Atom physics

Models of hydrogen atom, stimulated emission, laser. Multielectron atoms, Periodic table of elements, rules for electronic orbitals in atoms, Pauli exclusion principle, Hund's principle. Franck – Hertz experiment, ionization energy. Band structure of solids and its consequences. Chemical bonds – covalent, metallic and ionic. Characteristic properties of metals, semiconductors and isolators.

Atom physics

Atom physics is based on quantum effects and deals with atom properties

- chemical bonds, chemistry
- isotopes, physical parameters of atoms
- radiation spectra
- …

Atom

Atomos = indivisible particle

Démocritos

- Division of solids into parts, combination of solids (Avogadro’s law)
- Experiments with particle scattering (Rutherford, Thompson „plum-pudding“ model)

Atom structure

- Nucleus (10^{-15}m), built by nucleons (proton, neutron), most of the atom mass
- Electron orbitals (10^{-12}m), built by electrons with discrete energies (electron energy levels – shells, subshells), electron levels are responsible for the characteristics of radiation, periodic table of elements

“Plum-pudding” model of atom

1898 – J.J.Thompson

“plum-pudding“ model of atom

Atom is built by continuous positively charged material and negatively charged “plums” distributed randomly in it

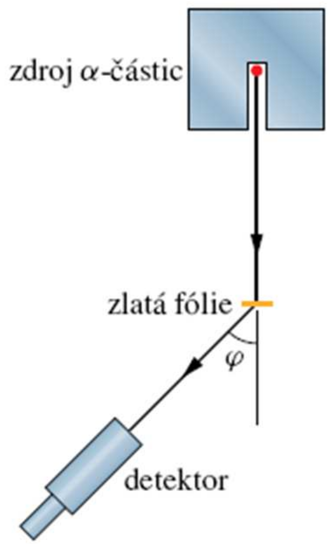
Atom nucleus

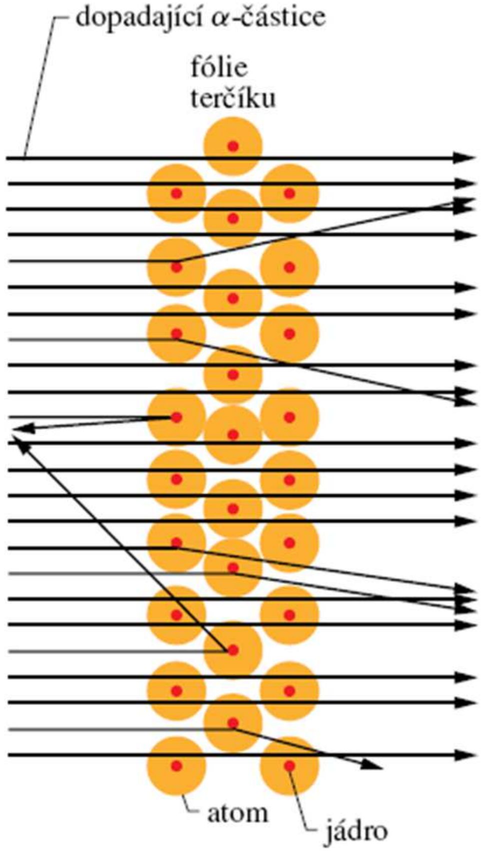
1911 – E.Rutherford,

Experiment - Marsden and Geiger

α-particles scattering

at thin Au-foil





Rutherford's planetary model

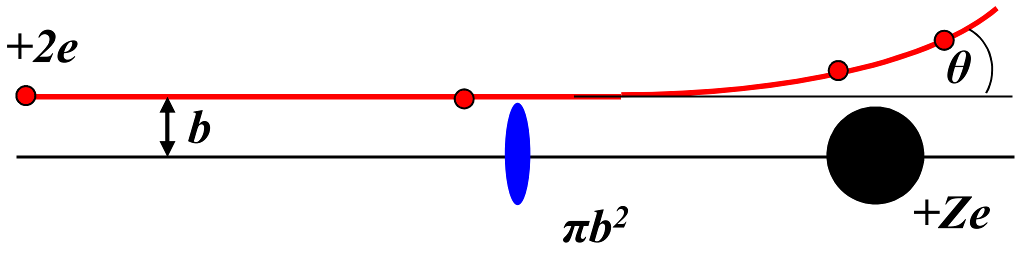
Some α-particles are scattered by high angles up to 180°, most particle did not scatter at all (without any direction change)

→ model of atom as an object with very small nucleus (positively charged) and electrons as satellites

Scattering of α-particles depend on atomic number Z

Scattering of α-particles

Scattering experiments allow for the estimate of nucleus size



b = scattering distance

T … kinetic energy

θ… scattering angle

Scattering angle

$$\cot(\frac{1}{2}\theta) = \frac{4\pi\varepsilon_0 T}{Ze^2} b$$

Scattering cross-section πb^2 = area with scattering angle of minimum magnitude θ

Atom size estimate

Kinetic energy at the closest distance between α-particle and nucleus is equal to the potential energy of electrostatic repulsion

$$T = \frac{1}{4\pi\varepsilon_0}\frac{(Ze)(2e)}{r_0} \rightarrow r_0 = \frac{2Ze^2}{4\pi\varepsilon_0 T}$$

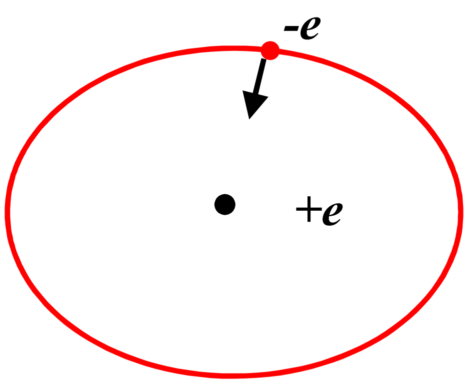
For T=7.7MeV it is $r_0=3.0\cdot 10^{-14}$m

Gold atomic number Z=79

Planetary model

Rutherford – electrons move similarly to planets around nucleus

Hydrogen



Centripetal force = electric attractive force

$$\frac{mv^2}{r} = \frac{1}{4\pi\varepsilon_0}\frac{e^2}{r^2} \rightarrow v = \frac{e}{\sqrt{4\pi\varepsilon_0 mr}}$$

