

Biophysics I

5. Structure of matter *Atoms, molecules, crystals*

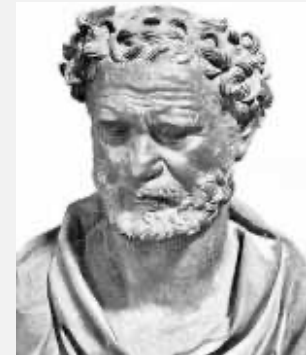
Károly LILIOM

04. 10. 2024.

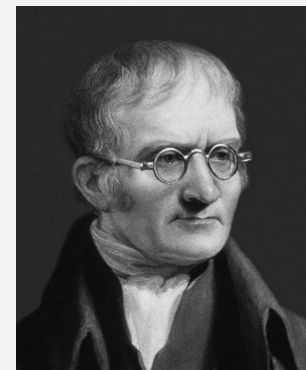
karoly.liliom.mta@gmail.com

Development of the atom concept

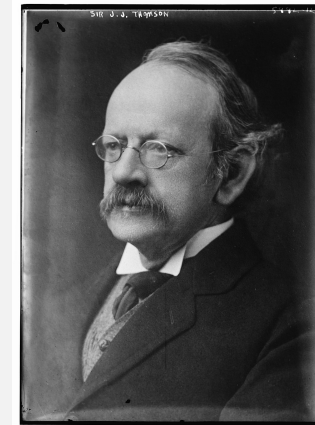
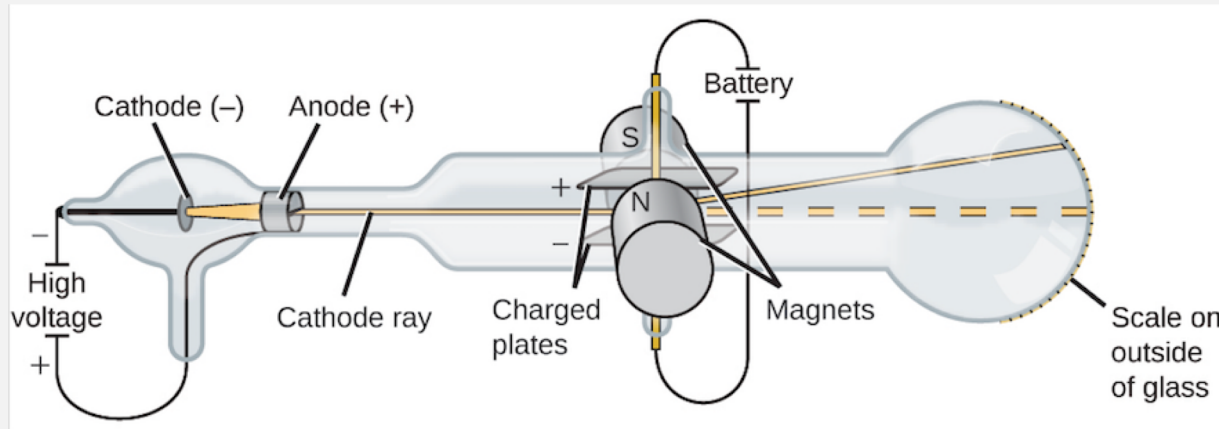
Democritus (460–370 BC): everything is composed of "atoms," which are physically, but not geometrically, indivisible; that between atoms, there lies empty space; that atoms are indestructible, and have always been and always will be in motion.
(greek *atomos* means uncuttable)



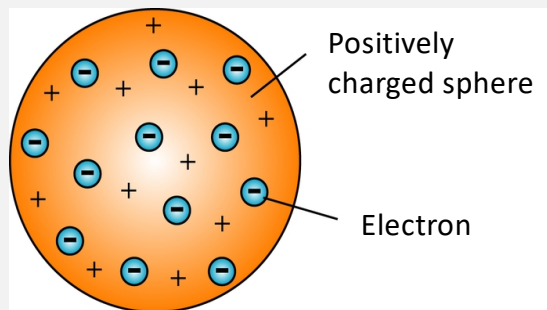
John Dalton (1803-1811) the law of multiple proportions: if the same two elements can be combined to form a number of different compounds, then the ratios of the masses of the two elements in their various compounds will be represented by small whole numbers – so elements react in multiples of some basic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



Development of the atom concept

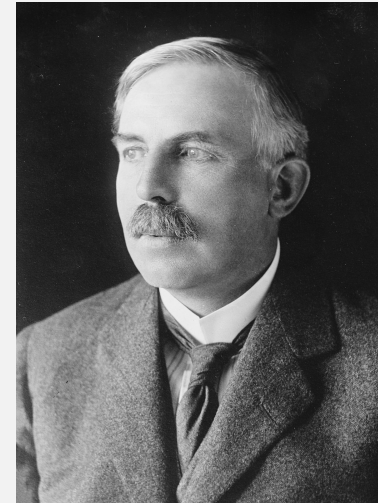
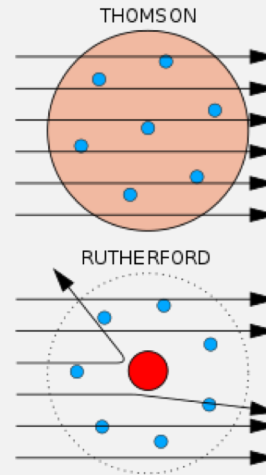
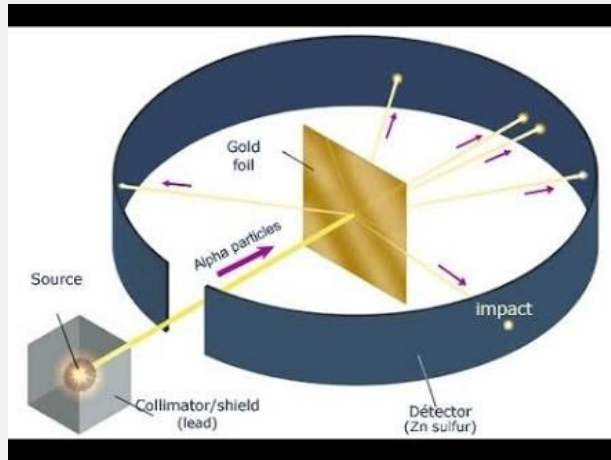


Joseph John Thomson (1897): Discovery of electrons by studying the cathode rays - identical particles with a mass $\sim 1/2000^{\text{th}}$ the mass of a H atom, independent of the cathode material – it must be the same constituent in all atoms.



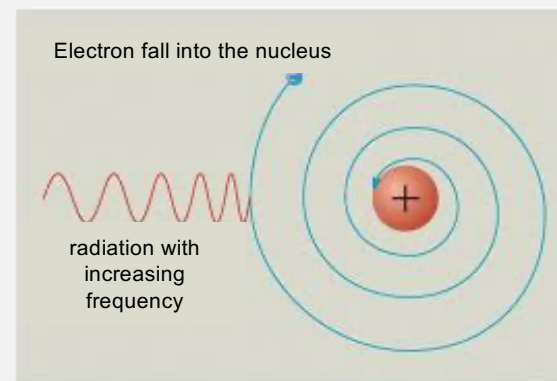
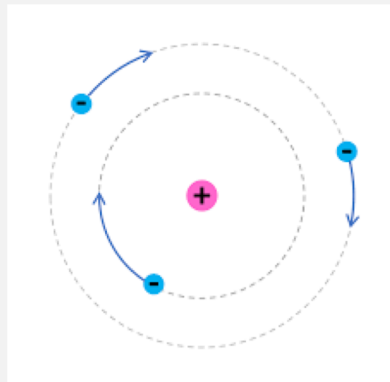
Joseph John Thomson "plum-puding model" (1904): the positively charged main mass is distributed evenly in the atom, whereas the negatively charged small electrons are moving in it.

