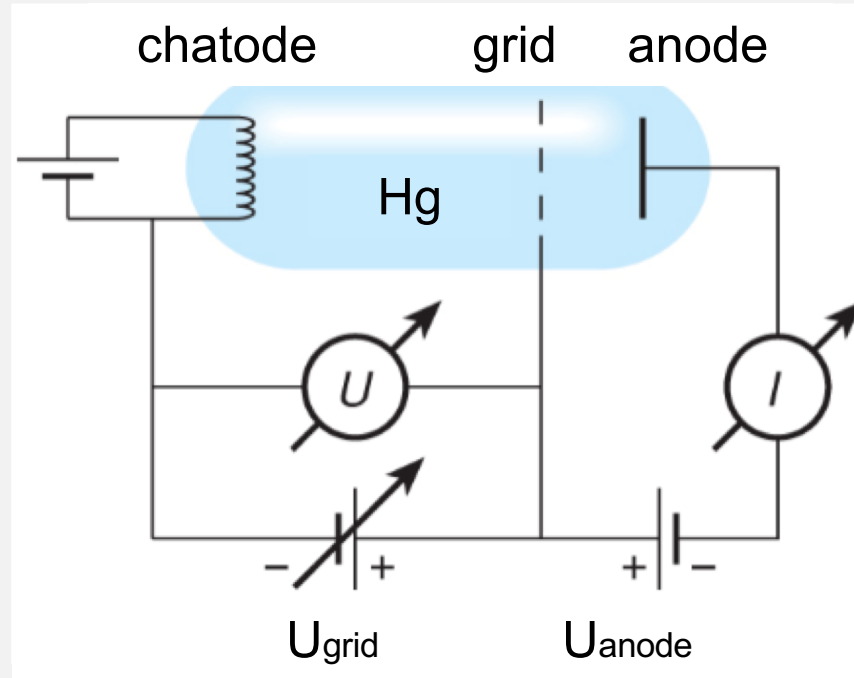


Development of the atom concept



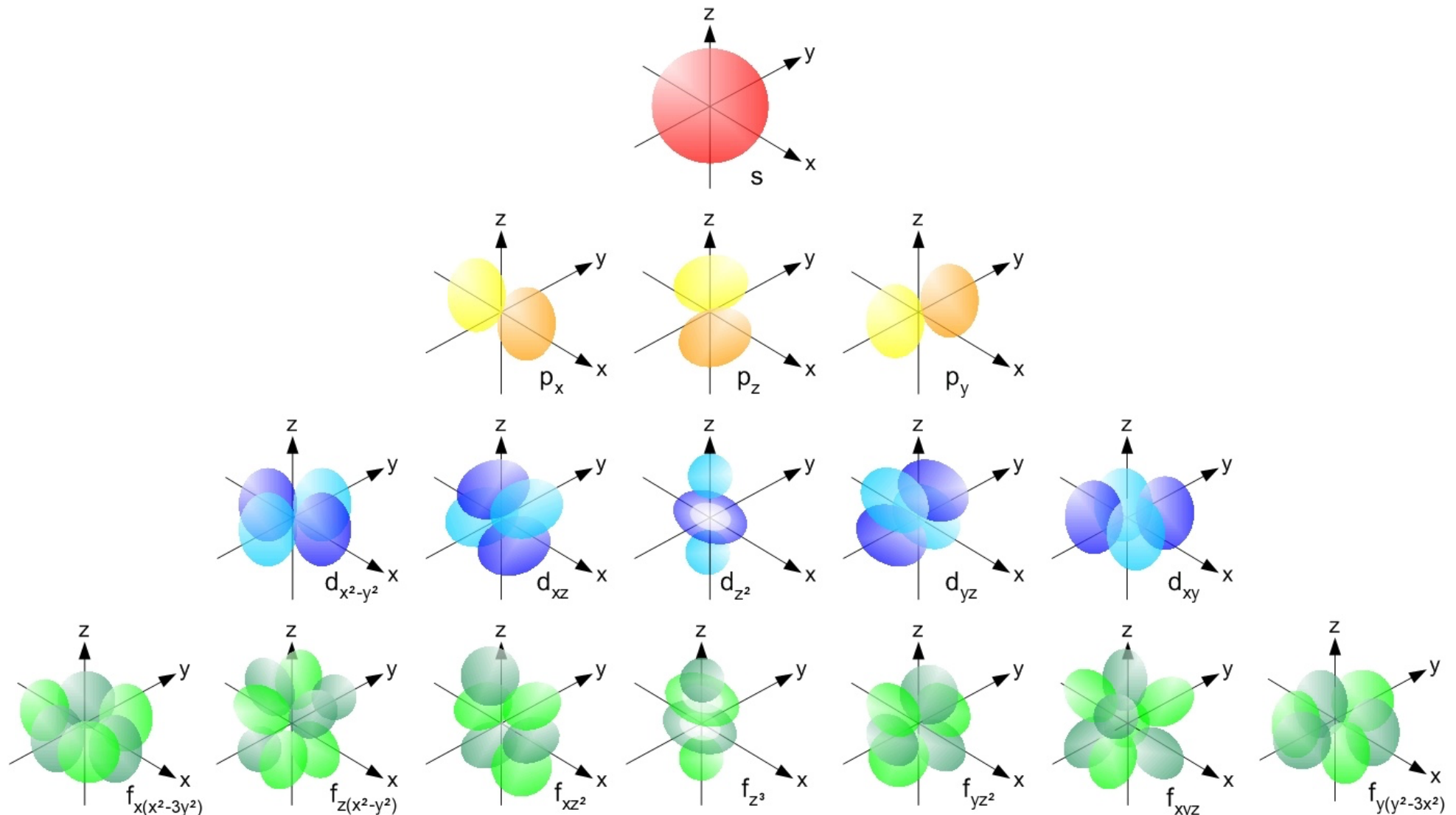
Niels Bohr (1913): There are stationary orbitals with well-defined (quantized) energy levels where electrons are not emitting radiations. Electrons can quantum-jump between these orbitals by absorbing or emitting the energy difference of the orbitals. The stationary orbitals are selected by the rule that the angular momentum is an integer multiple of $h/2\pi$.