Total electron energy

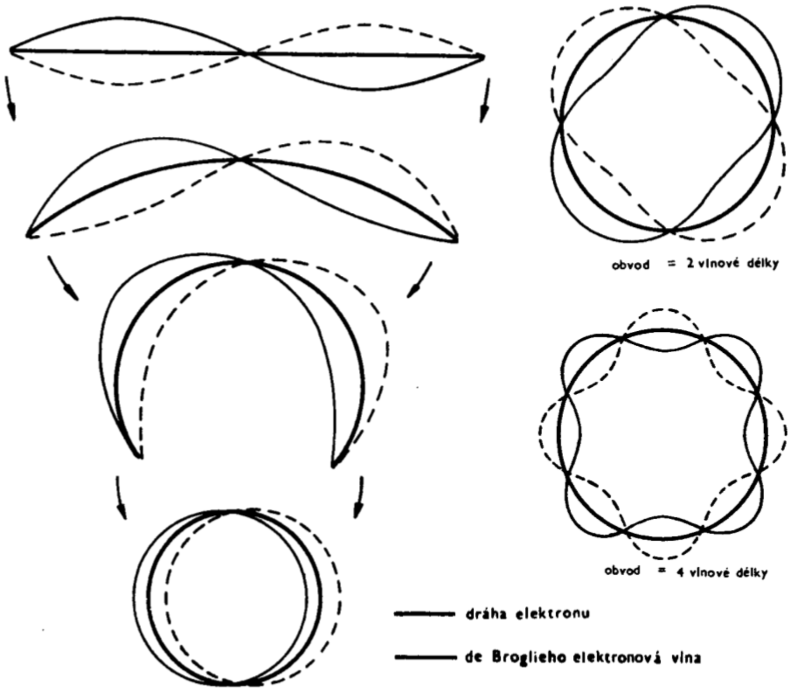
$$E = \frac{1}{2}mv^2 - \frac{e^2}{4\pi\varepsilon_0 r} = -\frac{e^2}{8\pi\varepsilon_0 r}$$

For hydrogen E = -13.6eV it is $r = 5.3\cdot10^{-11}$m

Misconception: Electron (accelerated charge) radiates energy – atom unstable!

The Bohr model

Electron as a planet moving around nucleus, but at constructive interference as standing wave



De Broglie's wavelength

$$\lambda = \frac{h}{mv} = \frac{h}{e}\sqrt{\frac{4\pi\varepsilon_0 r}{m}}$$

for $r = 5.3 \cdot 10^{-11}$m

it is $\lambda = 33 \cdot 10^{-11}\text{m} \approx 2\pi r$

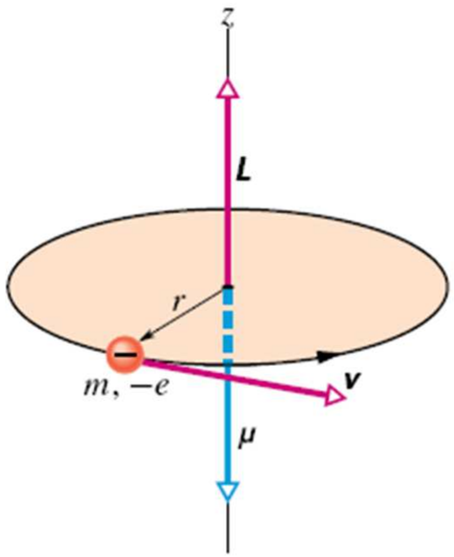
quantum condition

$2\pi r_n = n\lambda$

The Bohr model

N.Bohr, 1913

classical planetary model with quantum condition



Electron energy (Z=1)

$$E_P = -\frac{1}{4\pi\varepsilon_0}\frac{e^2}{r}$$

Quantum condition for angular momentum (Planck's constant)

$$m_e v r = n\frac{h}{2\pi}, \quad n = 1,2,3,...$$

The Bohr model

- Quantized radii of electrons

$$r_n = \frac{\varepsilon_0 h^2}{m_e \pi e^2} n^2 = a_0 n^2, a_0 = 5.3 \cdot 10^{-11} m$$

- Quantized speeds of electrons

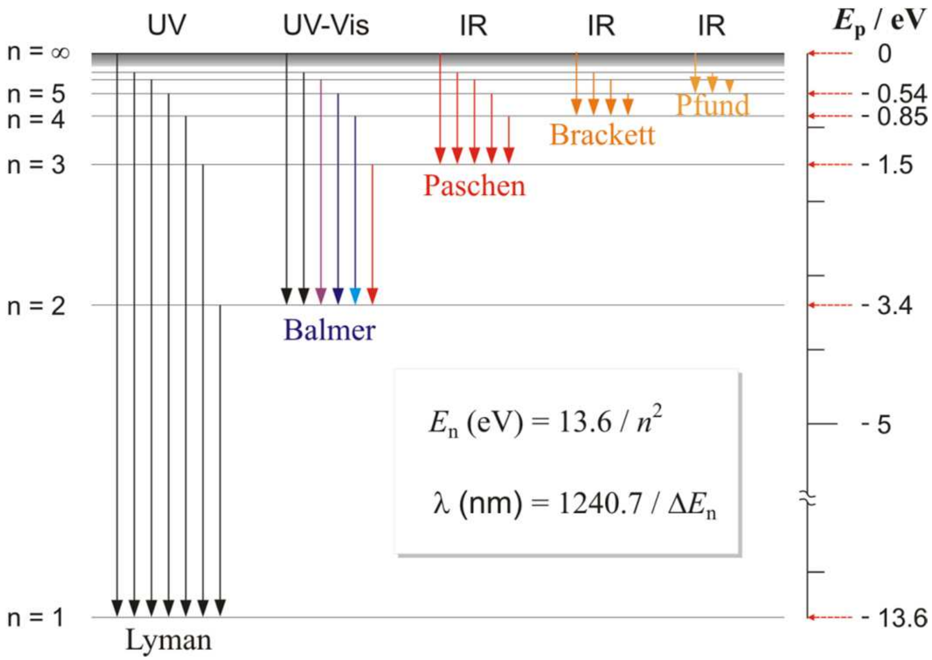
$$v_n = \frac{e^2}{2\varepsilon_0 h} \frac{1}{n}$$

- Quantized energies of electrons (principal quantum number n)

$$E = E_K + E_P = -\frac{e^4 m_e}{8\varepsilon_0^2 h^2} \frac{1}{n^2} = -\frac{13.6 eV}{n^2}$$

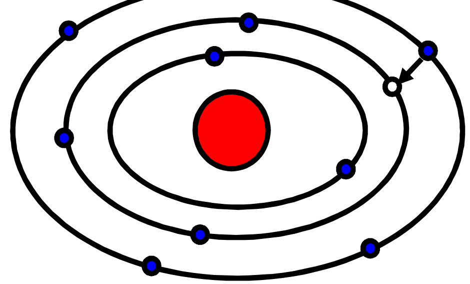
Energy levels of electrons for hydrogen atom