Development of the atom concept

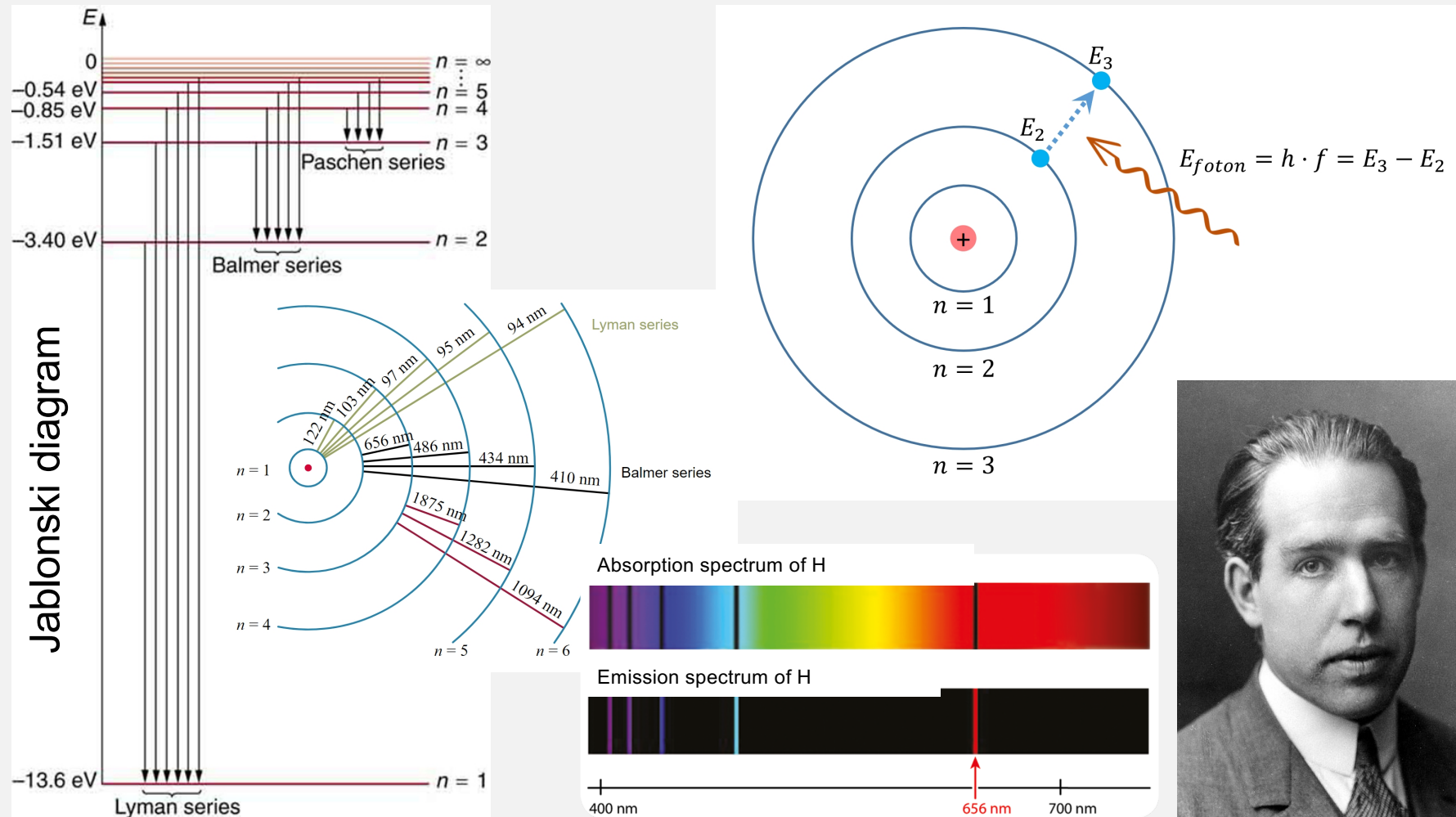


1909-1911: scattering of α -particles on gold

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.

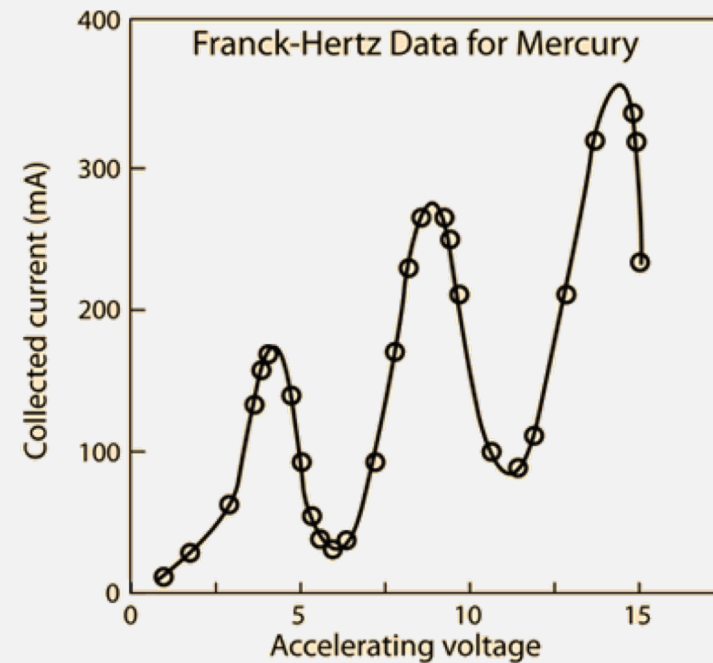
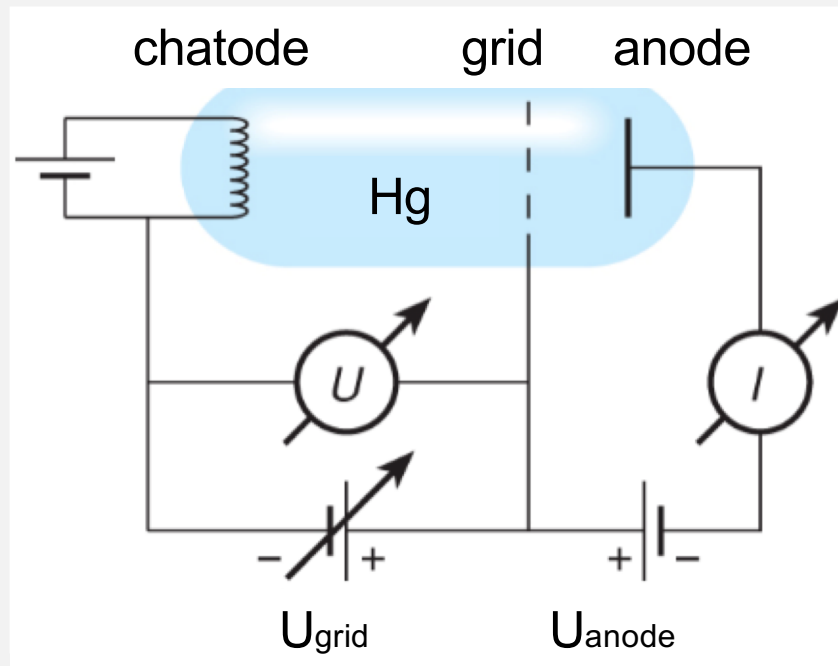


Development of the atom concept



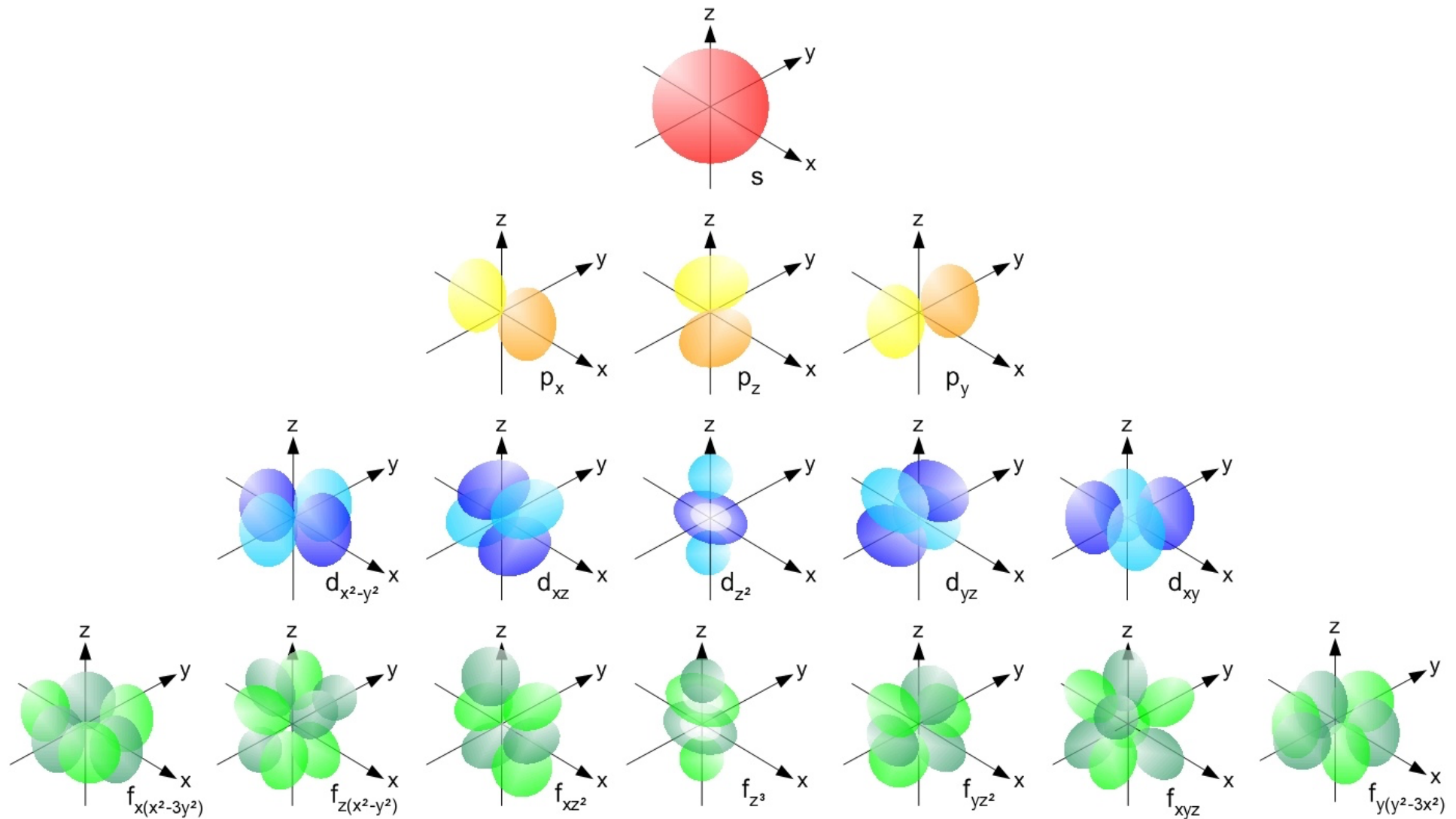
Niels Bohr (1913): There are stationary orbitals with quantized energy levels where electrons are not emitting radiations. Electrons can quantum-jump between these orbitals by absorbing or emitting the energy difference of the orbitals. The stationary orbitals are selected by the rule that the angular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