Franck – Hertz experiment (1914)



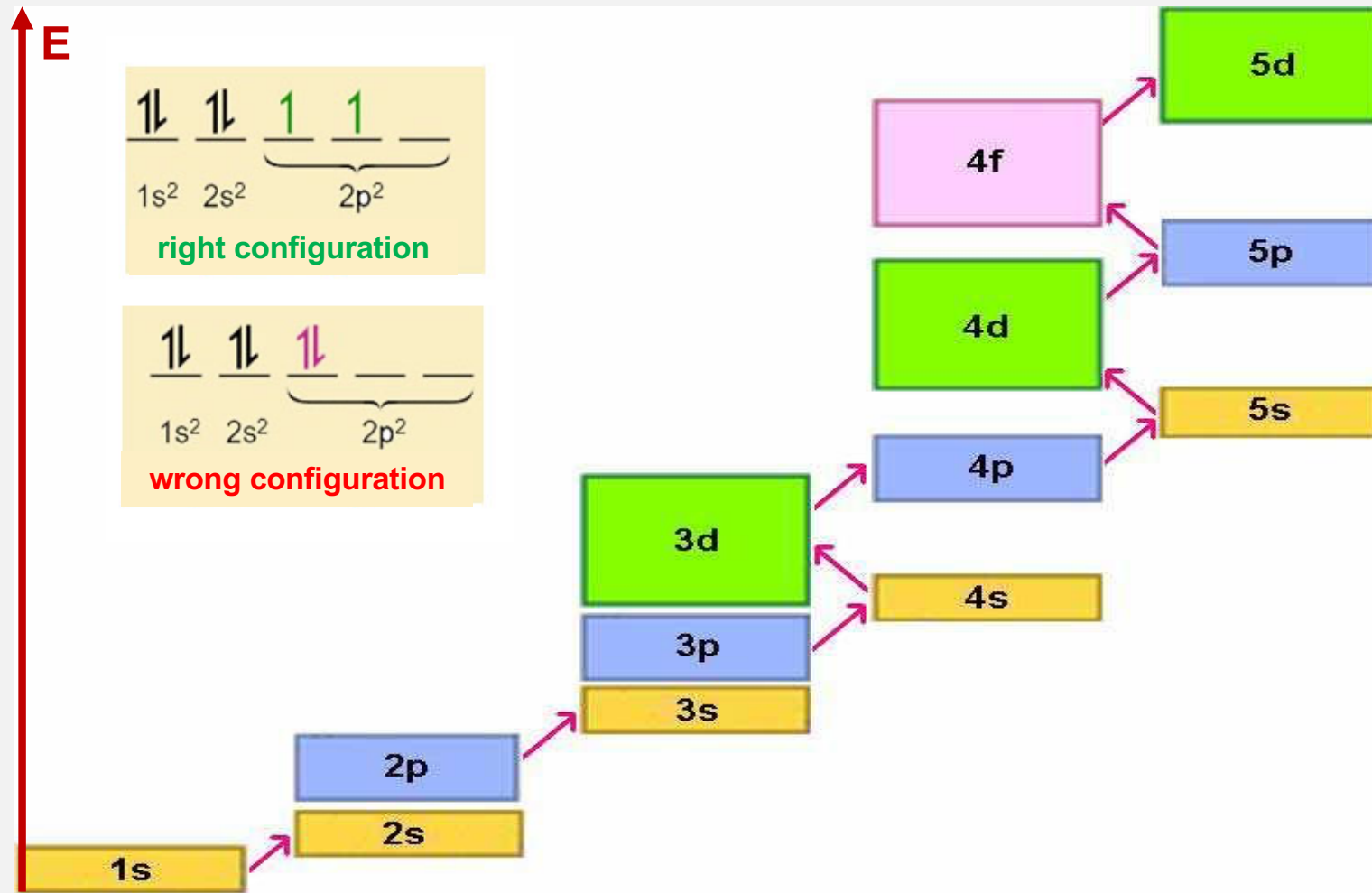
Electrons are colliding elastically with Hg atoms, until they get high enough energy, by increasing the grid voltage, to be able to excite the Hg atoms. At this accelerating voltage, the electrons lose their energy and are not able to reach the anode, so the current drops. Further increasing the accelerating voltage, the electrons collide again elastically until reaching the next energy level of the Hg atom, where they can excite the atoms again.

Development of the atom concept



Louis de Broglie: electron wave, Ervin Schrödinger: wavefunction, wave equation
4 quantum numbers (principal, azimuthal, magnetic and spin), Pauli principle.

Development of the atom concept



Pauli principle: in multi-electron systems all electrons are in different quantum states. As a consequence, there may be no two electrons within an atom or molecule with identical quantum numbers. **Hund's law:** in a given electron-configuration the lowest energy state is the one with the highest spin value (maximum multiplicity).

The Periodic Table of the Elements

group 1

1.00794

1

H

Hydrogen

3s¹

2

6.941

3

Li

Lithium

2s¹ 2s¹

3

9.012182

4

Be

Beryllium

1s² 2s²

11

22.98976

12

Na

Sodium

1s² 2s² 2p⁶ 3s¹

19

39.0983

20

K

Potassium

1s² 2s² 2p⁶ 3s² 3p⁶ 4s¹

37

85.4678

38

Rb

Rubidium

1s² 2s² 2p⁶ 3s² 3p⁶ 4s² 4p⁶ 5s¹

55

132.9054

56

Cs

Cesium

1s² 2s² 2p⁶ 3s² 3p⁶ 4s² 4p⁶ 5s² 5p⁶ 6s¹

87

(223)

Fr

Francium

1s² 2s² 2p⁶ 3s² 3p⁶ 4s² 4p⁶ 5s² 5p⁶ 6s² 6p⁶ 7s¹

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4.002602

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He

Helium

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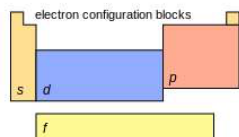
87

(223)

Fr

Francium

1s² 2s² 2p⁶ 3s² 3p



notes

- as of yet, elements 113, 115, 117 and 118 have no official name designated by the IUPAC.
- 1 kJ/mol = 96.485 eV.
- all elements are implied to have an oxidation state of zero.