Energy increases with principal quantum number n



$$E_n = -\frac{13.6eV}{n^2}$$

Emitted radiation



$$E_f - E_c = \frac{hc}{\lambda}, \quad h = 6{,}626 \cdot 10^{-34} Js$$

Spectral lines for hydrogen atom

Wavelength of spectral lines

$$\frac{1}{\lambda} = \frac{me^4}{8\varepsilon_0^2 ch^3}\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$$

Series of spectral lines – limit wavelength in series ($n_i \to \infty$)

n_f=1 Lyman series (UV)

n_f=2 Balmer series (visible)

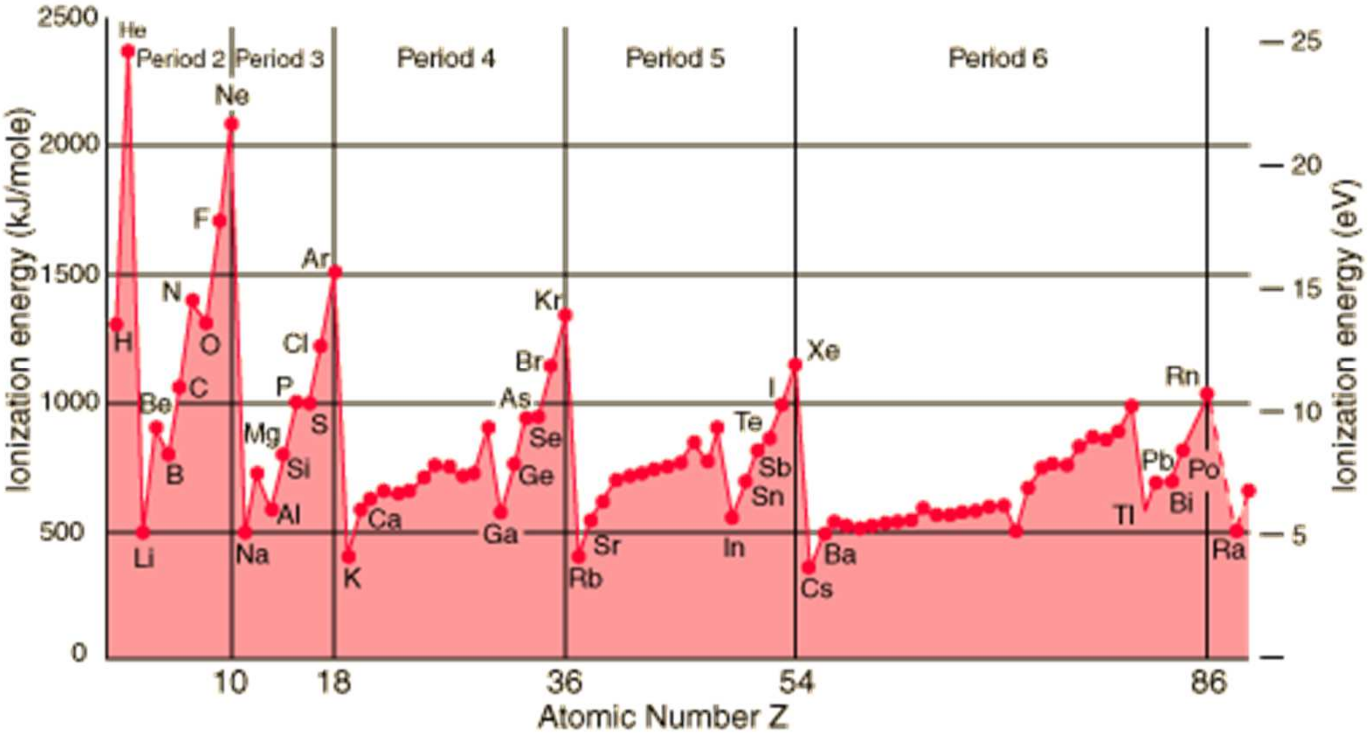
n_f=3 Paschen series (IR)

n_f=4 Brackett series (IR)

n_f=5 Pfund series (IR)

Ionization energy

Energy needed to release the weakest bonded electron from its orbital



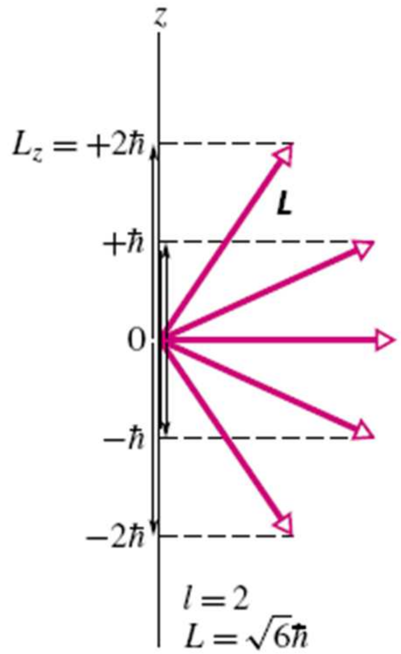
Angular momentum of electron

- Orbital quantum number l

$$L = \hbar\sqrt{l(l+1)} \qquad \mu_{orb,z} = -m_l \mu_B$$

$$L_z = m_l \hbar$$

Bohr magneton $\mu_B = \dfrac{e\hbar}{2m} = 9{,}274 \cdot 10^{-24}\ \mathrm{J{\cdot}T^{-1}}$



- Magnetic quantum number m_l
- Spin quantum number

$$S = \hbar\sqrt{s(s+1)} \qquad \mu_{s,z} = -2m_s \mu_B$$

$$S_z = m_s \hbar$$

Allowed values of quantum numbers

Quantum states of electron in atom

Number	Symbol	Possible Values
Principal Quantum Number	n	$1, 2, 3, 4, \ldots$
Angular Momentum Quantum Number	ℓ	$0, 1, 2, 3, \ldots, (n-1)$
Magnetic Quantum Number	m_l	$-\ell, \ldots, -1, 0, 1, \ldots, \ell$
Spin Quantum Number	m_s	$+1/2, -1/2$