Franck – Hertz experiment (1914)



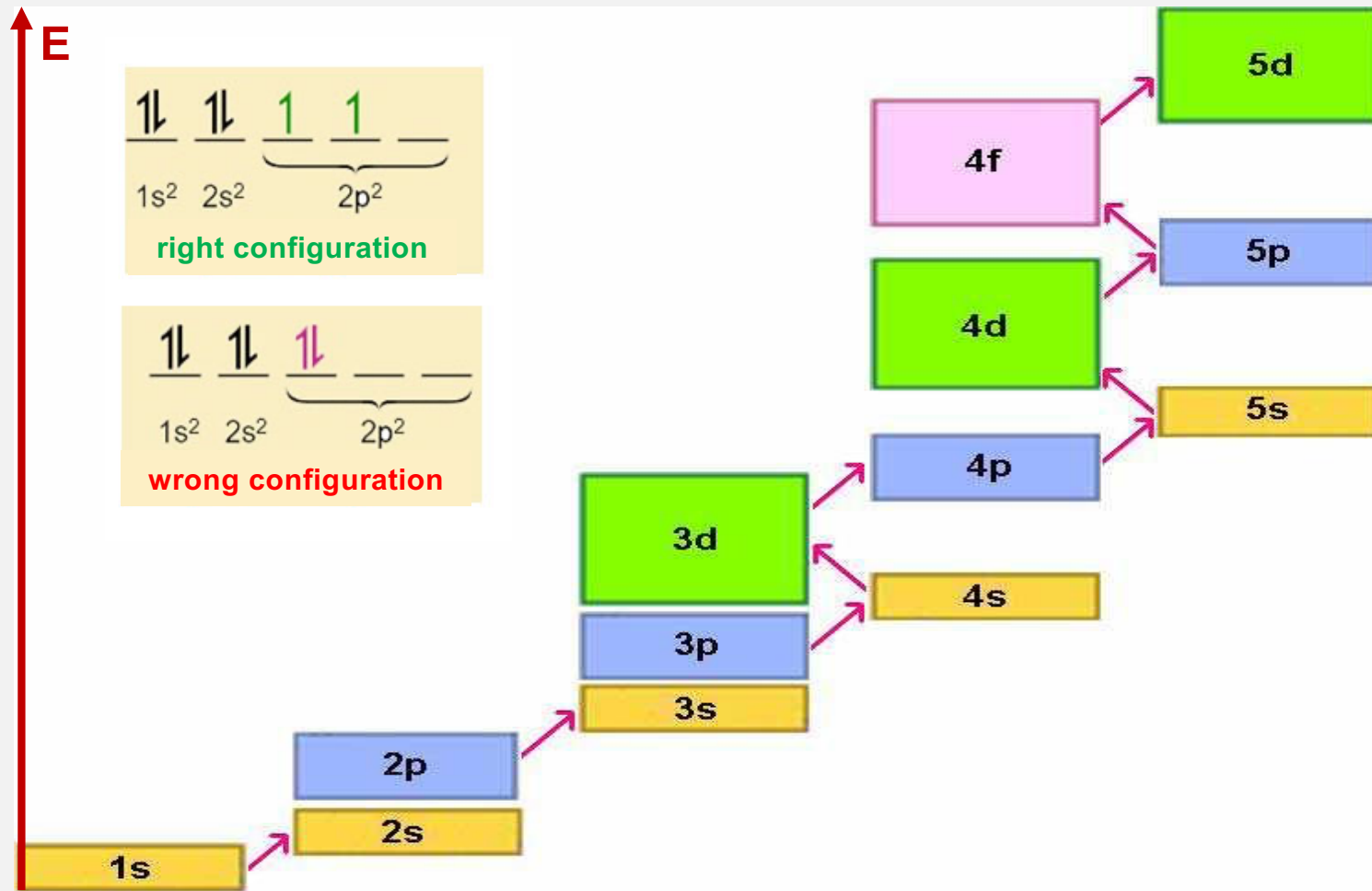
Electrons are colliding elastically with Hg atoms, until they get high enough energy, by increasing the grid voltage, to be able to excite the Hg atoms. At this accelerating voltage, the electrons lose their energy and are not able to reach the anode, so the current drops. Further increasing the accelerating 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 4 quantum numbers. **Hund's law:** in a given electron-configuration the lowest energy state is the one with the highest spin value (maximum multiplicity).