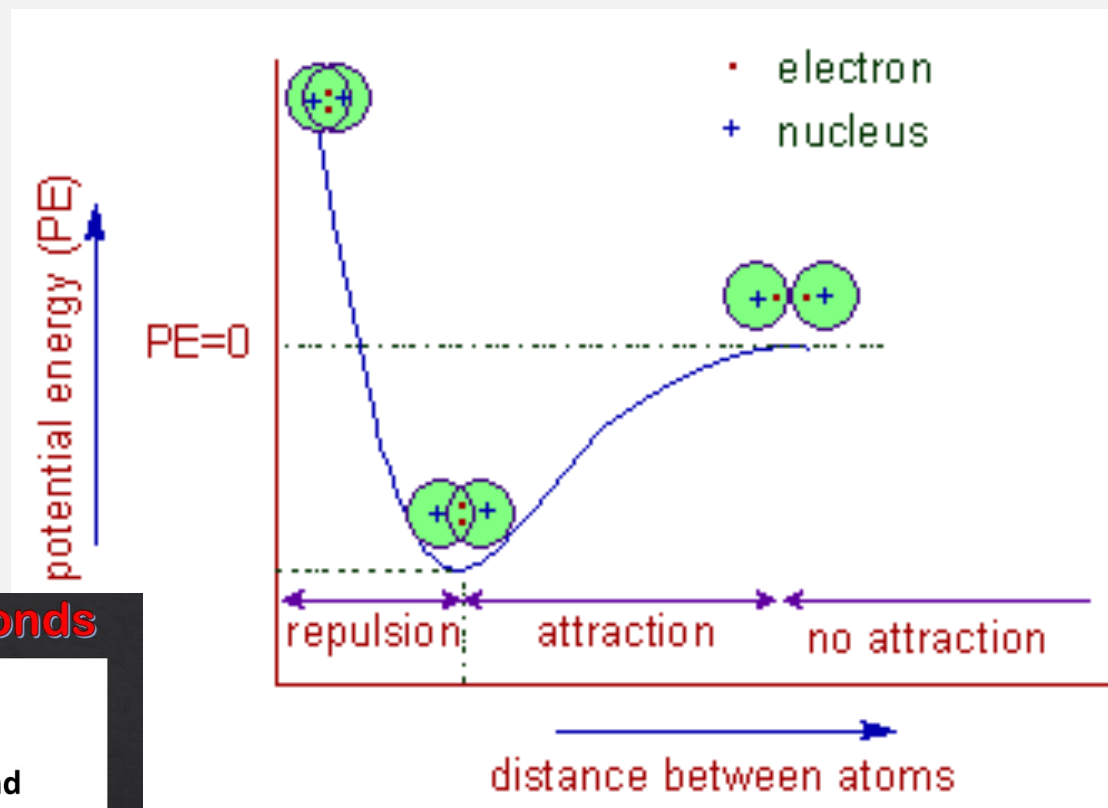
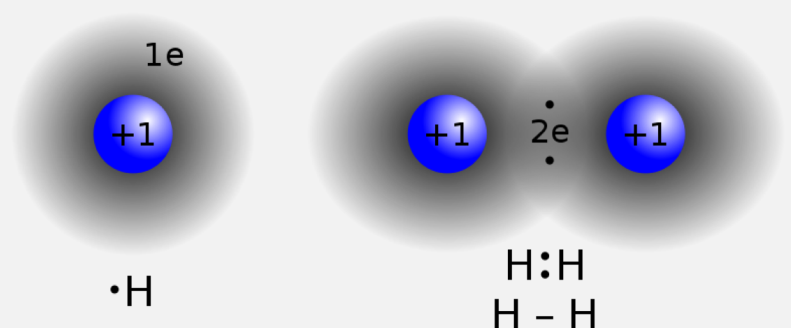
138.9054 57 La Lanthanum [Xe] 5d ¹ 6s ²	140.116 58 Ce Cerium [Xe] 4f ¹ 5d ¹ 6s ²	140.9076 59 Pr Praseodymium [Xe] 4f ³ 6s ²	144.242 60 Nd Neodymium [Xe] 4f ⁴ 6s ²	(145) 61 Pm Promethium [Xe] 4f ⁵ 6s ²	150.36 62 Sm Samarium [Xe] 4f ⁶ 6s ²	151.964 63 Eu Europium [Xe] 4f ⁷ 6s ²	157.25 64 Gd Gadolinium [Xe] 4f ⁷ 5d ¹ 6s ²	158.9253 65 Tb Terbium [Xe] 4f ⁹ 6s ²	162.500 66 Dy Dysprosium [Xe] 4f ¹⁰ 6s ²	164.9303 67 Ho Holmium [Xe] 4f ¹¹ 6s ²	167.259 68 Er Erbium [Xe] 4f ¹² 6s ²	168.9342 69 Tm Thulium [Xe] 4f ¹³ 6s ²	173.054 70 Yb Ytterbium [Xe] 4f ¹⁴ 6s ²
(227) 89 Ac Actinium [Rn] 6d ¹ 7s ²	232.0380 90 Th Thorium [Rn] 6d ² 7s ²	231.0358 91 Pa Protactinium [Rn] 5f ² 6d ¹ 7s ²	238.0289 92 U Uranium [Rn] 5f ³ 6d ¹ 7s ²	(237) 93 Np Neptunium [Rn] 5f ⁴ 6d ¹ 7s ²	(244) 94 Pu Plutonium [Rn] 5f ⁶ 7s ²	(243) 95 Am Americium [Rn] 5f ⁷ 7s ²	(247) 96 Cm Curium [Rn] 5f ⁷ 6d ¹ 7s ²	(247) 97 Bk Berkelium [Rn] 5f ⁹ 7s ²	(251) 98 Cf Californium [Rn] 5f ¹⁰ 7s ²	(252) 99 Es Einsteinium [Rn] 5f ¹¹ 7s ²	(257) 100 Fm Fermium [Rn] 5f ¹² 7s ²	(258) 101 Md Mendelevium [Rn] 5f ¹³ 7s ²	(259) 102 No Nobelium [Rn] 5f ¹⁴ 7s ²

Valence electrons (electrons of *s* and *p* subshells of the most outer shell) are determining the chemical nature and reactivity of the elements/atoms.

Primary chemical bonds

covalent, ionic, metallic

Covalent bond involves the sharing of electron pairs between atoms.