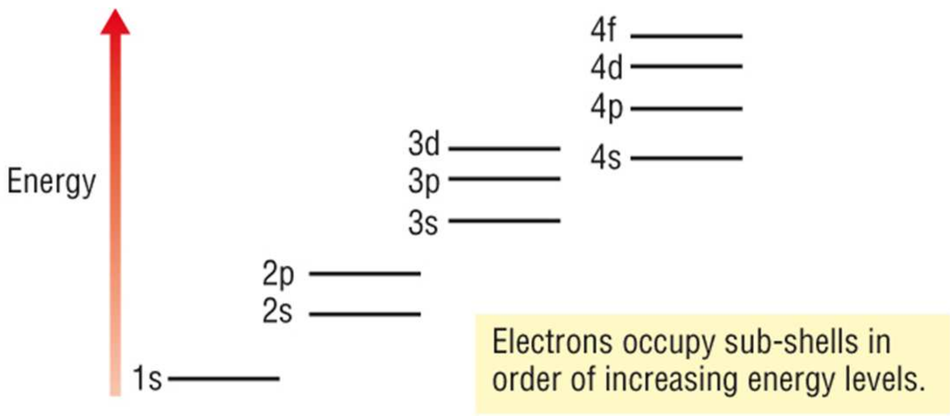
Numbering of shells and subshells

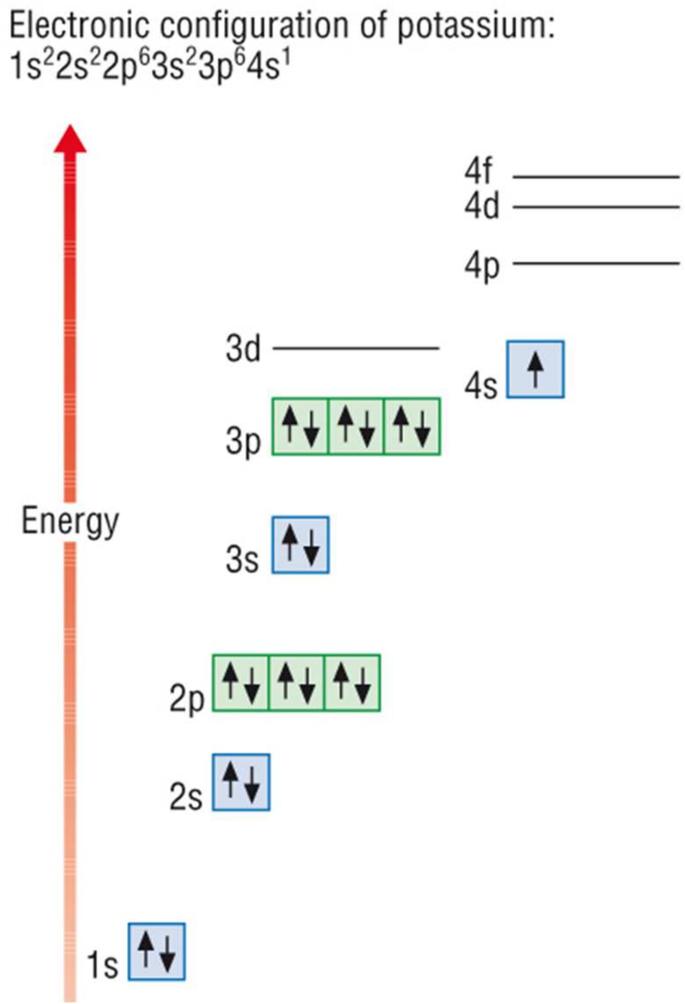
Shells: 1,2,3,…

Subshells: s,p,d,f

Electron level occupation rules

Minimum energy principle





Pauli exclusion principle and Hund’s rule

Pauli exclusion principle – no two electrons in an atom can occupy the same quantum state.

Hund’s rule – the lowest energy atomic state is the one that maximizes the total spin quantum number for the electrons in the open subshell.

Periodic Table of the Elements

Atomic Number	Boiling Point
Symbol	
Name	
Atomic Mass	

Normal boiling points are in °C.
SP = Triple Point
Pressure is listed if not 1 atm.
Allotrope is listed if more than one allotrope.