group 1

1

1.00794

1310.0

2.20

-1

1

H

Hydrogen

1s¹

2

6.941

520.2

0.98

-1

2

Li

Lithium

1s² 2s¹

3

9.012182

999.5

1.57

-2

3

Be

Beryllium

1s² 2s²

4

22.98976

405.8

0.93

-1

4

Na

Sodium

[Ne] 3s¹

5

24.3050

737.7

1.31

-1

5

Mg

Magnesium

[Ne] 3s²

atomic mass
or most stable mass number

1st ionization energy
in kJ/mol

chemical symbol

name

electron configuration

55.845

762.5

1.83

26

Fe

Iron

[Ar] 3d⁶ 4s²

atomic number

electronegativity

oxidation states
most common are bold

alkali metals

alkaline metals

other metals

transition metals

lanthanoids

actinoids

metalloids

nonmetals

halogens

noble gases

unknown elements

radioactive elements have
masses in parentheses

13

10.811

800.5

2.04

-2

5

B

Boron

1s² 2s² 2p¹

14

12.0107

1086.5

2.25

-2

6

C

Carbon

1s² 2s² 2p²

15

14.0067

1402.3

3.04

-2

7

N

Nitrogen

1s² 2s² 2p³

16

15.9994

1313.9

3.44

-2

8

O

Oxygen

1s² 2s² 2p⁴

17

18.998403

1681.0

3.98

-1

9

F

Fluorine

1s² 2s² 2p⁵

18

20.1797

2081.0

3.98

-1

10

Ne

Neon

1s² 2s² 2p⁶

13

26.98153

577.5

1.61

-2

13

Al

Aluminium

[Ne] 3s² 3p¹

14

28.0855

786.5

1.90

-2

14

Si

Silicon

[Ne] 3s² 3p²

15

30.97696

1011.8

2.19

-2

15

P

Phosphorus

[Ne] 3s² 3p³

16

32.065

999.6

2.20

-2

16

S

Sulfur

[Ne] 3s² 3p⁴

17

35.453

1251.2

3.16

-2

17

Cl

Chlorine

[Ne] 3s² 3p⁵

18

39.948

1520.6

3.16

-2

18

Ar

Argon

[Ne] 3s² 3p⁶

19

39.0983

438.8

0.82

-1

19

K

Potassium

[Ar] 4s¹

20

40.078

598.8

1.00

-2

20

Ca

Calcium

[Ar] 4s²

21

44.95591

633.1

1.36

-2

21

Sc

Scandium

[Ar] 3d¹ 4s²

22

47.867

658.8

1.54

-2

22

Ti

Titanium

[Ar] 4s² 3d²

23

50.9415

690.9

1.63

-2

23

V

Vanadium

[Ar] 4s² 3d³

24

51.9962

692.9

1.60

-2

24

Cr

Chromium

[Ar] 4s¹ 3d⁵

25

54.93804

737.3

1.70

-2

25

Mn

Manganese

[Ar] 4s² 3d⁵

26

55.845

762.5

1.83

-2

26

Fe

Iron

[Ar] 4s² 3d⁶

27

58.93319

790.4

1.91

-2

27

Co

Cobalt

[Ar] 4s² 3d⁷

28

58.6934

737.1

1.88

-2

28

Ni

Nickel

[Ar] 4s² 3d⁸

29

63.546

746.5

1.90

-2

29

Cu

Copper

[Ar] 4s¹ 3d¹⁰

30

65.38

900.4

1.05

-2

30

Zn

Zinc

[Ar] 4s² 3d¹⁰

31

69.723

758.8

1.81

-2

31

Ga

Gallium

[Ar] 4s² 3d¹⁰ 4p¹

32

72.64

760.0

2.01

-2

32

Ge

Germanium

[Ar] 4s² 3d¹⁰ 4p²

33

74.92160

747.0

2.35

-2

33

As

Arsenic

[Ar] 4s² 3d¹⁰ 4p³

34

78.96

944.0

2.55

-2

34

Se

Selenium

[Ar] 4s² 3d¹⁰ 4p⁴

35

79.904

1129.9

2.95

-2

35

Br

Bromine

[Ar] 4s² 3d¹⁰ 4p⁵

36

83.798

1300.8

3.00

-2

36

Kr

Krypton

[Ar] 4s² 3d¹⁰ 4p⁶

37

85.4678

803.0

0.82

-1

37

Rb

Rubidium

[Kr] 5s¹

38

87.62

549.5

0.95

-2

38

Sr

Strontium

[Kr] 5s²

39

88.90585

600.0

1.22

-2

39

Y

Yttrium

[Kr] 4d¹ 5s²

40

91.224

658.1

1.33

-2

40

Zr

Zirconium

[Kr] 4d² 5s²

41

92.90638

680.1

1.60

-2

41

Nb

Niobium

[Kr] 4d⁴ 5s¹

42

95.96

694.3

2.16

-2

42

Mo

Molybdenum

[Kr] 4d⁵ 5s¹

43

(98)

703.0

1.90

-2

43

Tc

Technetium

[Kr] 4d⁵ 5s²

44

101.07

710.0

2.20

-2

44

Ru

Ruthenium

[Kr] 4d⁷ 5s¹

45

102.9055

719.7

2.28

-2

45

Rh

Rhodium

[Kr] 4d⁸ 5s¹

46

106.42

804.4

2.30

-2

46

Pd

Palladium

[Kr] 4d¹⁰

47

107.8682

843.6

2.28

-2

47

Ag

Silver

[Kr] 4d¹⁰ 5s¹

48

112.414

867.8

1.09

-2

48

Cd

Cadmium

[Kr] 4d¹⁰ 5s²

49

114.818

898.0

1.78

-2

49

In

Indium

[Kr] 4d¹⁰ 5s² 5p¹

50

118.710

908.8

1.96

-2

50

Sn

Tin

[Kr] 4d¹⁰ 5s² 5p²

51

121.760

940.0

2.05

-2

51

Sb

Antimony

[Kr] 4d¹⁰ 5s² 5p³

52

126.904

976.3

2.10

-2

52

Te

Tellurium

[Kr] 4d¹⁰ 5s² 5p⁴

53

126.9044

1008.4

2.60

-2

53

I

Iodine

[Kr] 4d¹⁰ 5s² 5p⁵

54

131.293

1099.4

2.60

-2

54

Xe

Xenon

[Kr] 4d¹⁰ 5s² 5p⁶

55

132.9054

1375.7

0.79

-1

55

Cs

Caesium

[Xe] 6s¹

56

137.327

1022.9

0.89

-2

56

Ba

Barium

[Xe] 6s²

57

174.9668

503.5

1.27

-2

57

La

Lanthanum

[Xe] 5d¹ 6s²

58

178.49

505.5

1.27

-2

58

Hf

Hafnium

[Xe] 5d² 6s²

59

180.9478

703.0

1.50

-2

59

Ta

Tantalum

[Xe] 5d³ 6s²

60

183.84

703.0

2.36

-2

60

W

Tungsten

[Xe] 5d⁴ 6s²

61

186.207

703.0

1.90

-2

61

Re

Rhenium

[Xe] 5d⁵ 6s²

62

190.23

703.0

2.20

-2

62

Os

Osmium

[Xe] 5d⁶ 6s²

63

192.217

890.0

2.20

-2

63

Ir

Iridium

[Xe] 5d⁷ 6s²

64

195.084

890.0

2.20

-2

64

Pt

Platinum

[Xe] 5d⁹ 6s¹

65

196.9665

890.0

2.54

-2

65

Au

Gold

[Xe] 5d¹⁰ 6s¹

66

200.59

900.0

2.00

-2

66

Hg

Mercury

[Xe] 5d¹⁰ 6s²

67

204.3833

989.4

1.82

-2

67

Tl

Thallium

[Xe] 5d¹⁰ 6s² 6p¹

68

207.2

1035.0

1.78

-2

68

Pb

Lead

[Xe] 5d¹⁰ 6s² 6p²

69

208.9804

1035.0

2.02

-2

69

Bi

Bismuth

[Xe] 5d¹⁰ 6s² 6p³

70

(210)

1035.0

2.00

-2

70

Po

Polonium

[Xe] 5d¹⁰ 6s² 6p⁴

71

(210)

1035.0

2.30

-2

71

At

Astatine

[Xe] 5d¹⁰ 6s² 6p⁵

72

(220)

1035.0

2.30

-2

72

Rn

Radon

[Xe] 5d¹⁰ 6s² 6p⁶

87

(223)

380.0

0.70

-1

87

Fr

Francium

[Rn] 7s¹

88

(226)

390.5

0.90

-2

88

Ra

Radium

[Rn] 7s²

89

(262)

470.0

1.03

-2

89

Lr

Lawrencium

[Rn] 5f¹⁴ 7s² 7p⁶

90

(261)

580.0

1.04

-2

90

Rf

Rutherfordium

[Rn] 5f¹⁴ 7s² 7p⁶

91

(262)

580.0

1.05

-2

91

Db

Dubnium

[Rn] 5f¹⁴ 7s² 7p⁶

92

(266)

580.0

1.06

-2

92

Sg

Seaborgium

[Rn] 5f¹⁴ 7s² 7p⁶

93

(264)

580.0

1.07

-2

93

Bh

Bohrium

[Rn] 5f¹⁴ 7s² 7p⁶

94

(277)

580.0

1.08

-2

94

Hs

Hassium

[Rn] 5f¹⁴ 7s² 7p⁶

95

(268)

580.0

1.09

-2

95

Mt

Meitnerium

[Rn] 5f¹⁴ 7s² 7p⁶

96

(271)

580.0

1.10

-2

96

Ds

Darmstadtium

[Rn] 5f¹⁴ 7s² 7p⁶

97

(272)

580.0

1.11

-2

97

Rg

Roentgenium

[Rn] 5f¹⁴ 7s² 7p⁶

98

(285)

580.0

1.12

-2

98

Cn

Copernicium

[Rn] 5f¹⁴ 7s² 7p⁶

99

(284)

580.0

1.13

-2

99

Uut

Ununtrium

[Rn] 5f¹⁴ 7s² 7p⁶

100

(289)

580.0

1.14

-2

100

Fl

Flerovium

[Rn] 5f¹⁴ 7s² 7p⁶

101

(288)

580.0

1.15

-2

101

Uup

Ununpentium

[Rn] 5f¹⁴ 7s² 7p⁶

102

(292)

580.0

1.16

-2

102

Lv

Livermorium

[Rn] 5f¹⁴ 7s² 7p⁶

103

(294)

580.0

1.17

-2

103

Uus

Ununseptium

[Rn] 5f¹⁴ 7s² 7p⁶

104

(294)