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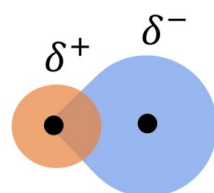
Polar and non-polar bonds

Non-polar
covalent bond



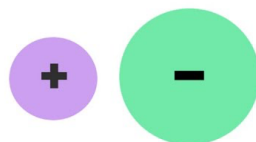
Equal sharing of
electrons

Polar covalent
bond



Unequal sharing
of electrons

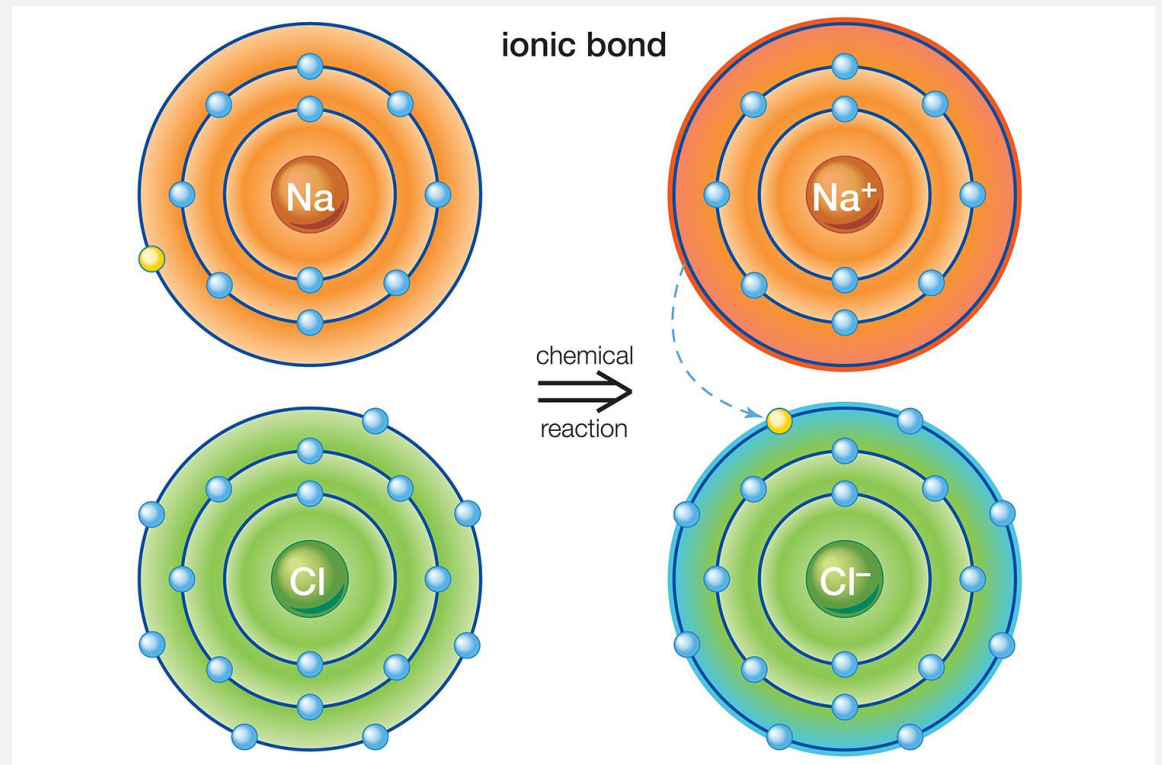
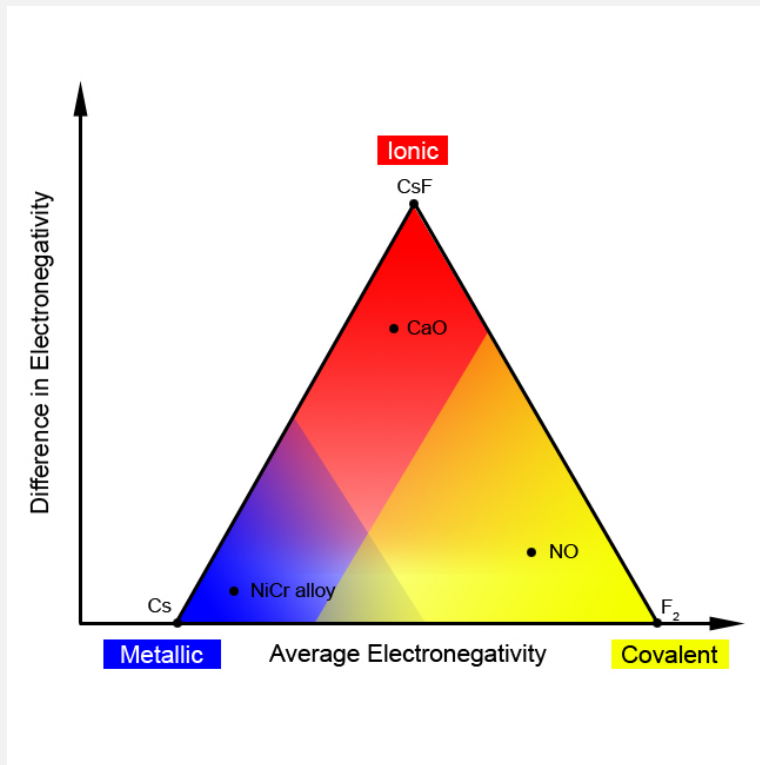
Ionic bond