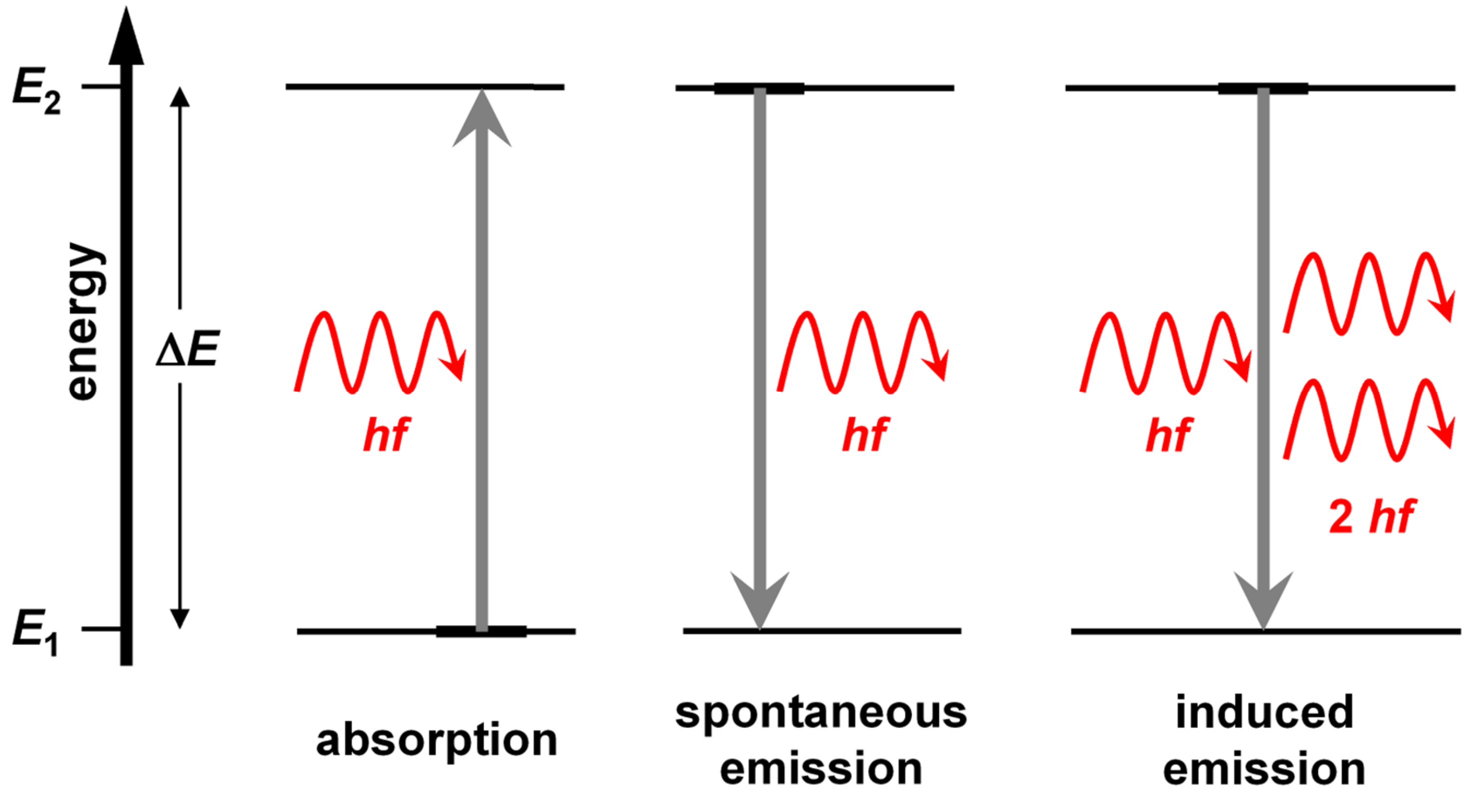
1 IA 1A	2 IIA 2A	3 IIIB 3B	4 IVB 4B	5 VB 5B	6 VIB 6B	7 VIIB 7B	8	9 VIII 8	10	11 IB 1B	12 IIB 2B	13 IIIA 3A	14 IVA 4A	15 VA 5A	16 VIA 6A	17 VIIA 7A	18 VIIIA 8A
1 -252.762 H Hydrogen 1.008																	2 -268.93 He Helium 4.003
3 1342 Li Lithium 6.941	4 2471 Be Beryllium 9.012											5 4000 B Boron 10.811	6 graphite 3825 SP C Carbon 12.011	7 -195.798 N Nitrogen 14.007	8 -182.953 O Oxygen 15.999	9 -188.12 F Fluorine 18.998	10 -246.053 Ne Neon 20.180
11 882.940 Na Sodium 22.990	12 1090 Mg Magnesium 24.305											13 2519 Al Aluminum 26.982	14 3265 Si Silicon 28.086	15 white 280.5 P Phosphorus 30.974	16 444.61 S Sulfur 32.066	17 -101.5 Cl Chlorine 35.453	18 -185.847 Ar Argon 39.948
19 759 K Potassium 39.098	20 1484 Ca Calcium 40.078	21 2836 Sc Scandium 44.956	22 3287 Ti Titanium 47.88	23 3407 V Vanadium 50.942	24 2671 Cr Chromium 51.996	25 2061 Mn Manganese 54.938	26 2861 Fe Iron 55.933	27 2927 Co Cobalt 58.933	28 2913 Ni Nickel 58.693	29 2562 Cu Copper 63.546	30 907 Zn Zinc 65.39	31 2204 Ga Gallium 69.732	32 2833 Ge Germanium 72.61	33 616 SP As Arsenic 74.922	34 685 Se Selenium 78.972	35 58.8 Br Bromine 79.904	36 -153.34 Kr Krypton 84.80
37 688 Rb Rubidium 84.468	38 1382 Sr Strontium 87.62	39 3345 Y Yttrium 88.906	40 4409 Zr Zirconium 91.224	41 4744 Nb Niobium 92.906	42 4639 Mo Molybdenum 95.95	43 4265 Tc Technetium 98.907	44 4150 Ru Ruthenium 101.07	45 3695 Rh Rhodium 102.906	46 2963 Pd Palladium 106.42	47 2162 Ag Silver 107.868	48 767 Cd Cadmium 112.411	49 2072 In Indium 114.818	50 2602 Sn Tin 118.71	51 1587 Sb Antimony 121.760	52 988 Te Tellurium 127.6	53 184.4 I Iodine 126.904	54 -108.09 Xe Xenon 131.29
55 671 Cs Cesium 132.905	56 1897 Ba Barium 137.327	57-71	72 4603 Hf Hafnium 178.49	73 5458 Ta Tantalum 180.948	74 5555 W Tungsten 183.85	75 5596 Re Rhenium 186.207	76 5012 Os Osmium 190.23	77 4428 Ir Iridium 192.22	78 3825 Pt Platinum 195.08	79 2856 Au Gold 196.967	80 356.62 Hg Mercury 200.59	81 1473 Tl Thallium 204.383	82 1749 Pb Lead 207.2	83 1564 Bi Bismuth 208.980	84 962 Po Polonium [208.982]	85 337 At Astatine 209.987	86 -61.7 Rn Radon 222.018
87 677 Fr Francium 223.020	88 1737 Ra Radium 226.025	89-103	104 unknown Rf Rutherfordium [261]	105 unknown Db Dubnium [262]	106 unknown Sg Seaborgium [266]	107 unknown Bh Bohrium [264]	108 unknown Hs Hassium [269]	109 unknown Mt Meitnerium [268]	110 unknown Ds Darmstadtium [269]	111 unknown Rg Roentgenium [272]	112 unknown Cn Copernicium [277]	113 unknown Uut Ununtrium unknown	114 unknown Fl Flerovium [289]	115 unknown Uup Ununpentium unknown	116 unknown Lv Livermorium [298]	117 unknown Uus Ununseptium unknown	118 unknown Uuo Ununoctium unknown

Lanthanide Series	57 3464 La Lanthanum 138.906	58 3443 Ce Cerium 140.115	59 3520 Pr Praseodymium 140.908	60 3074 Nd Neodymium 144.24	61 3000 Pm Promethium 144.913	62 1794 Sm Samarium 150.36	63 1529 Eu Europium 151.966	64 3273 Gd Gadolinium 157.25	65 3230 Tb Terbium 158.925	66 2567 Dy Dysprosium 162.50	67 2700 Ho Holmium 164.930	68 2868 Er Erbium 167.26	69 1950 Tm Thulium 168.934	70 1196 Yb Ytterbium 173.04	71 3402 Lu Lutetium 174.967
Actinide Series	89 3198 Ac Actinium 227.028	90 4788 Th Thorium 232.038	91 4027 Pa Protactinium 231.036	92 4131 U Uranium 238.029	93 4174 Np Neptunium 237.048	94 3228 Pu Plutonium 244.064	95 2011 Am Americium 243.061	96 3100 Cm Curium 247.070	97 2627 Bk Berkelium 247.070	98 unknown Cf Californium 251.080	99 unknown Es Einsteinium [254]	100 unknown Fm Fermium 257.095	101 unknown Md Mendelevium 258.1	102 unknown No Nobelium 259.101	103 unknown Lr Lawrencium [262]

Alkali Metal · **Alkaline Earth** · **Transition Metal** · **Basic Metal** · **Semimetal** · **Nonmetal** · **Halogen** · **Noble Gas** · **Lanthanide** · **Actinide**