580.0

1.18

-2

104

Uuo

Ununoctium

[Rn] 5f¹⁴ 7s² 7p⁶

group 1

1

1.00794

1310.0

2.20

-1

1

H

Hydrogen

1s¹

2

6.941

520.2

0.98

-1

2

Li

Lithium

1s² 2s¹

3

9.012182

999.5

1.57

-2

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Beryllium

1s² 2s²

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405.8

0.93

-1

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Na

Sodium

[Ne] 3s¹

5

24.3050

737.7

1.31

-1

5

Mg

Magnesium

[Ne] 3s²

atomic mass
or most stable mass number

1st ionization energy
in kJ/mol

chemical symbol

name

electron configuration

55.845

762.5

1.83

26

Fe

Iron

[Ar] 3d⁶ 4s²

atomic number

electronegativity

oxidation states
most common are bold

alkali metals

alkaline metals

other metals

transition metals

lanthanoids

actinoids

metalloids

nonmetals

halogens

noble gases

unknown elements

radioactive elements have
masses in parentheses

13

10.811

800.5

2.04

-2

5

B

Boron

1s² 2s² 2p¹

14

12.0107

1086.5

2.25

-2

6

C

Carbon

1s² 2s² 2p²

15

14.0067

1402.3

3.04

-2

7

N

Nitrogen

1s² 2s² 2p³

16

15.9994

1313.9

3.44

-2

8

O

Oxygen

1s² 2s² 2p⁴

17

18.998403

1681.0

3.98

-1

9

F

Fluorine

1s² 2s² 2p⁵

18

20.1797

2081.0

3.98

-1

10

Ne

Neon

1s² 2s² 2p⁶

13

26.98153

577.5

1.61

-2

13

Al

Aluminium

[Ne] 3s² 3p¹

14

28.0855

786.5

1.90

-2

14

Si

Silicon

[Ne] 3s² 3p²

15

30.97696

1011.8

2.19

-2

15

P

Phosphorus

[Ne] 3s² 3p³

16

32.065

999.6

2.20

-2

16

S

Sulfur

[Ne] 3s² 3p⁴

17

35.453

1251.2

3.16

-2

17

Cl

Chlorine

[Ne] 3s² 3p⁵

18

39.948

1520.6

3.16

-2

18

Ar

Argon

[Ne] 3s² 3p⁶

19

39.0983

438.8

0.82

-1

19

K

Potassium

[Ar] 4s¹

20

40.078

598.8

1.00

-2

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1.36

-2

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Scandium

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1.54

-2

22

Ti

Titanium

[Ar] 4s² 3d²

23

50.9415

690.9

1.63

-2

23

V

Vanadium

[Ar] 4s² 3d³

24

51.9962

692.9

1.60

-2

24

Cr

Chromium

[Ar] 4s¹ 3d⁵

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54.93804

737.3

1.70

-2

25

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55.845

762.5

1.83

-2

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Fe

Iron

[Ar] 4s² 3d⁶

27

58.93319

790.4

1.91

-2

27

Co

Cobalt

[Ar] 4s² 3d⁷

28

58.6934

737.1

1.88

-2

28

Ni

Nickel

[Ar] 4s² 3d⁸

29

63.546

746.5

1.90

-2

29

Cu

Copper

[Ar] 4s¹ 3d¹⁰

30

65.38

900.4

1.05

-2

30

Zn

Zinc

[Ar] 4s² 3d¹⁰

31

69.723

758.8

1.81

-2

31

Ga

Gallium

[Ar] 4s² 3d¹⁰ 4p¹

32

72.64

760.0

2.01

-2

32

Ge

Germanium

[Ar] 4s² 3d¹⁰ 4p²

33

74.92160

747.0

2.35

-2

33

As

Arsenic

[Ar] 4s² 3d¹⁰ 4p³

34

78.96

944.0

2.55

-2

34

Se

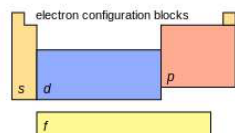
Selenium

[Ar] 4s² 3d¹⁰ 4p⁴

35

79.904

112



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.

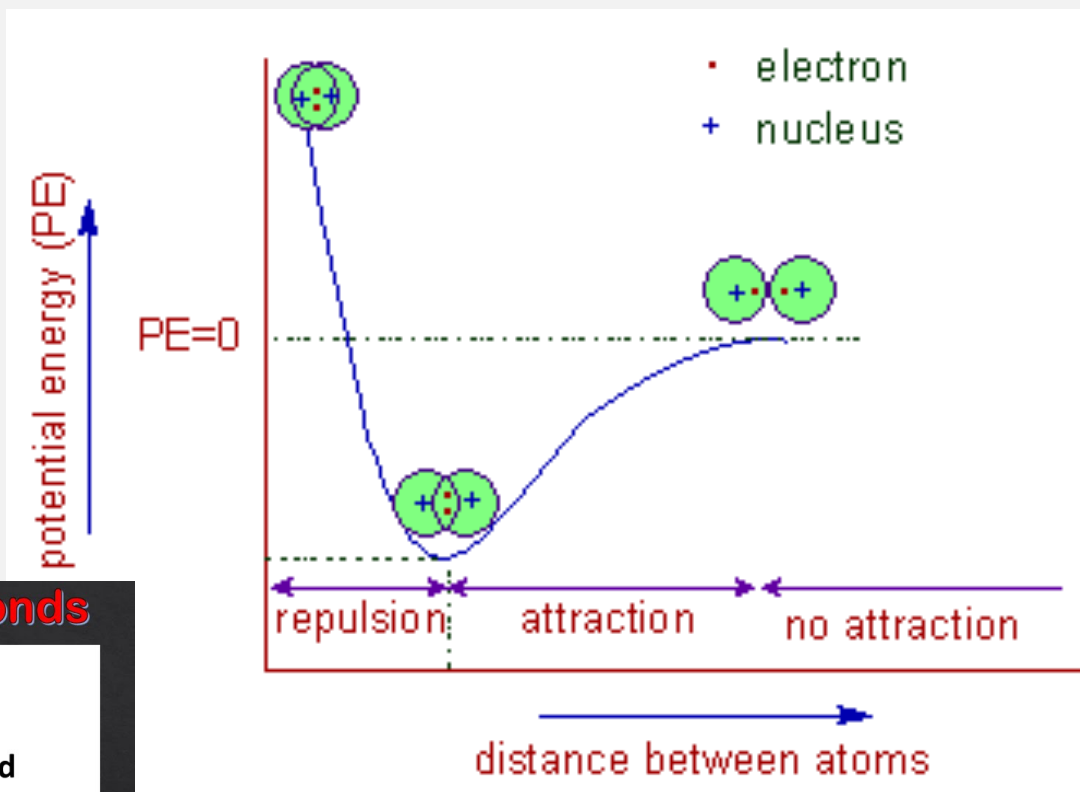
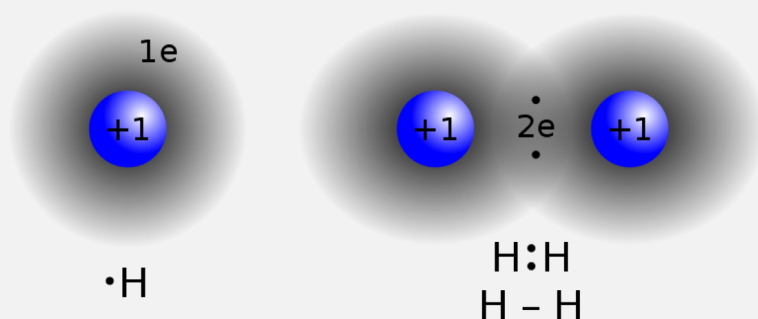
138.9054 57 La Lanthanum [Xe] 5d ¹ 6s ²	140.116 58 Ce Cerium [Xe] 4f ¹ 5d ¹ 6s ²	140.9076 59 Pr Praseodymium [Xe] 4f ³ 6s ²	144.242 60 Nd Neodymium [Xe] 4f ⁴ 6s ²	(145) 61 Pm Promethium [Xe] 4f ⁵ 6s ²	150.36 62 Sm Samarium [Xe] 4f ⁶ 6s ²	151.964 63 Eu Europium [Xe] 4f ⁷ 6s ²	157.25 64 Gd Gadolinium [Xe] 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

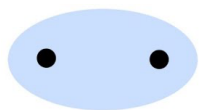
Covalent bond involves the sharing of electron pairs between atoms.



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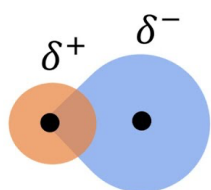
Polar and non-polar bonds