No sharing of
electrons in bond

Increasing difference in electronegativity

Primary chemical bonds



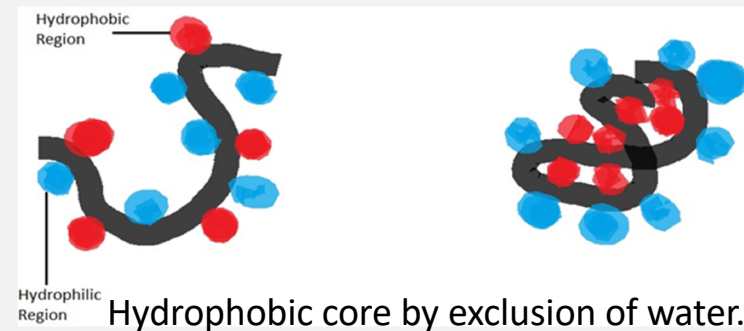
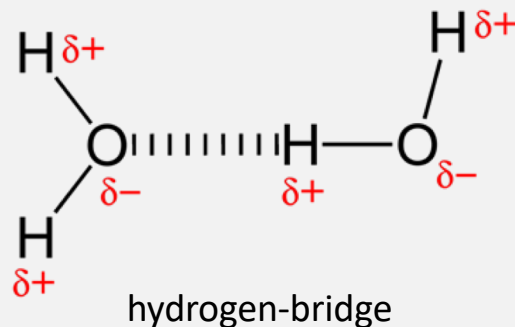
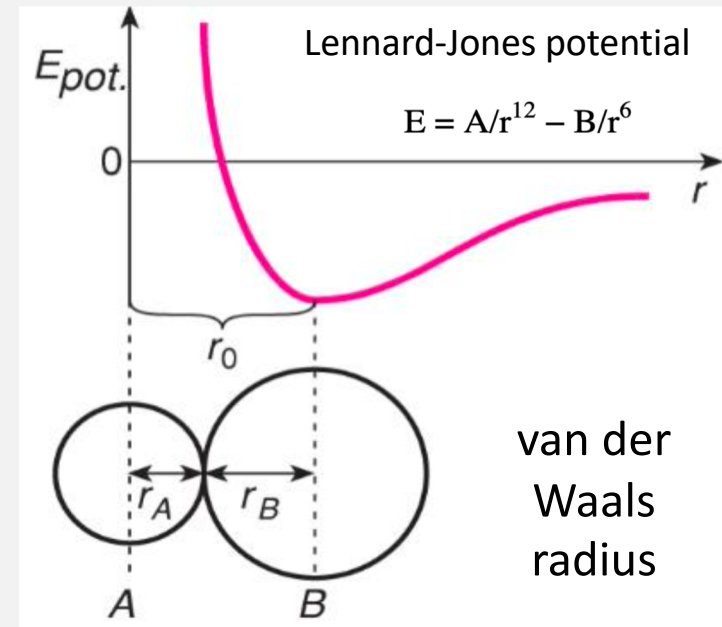
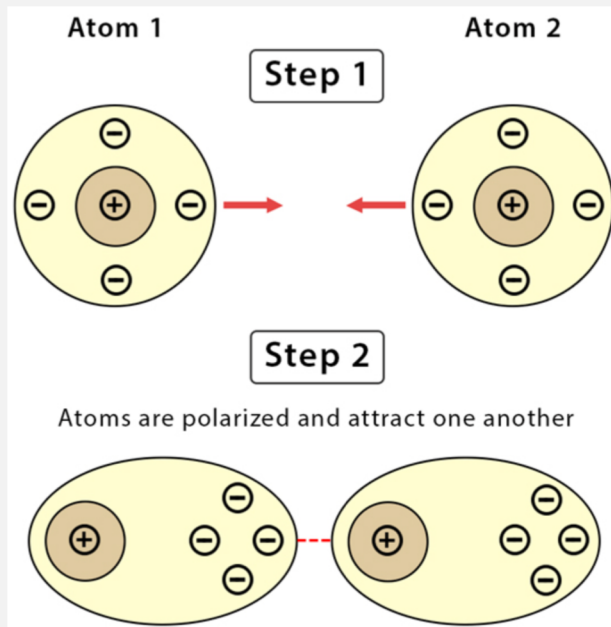
Elektronegativity (Linus Pauling): sum of the energies needed to produce a positive and a negative ion from an element.

Ionic bond: if there is a great difference in electronegativity of the atoms (*e.g.* NaCl).

Metallic bond: there is an ordered, periodic lattice of the positive ions. The electrons are delocalized, stabilizing the whole structure.

Secondary interactions

dipole-dipole, van der Waals, H-bridge, hydrophobic
weaker by one-two orders of magnitude

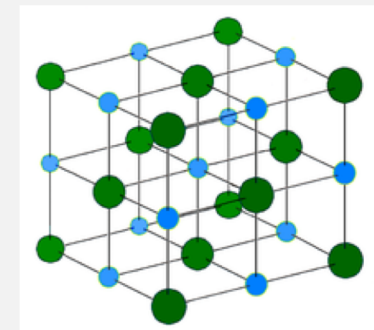
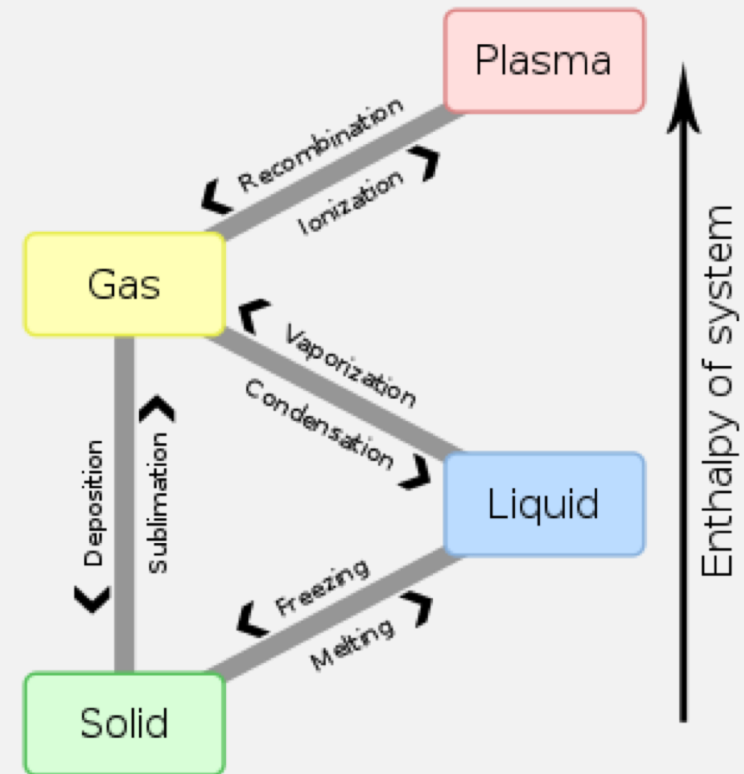