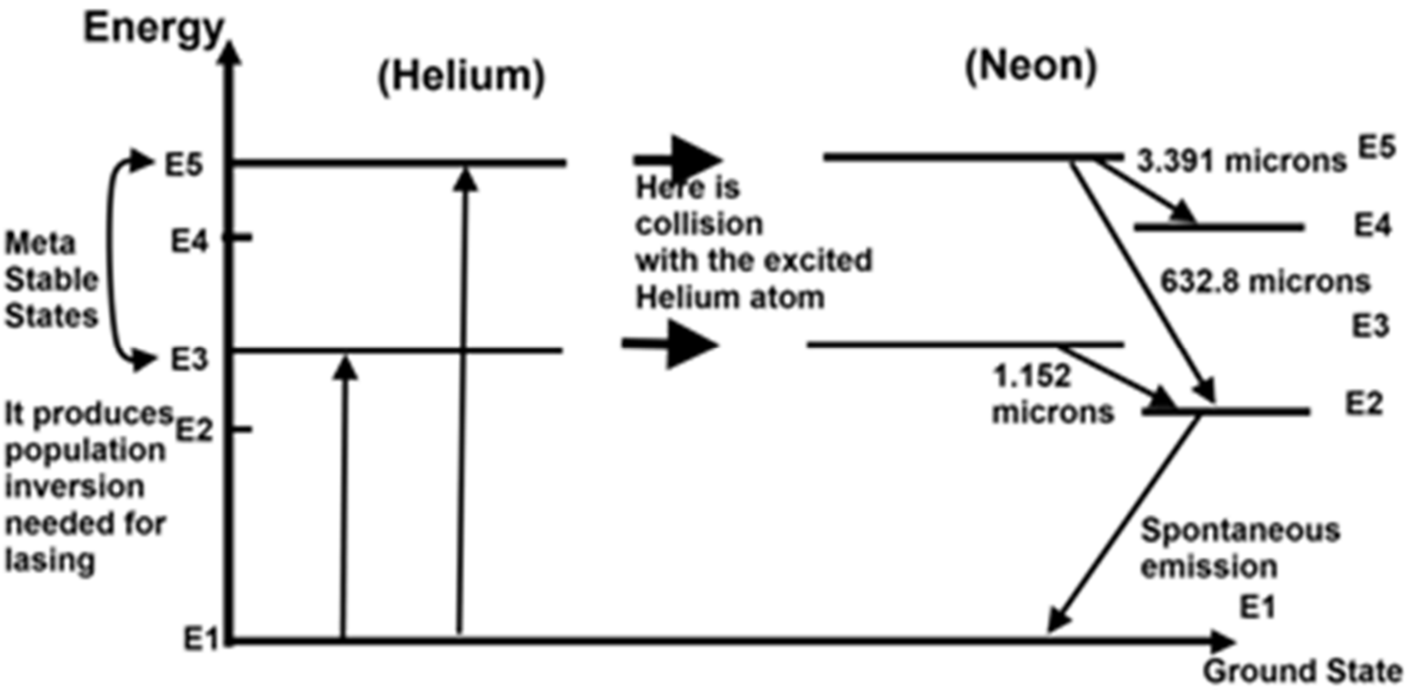
Absorption and emission of photon

Electron level occupation



He-Ne laser

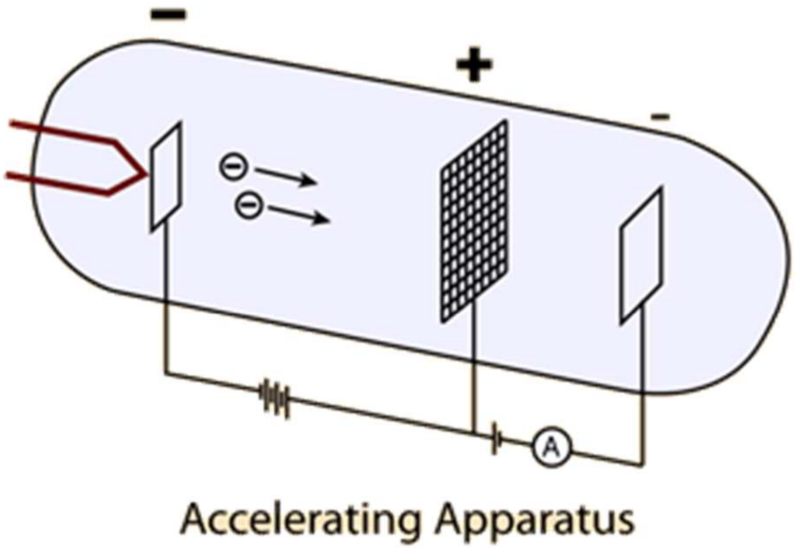
Stimulated electron emission

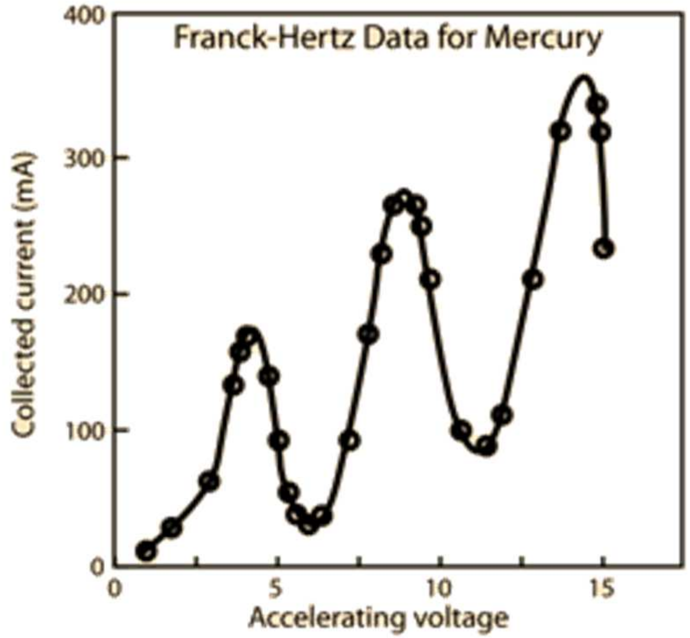


Photon has the same properties as stimulating one

Franck – Hertz experiment

1914 – J.Franck, G.Hertz, collisions of accelerated electrons with atoms → maxima/minima in current





Franck – Hertz experiment

Electrons emitted from cathode collide elastically with atoms of gas in tube

Expected – monotonous increase of current with increase of voltage

Experiment – current increased non-monotonically with distinct minima!