Non-polar
covalent bond



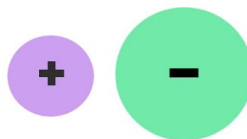
Equal sharing of
electrons

Polar covalent
bond



Unequal sharing
of electrons

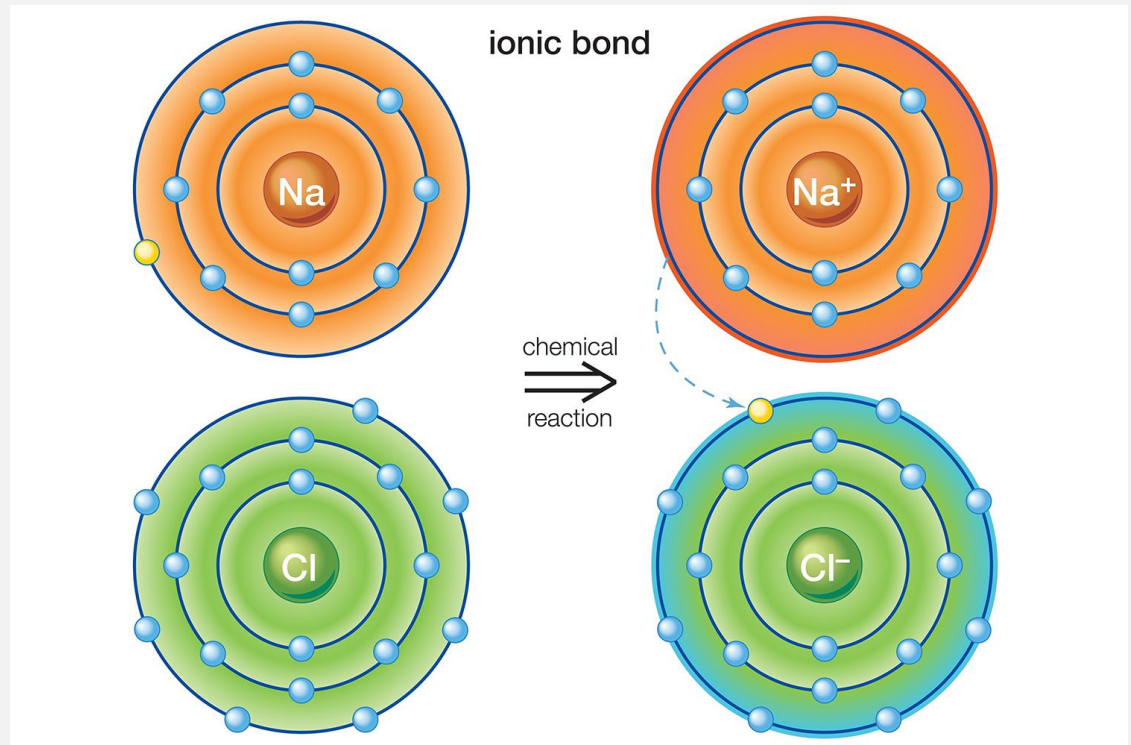
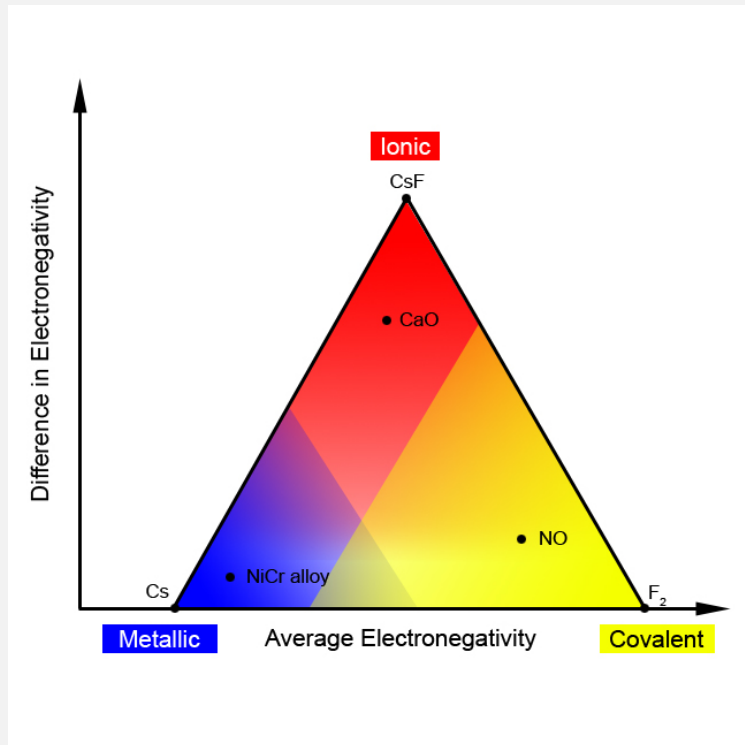
Ionic bond



No sharing of
electrons in bond

Increasing difference in electronegativity

Primary chemical bonds



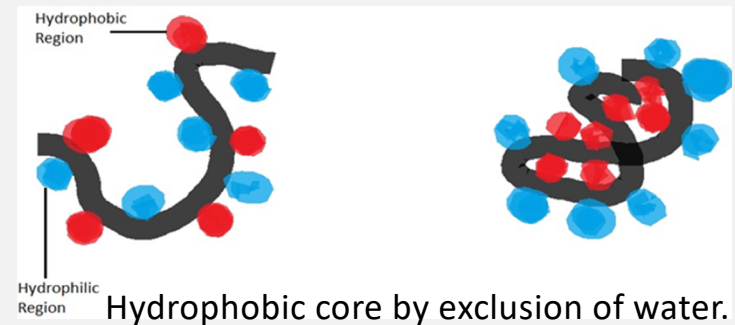
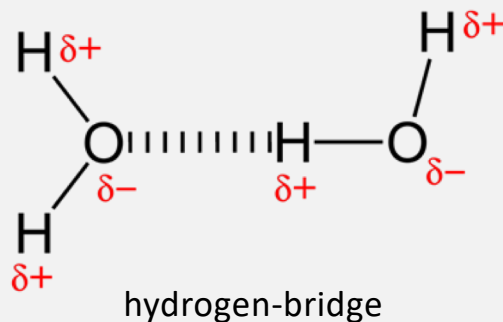
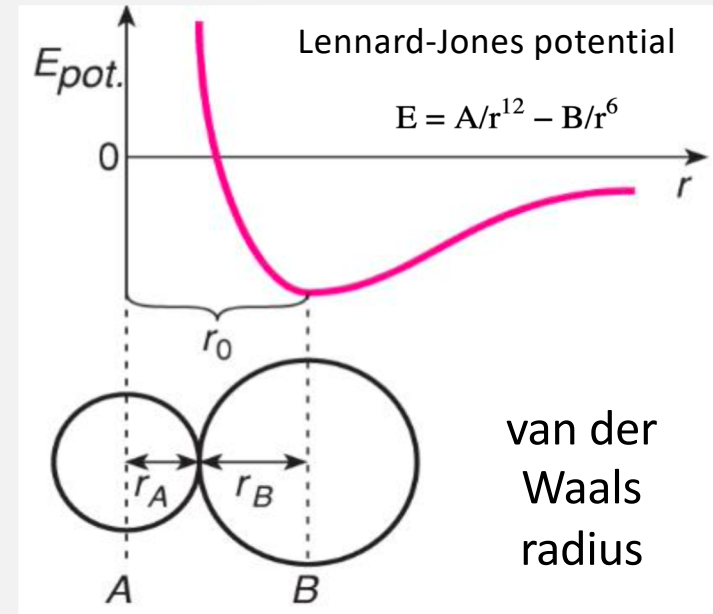
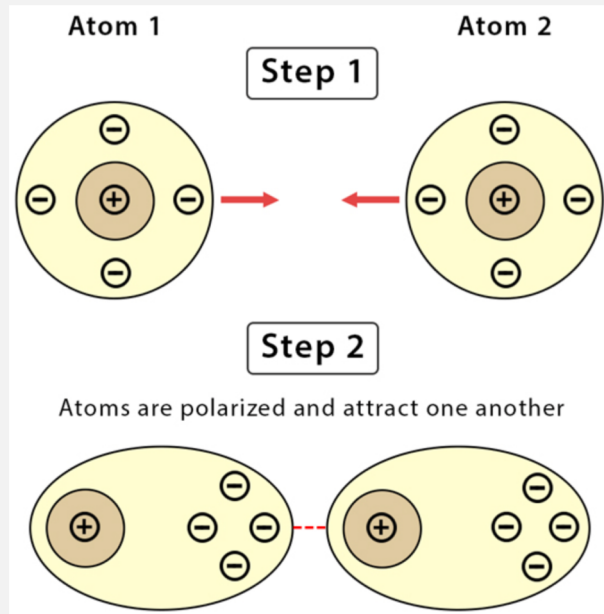
Elektronegativity (Linus Pauling): sum of the energies needed to produce a positive and a negative ion from an atom.

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

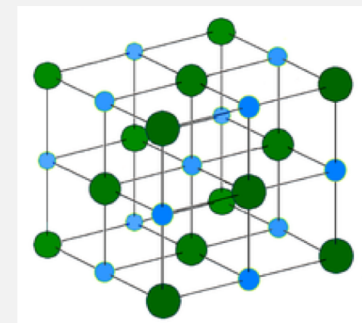
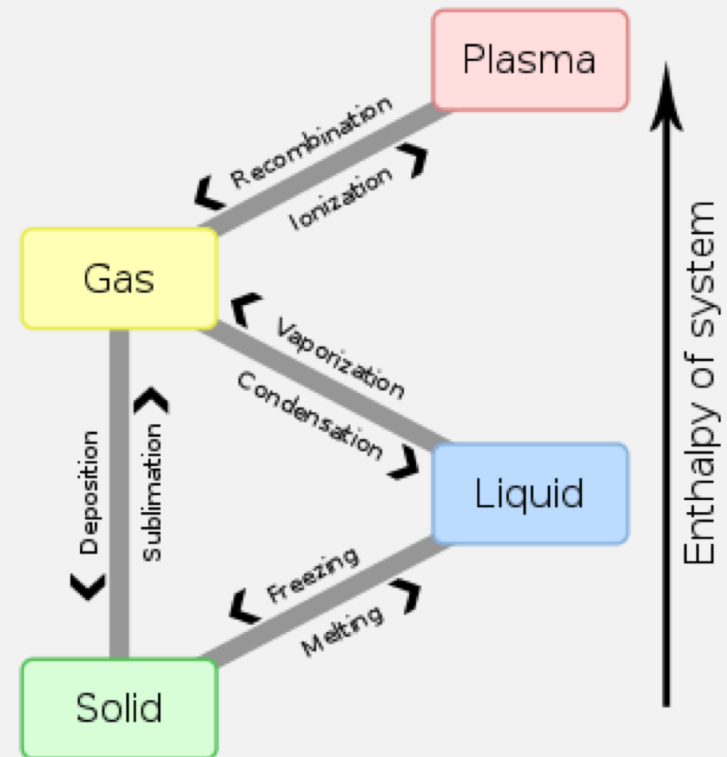