Phases of matter

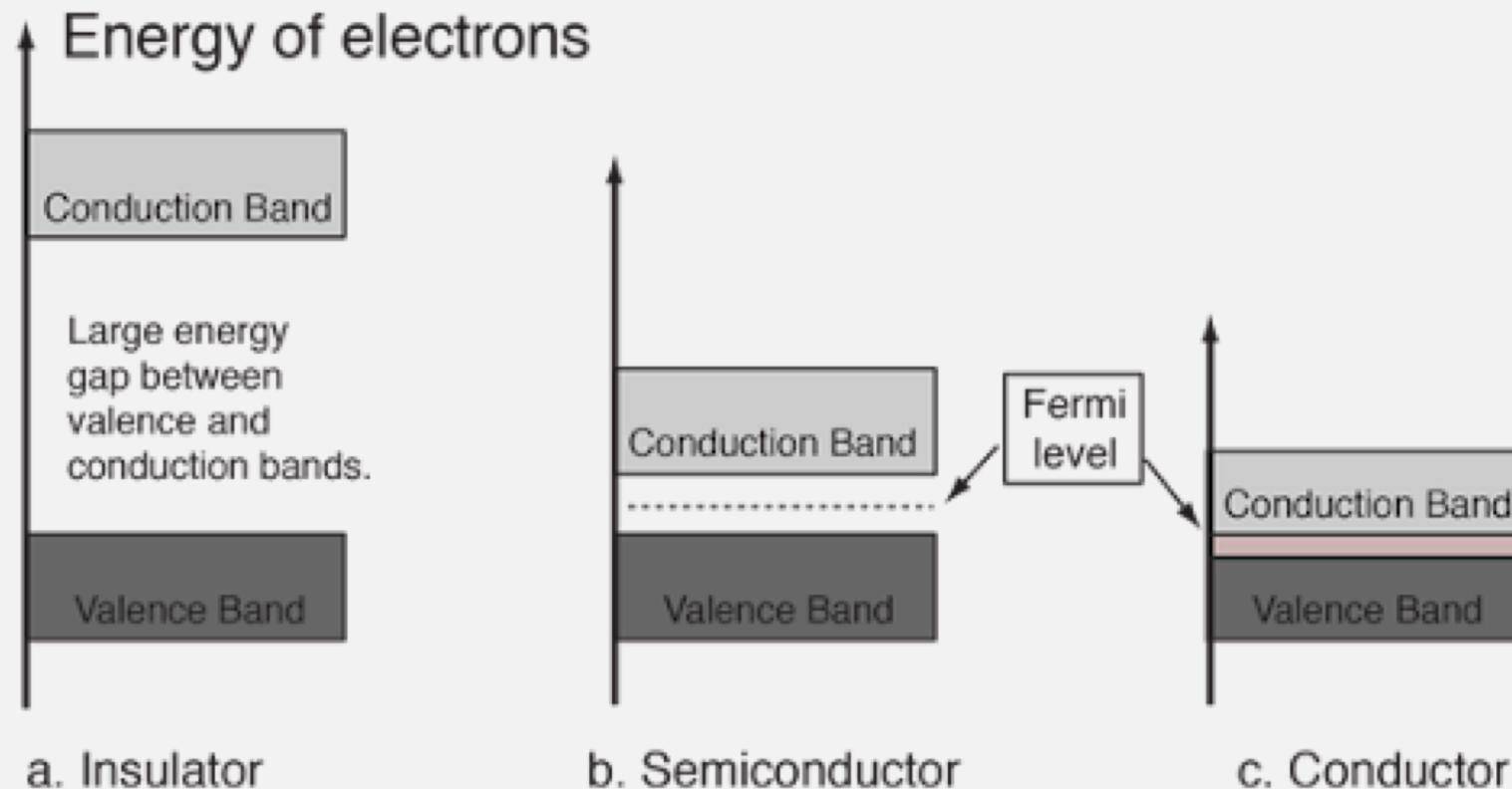
Gases: the particles are moving independently, colliding with each other and with the wall of the container. Ideal gas: the particles are point-like without a volume.

Liquids: there are only short-range order which is dynamic in nature. Particles can roll on each other. A liquid is a nearly incompressible fluid that conforms to the shape of its container but retains a constant volume independent of the pressure. Liquids are usually isotropic.

Crystalline materials: long-range, periodic order exists with many repetition of an elementary cell. Anisotropic.



Band structures of crystals



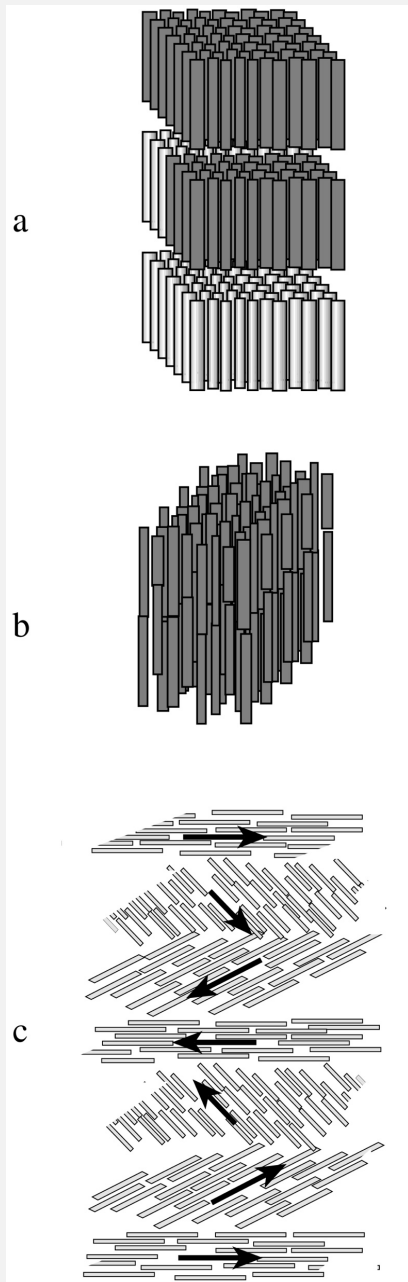
Energy gap between valence and conduction bands is called forbidden gap. Fermi energy is a hypothetical energy level for the electrons, related to a 50% occupancy.

If the energy gap is bigger than $>3,1$ eV, the maximum photon energy of a visible light, then the crystal is transparent. Conductors are non-transparent as there are electrons in the conduction band which can absorb visible photon energies.

Liquid crystal phases

Mesophases can be characterized by the type of ordering. One can distinguish positional order (whether molecules are arranged in any sort of ordered lattice) and orientational order (whether molecules are mostly pointing in the same direction).