Explanation – certain values of electron kinetic energies are absorbed by electrons in gas atoms, electron is excited to higher energy level and emits photon, these absorbed electrons have lower energies and current decreases subsequently

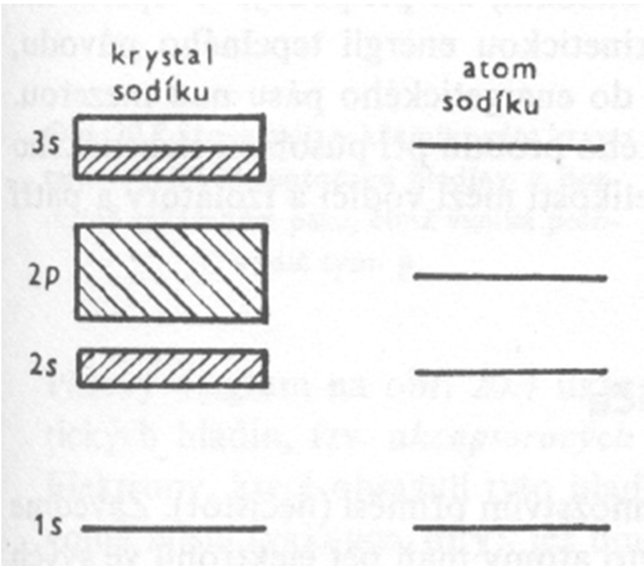
Example: mercury $E = 4.9\text{eV}$ for $\lambda = 254\text{nm}$

Band structure of electron energy levels

- Energies of electron orbitals in atoms overlap – bands
- Energy bands might overlap
- Band gap separates two bands without any overlap
- Valency and conductivity bands of energies