Phases of matter

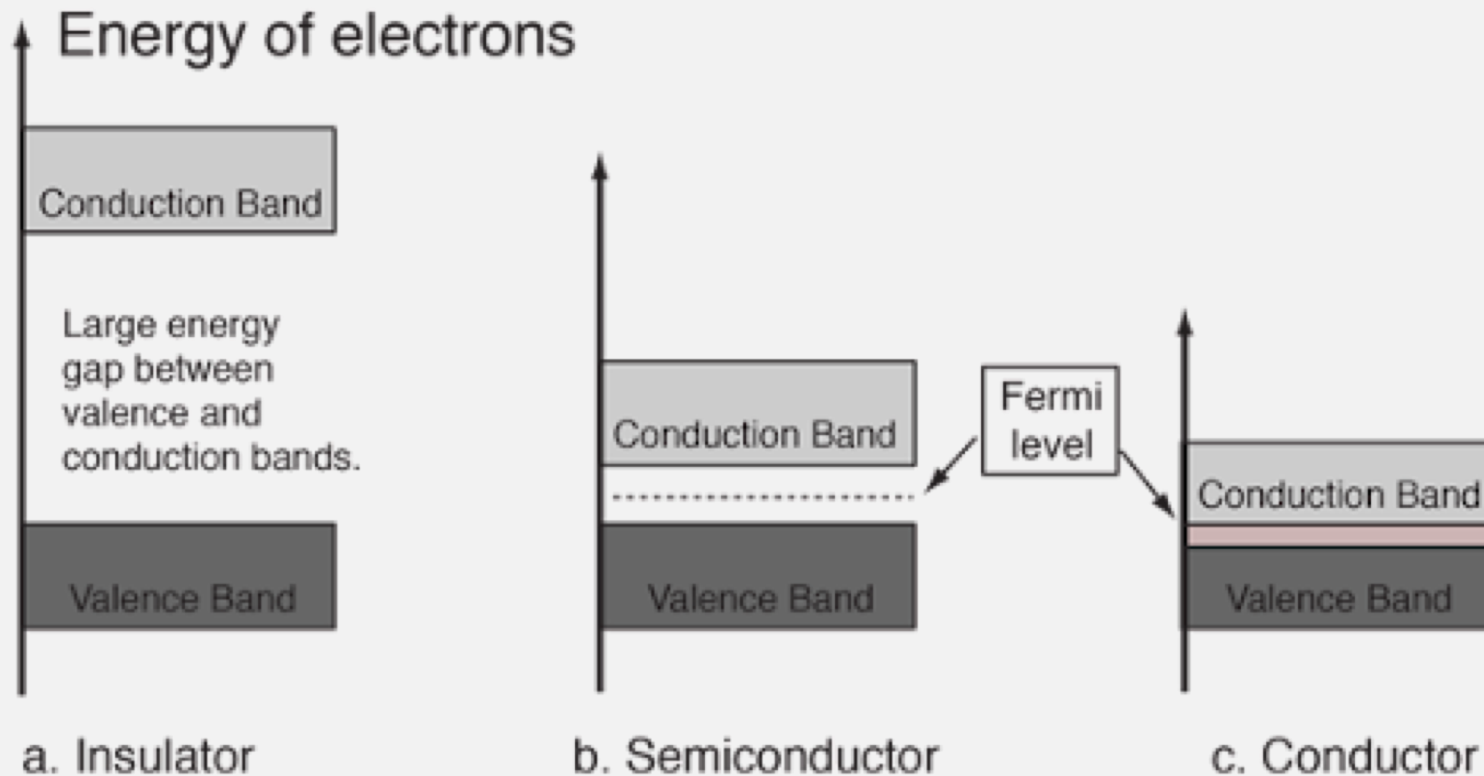
Gases: the particles are moving independently, colliding with each other and with the wall of the container. Ideal gas: the particles are point-like without a volume.

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



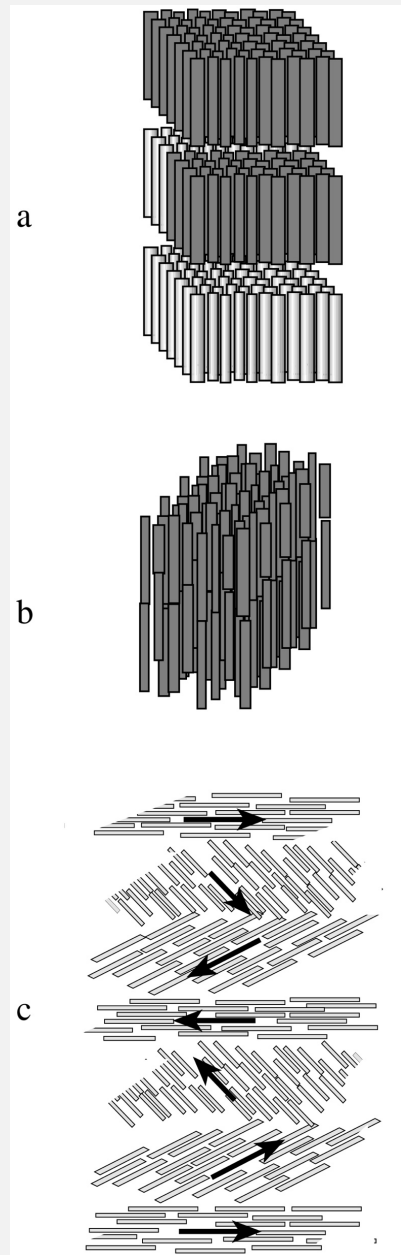
Energy gap between valence and conduction bands is called forbidden gap. Fermi energy is a hypothetical energy level for the electrons, related to a 50% occupancy.

If the energy gap is bigger than $>3,1$ eV, the maximum photon energy of a visible light, than 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).

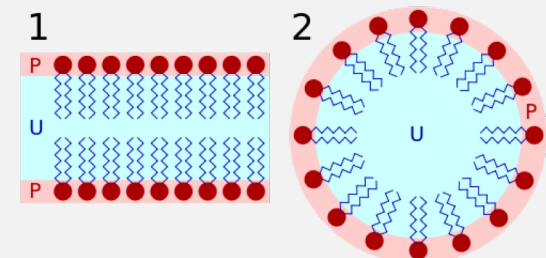
- a) smectic phase: both ordering are present
- b) nematic phase: only the orientational ordering is present
- c) cholesteric or twisted nematic phase: a chiral order can be observed due to a fixed angle rotation of asymmetric molecules in the adjacent layers



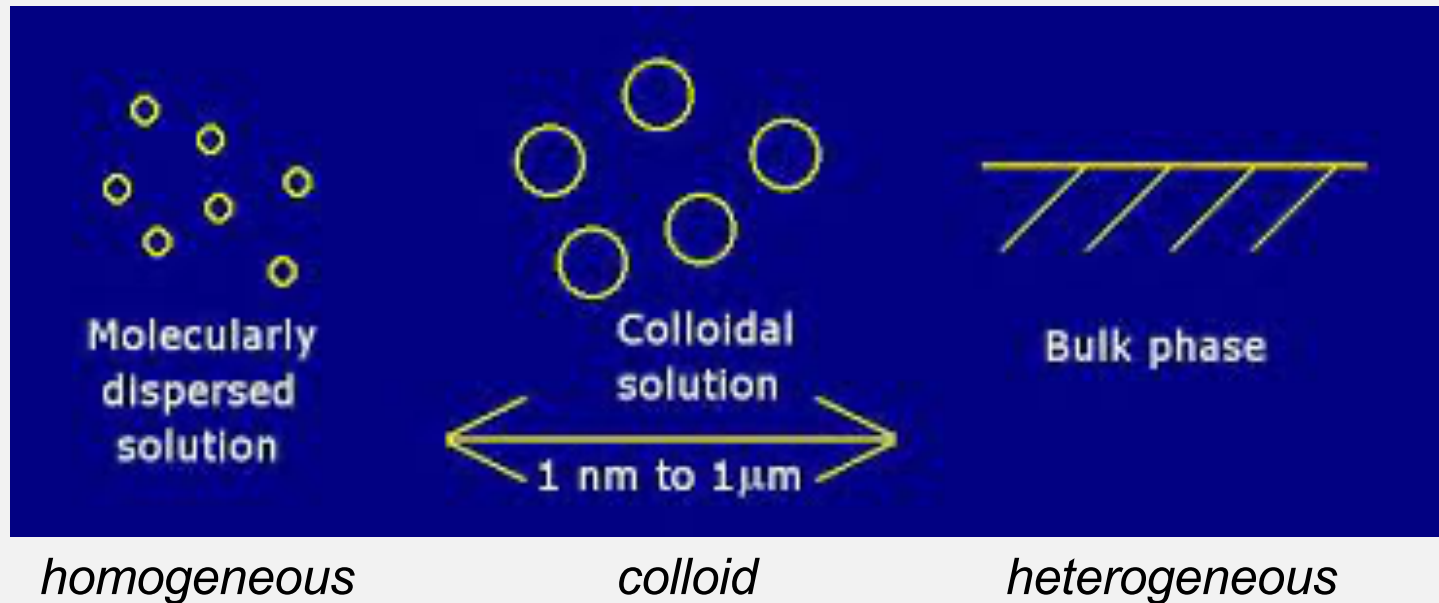
Thermotropic liquid crystals: the ordering depends on the temperature, present only in a certain temperature range.