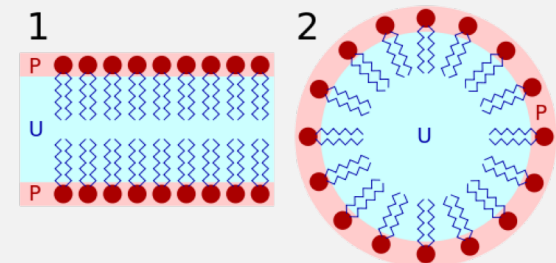
- a) smectic phase: both ordering are present
- b) nematic phase: only the orientational ordering is present
- c) cholesteric or twisted nematic phase: a chiral order can be observed due to a fixed angle rotation of asymmetric molecules in the adjacent layers



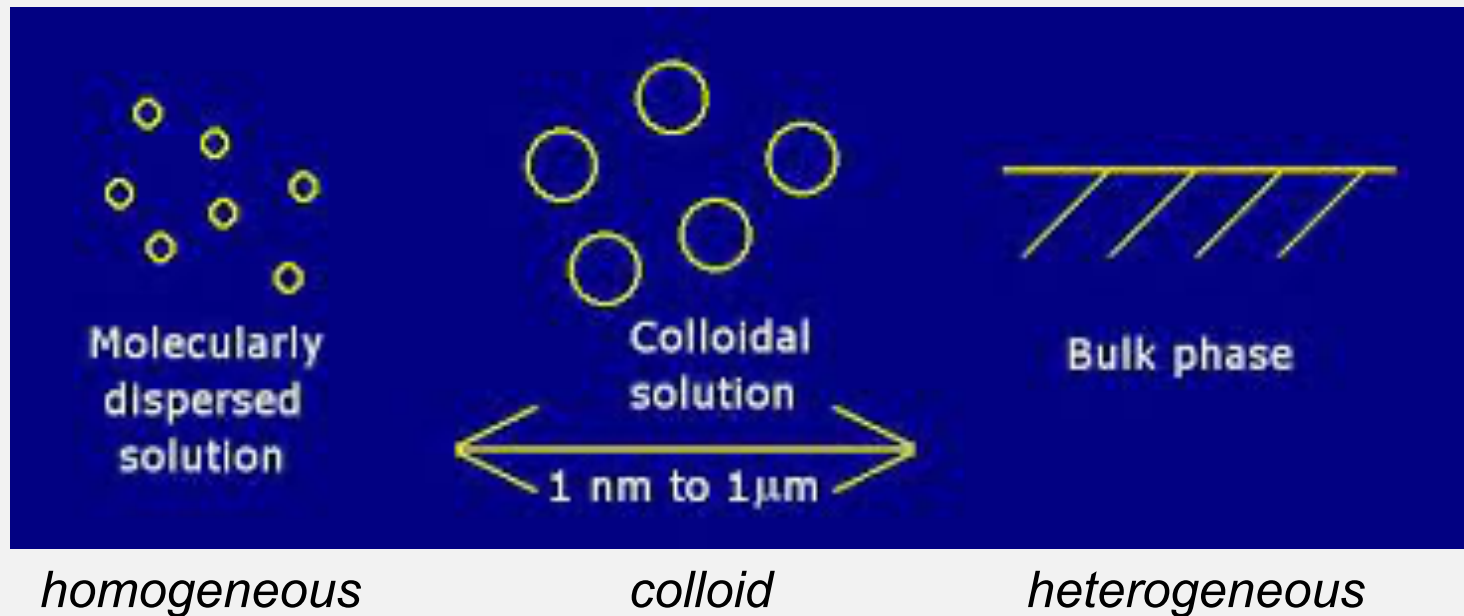
Thermotropic liquid crystals: the ordering depends on the temperature, present only in a certain temperature range.

Lyotropic liquid crystals: the ordering can be observed in certain concentration range, characteristic for amphiphilic molecules.