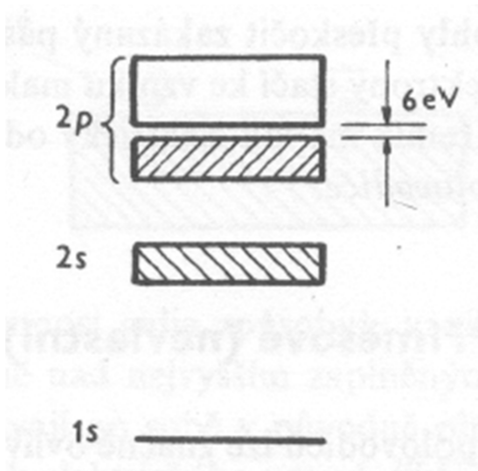
Energy bands

Sodium – metal

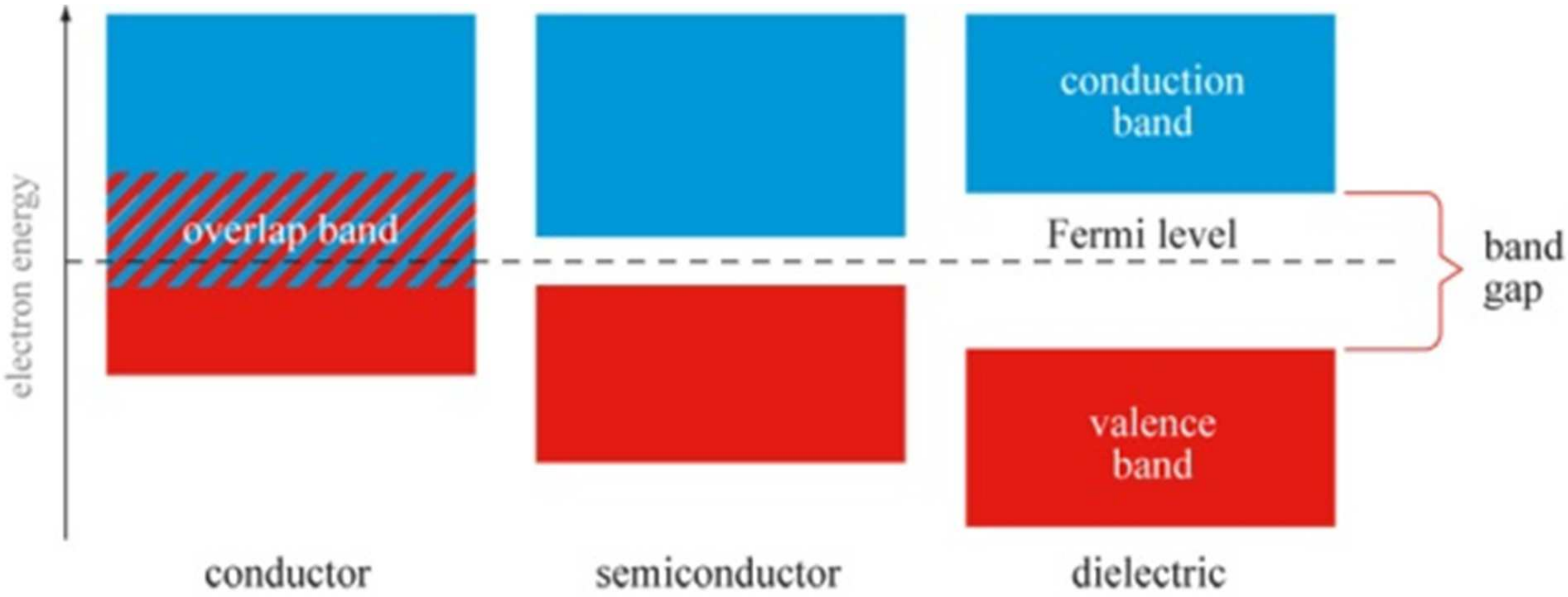


diamond - insulator

band gap 6eV



Solids by band structure



Chemical bond of atoms

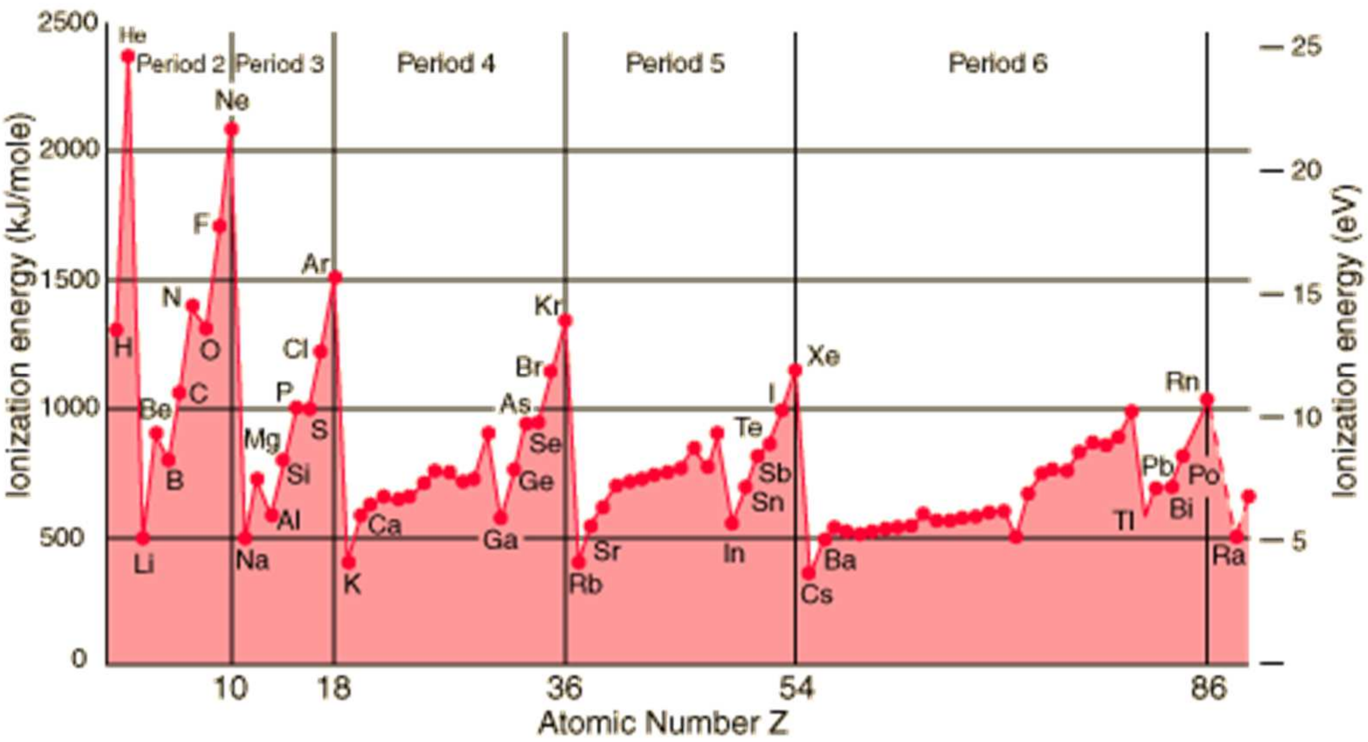
Lowers energy of atomic system in molecule

Bond types:

- Covalent bond – one or more electrons common for both atoms
- Ionic bond – one or more electrons is transferred from one to another atom, ions interact more or less electrostatically
- Metallic bond – many electrons shared within all volume of solid
- Combined bond types (Van der Waals, hydrogen bonds)
- No bond – e.g. due to Pauli exclusion principle

Ionization energy

Energy needed to release the weakest bonded electron from its orbital



Alkali metals

1st group of Periodic table – one electron at partially filled valency energy level

$_3Li$ $1s^2\ 2s^1$

$_{11}Na$ $1s^2\ 2s^2\ 2p^6\ 3s^1$

$_{19}K$ $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^1$

Inner shells are fully filled and their charges screen valency orbital, effective charge $+e$ only → low energy needed to ionize atom

Alkali metals can easily built 1+ valent ions (Na^{1+}, K^{1+}, etc.) and ionic bonds

Halogens

7^{th} group of Periodic table – one electron is missing to complete valency energy level

$_{9}F$	$1s^2\ 2s^2\ 2p^5$
$_{17}Cl$	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^5$
$_{35}Br$	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^5$

Atoms can easily complete valency orbital (non-complete p-shell), they built 1- valency ions (F^{1-}, Cl^{1-}, etc.) and ionic bond

LiF, LiCl, NaCl, NaF, KBr, KI, …

Electron affinity

Energy released by adding electron to the atom. Higher affinity means stronger electron bond

F	3.45eV
Cl	3.61eV
Br	3.36eV
I	3.06eV

E.g. in NaCl ions Na^{+} and Cl^{-} are not close each other to overlap electron orbitals, electric dipole structure

Ionic crystals

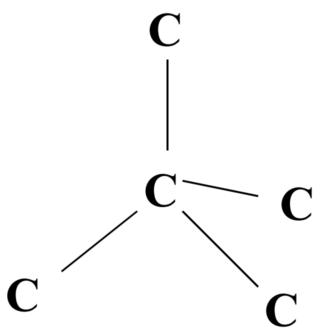
E.g. NaCl – two ions build dipole, attractive forces in dipole are stronger than repulsive forces between neighboring dipoles

Ionic crystals – hard, but brittle, high melting point, soluble in polar solvents (e.g. H_2O)

Covalent crystals

Overlap of electron orbitals and by sharing elektrons between two atoms, directional bonds

E.g. C (diamond), SiC, Si, Ge

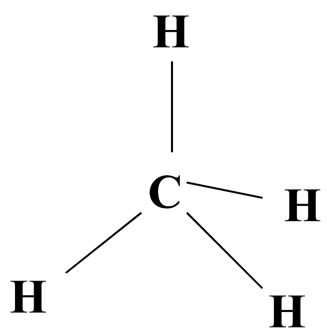


covalent crystals are hard,
high melting point,
not soluble in liquids

Van der Waals forces

Week attractive (short range) forces between atoms, polar molecules are attracted by oppositely charged ends

These week forces may cause e.g. gas condensation, viscosity, surface tension etc.



Molecular crystals have low melting and boiling point, low mechanical strength

e.g. methane CH_4

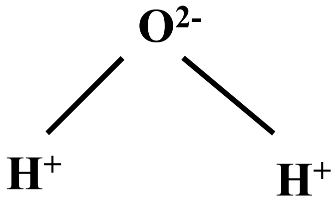
Hydrogen bonds

E.g. H_2O, ammonium NH_3, hydrogen fluoride HF

Hydrogen atom combines easily with electronegative elements, that all negative charge is located on such atom and hydrogen stays almost as single proton

Strongly polar bond, water anomaly

$_8O$ $1s^2\ 2s^2\ 2p^4$



each water molecule may create hydrogen bonds with up to 4 other molecules

Metallic bond

Electrons are sheared by all metallic crystal volume

„electronic gas“ of free electrons

Collective interaction of electrons in crystal volume

Electronic energy levels build continuous band of energies, possibility of absorption of any photon and non-transparency of metals

Crystals are very good electrical and heat conductors, ductility, non-transparency, reflecting surface, but lower hardness than ionic crystals

Atomic arrangement

- Short-range (interatomic forces, chemical bond, phase structure)
- Long-range (crystallographic lattice, amorphous solids)

Liquid crystals have partial atomic/molecular arrangement in 1D or 2D – solids between crystallic and amorphous materials

- Nematic LC – molecular arrangement in one direction (1D)
- Smectic LC – molecular arrangement in layers (2D)
- Chiral, cholesteric LC – molecular arrangement in screw structure

Literature

Pictures used from the books:

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Ch.Kittel: Úvod do fyziky pevných látek, Academia Praha 1985

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