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

1) bilayers, 2) micelles



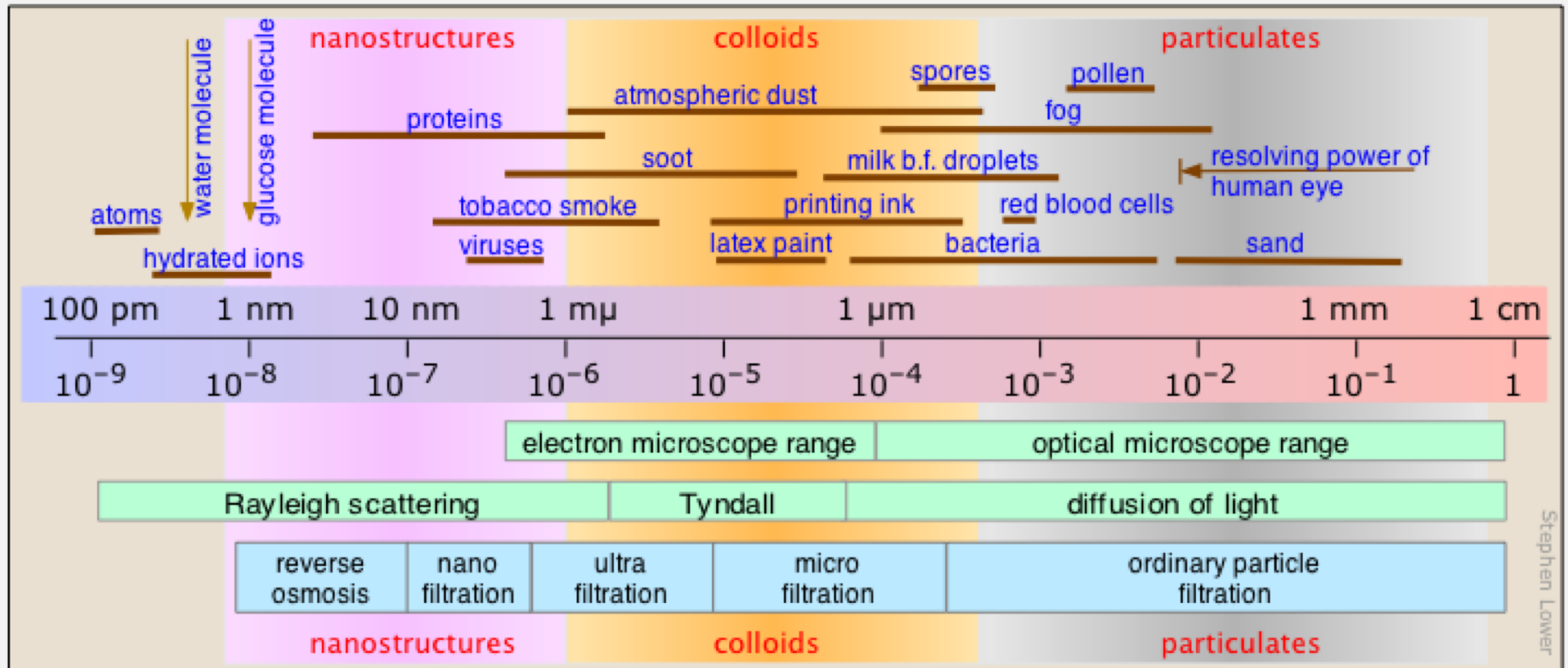
Colloid state



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.

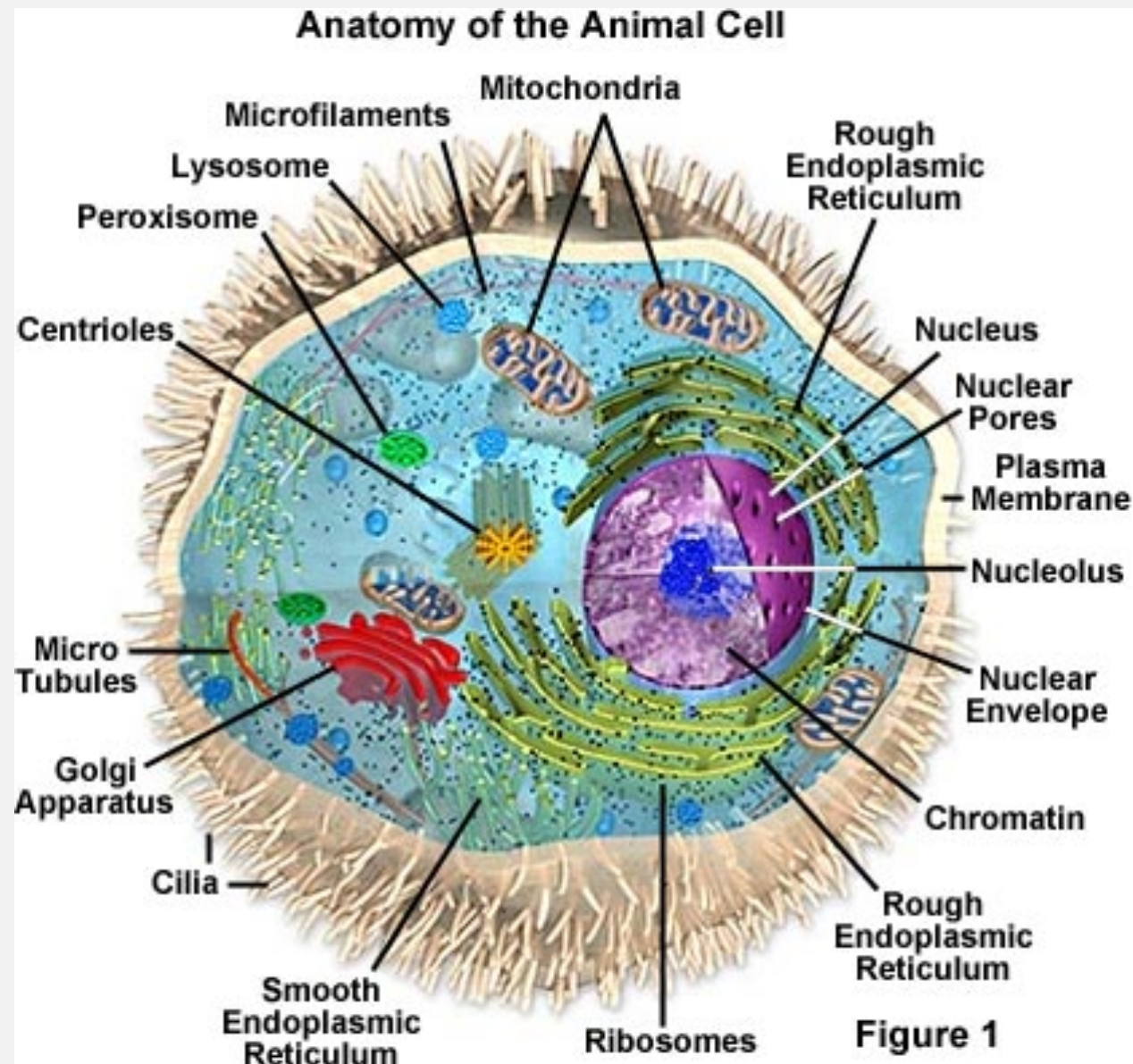
A colloid consists of two distinct phases, a continuous phase (the dispersion medium) and a particulate phase, where the particles generally have dimensions ranging between 2 and 200 nm. The two phases can be liquid-in-liquid (milk), solid-in-liquid (paint), liquid-in-gas (aerosol) and other combinations.

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 christals

colloids

Related chapters in
Damjanovich, Fidy, Szöllősi: Medical Biophysics

I. chapter

1.1.1	3.1.1
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	