1) bilayers, 2) micelles



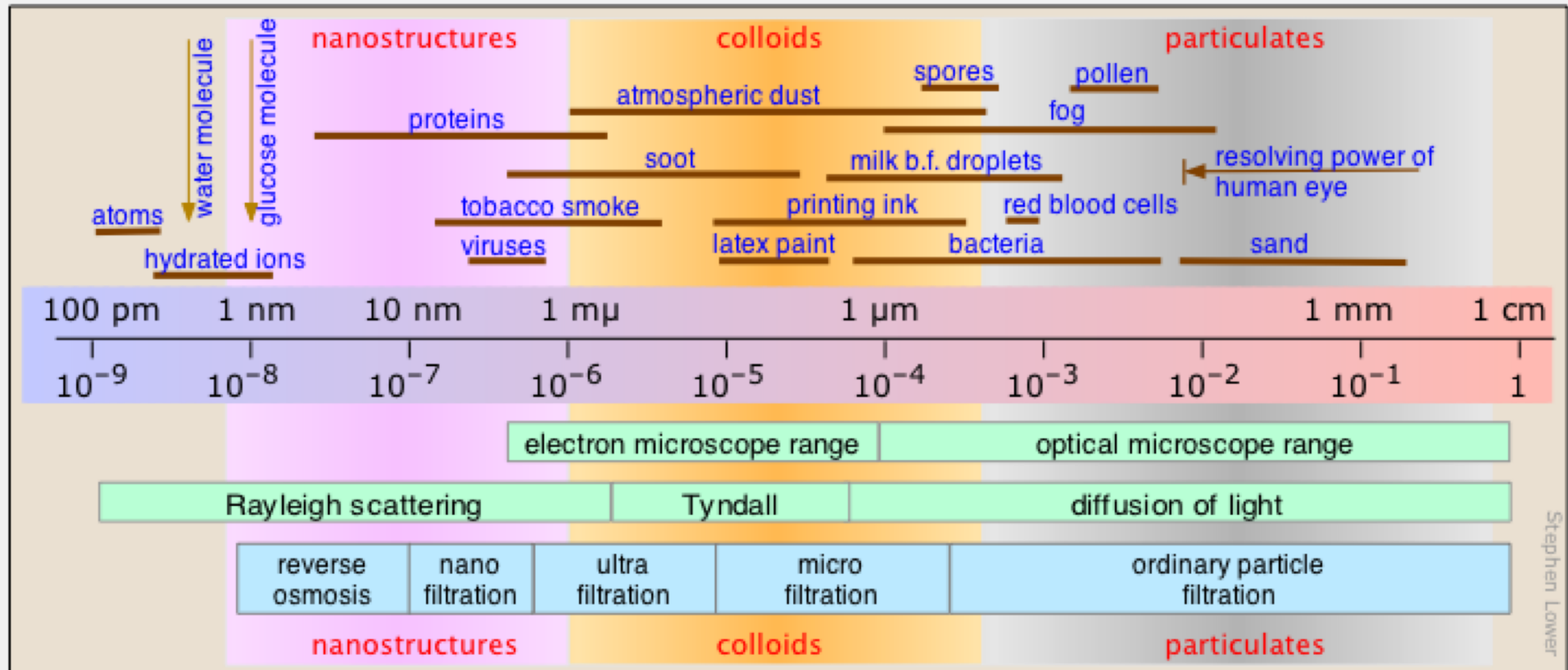
Colloid state



If particulate matter is dispersed in a homogeneous medium the way that particles have real surfaces (there are inner molecules in the particles which are not in contact with the dispersion medium) then we call this state as colloid phase. Many important biological molecule is forming colloids, like macromolecular colloids (proteins, polysaccharides), or association colloids like cell membranes.

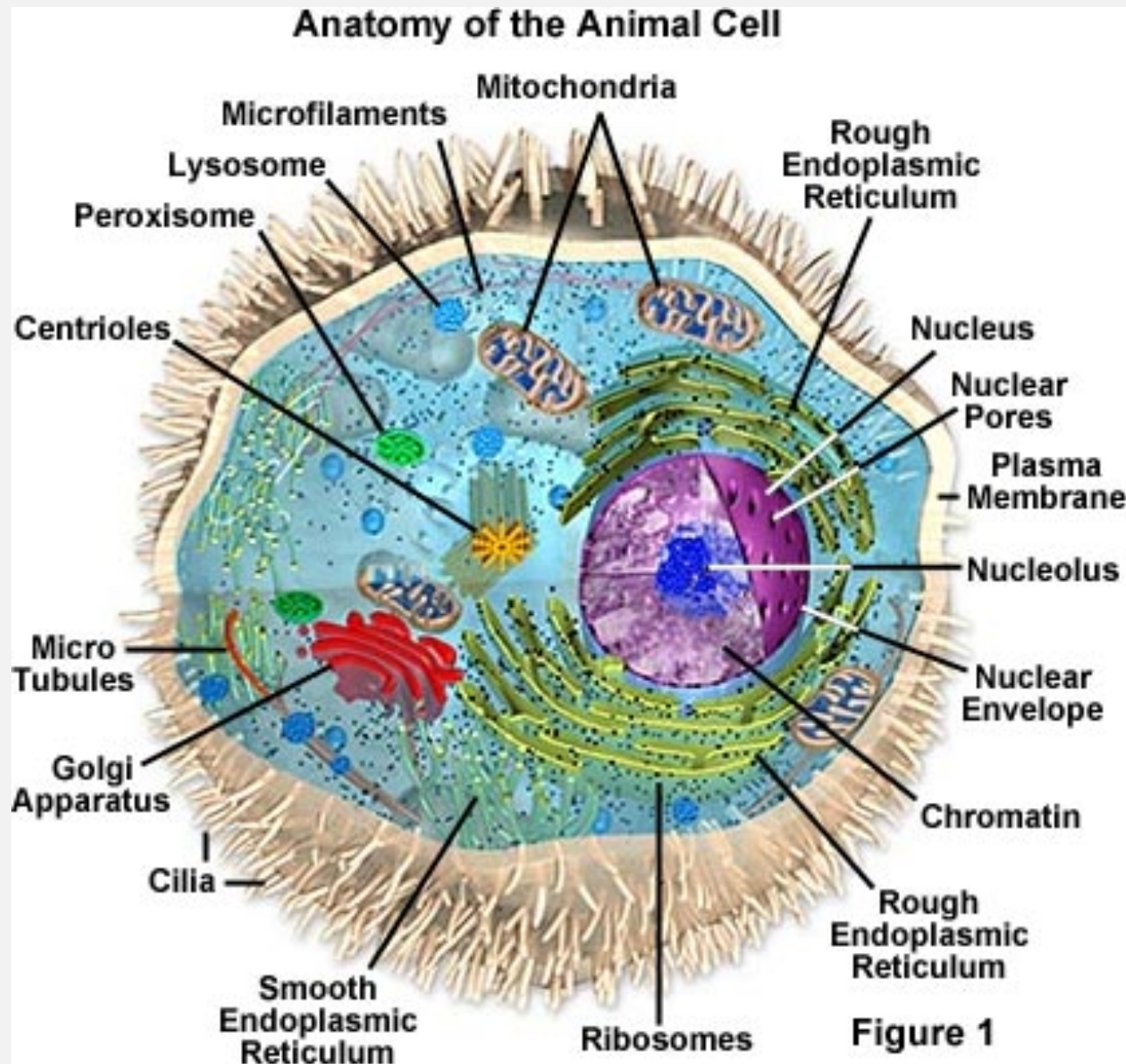
A colloid consists of two distinct phases, a continuous phase (the dispersion medium) and a particulate phase, where the particles generally have dimensions ranging between 2 and 200 nm. The two phases can be liquid-in-liquid (milk), solid-in-liquid (paint), liquid-in-gas (aerosol) and other combinations.

Typical colloid sizes



Any matter can form colloids. The colloid state depends only on particle sizes, independently of chemical compositions or material characteristics.

Many biological materials are colloids



Checklist

developing models of atom

quantized energy levels

Franck-Hertz experiment

Spectrum of the H atom

quantum numbers

Pauli principle

Hund's low

bond types

gas, liquid, solid states

liquid crystals

colloids

Related chapters in
Damjanovich, Fidy, Szöllősi: Medical Biophysics

I. chapter

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1.1.2	3.2.1
1.2.1	3.3.1
1.2.2	3.3.2
1.3.1	3.3.3
1.3.3	3.4.1
1.4.1	3.4.2
1.4.2	4.1.1
1.4.3	4.1.2
2.1.1	4.1.3
2.1.2	
2.1.3	
2.1.4	
2.1.5	