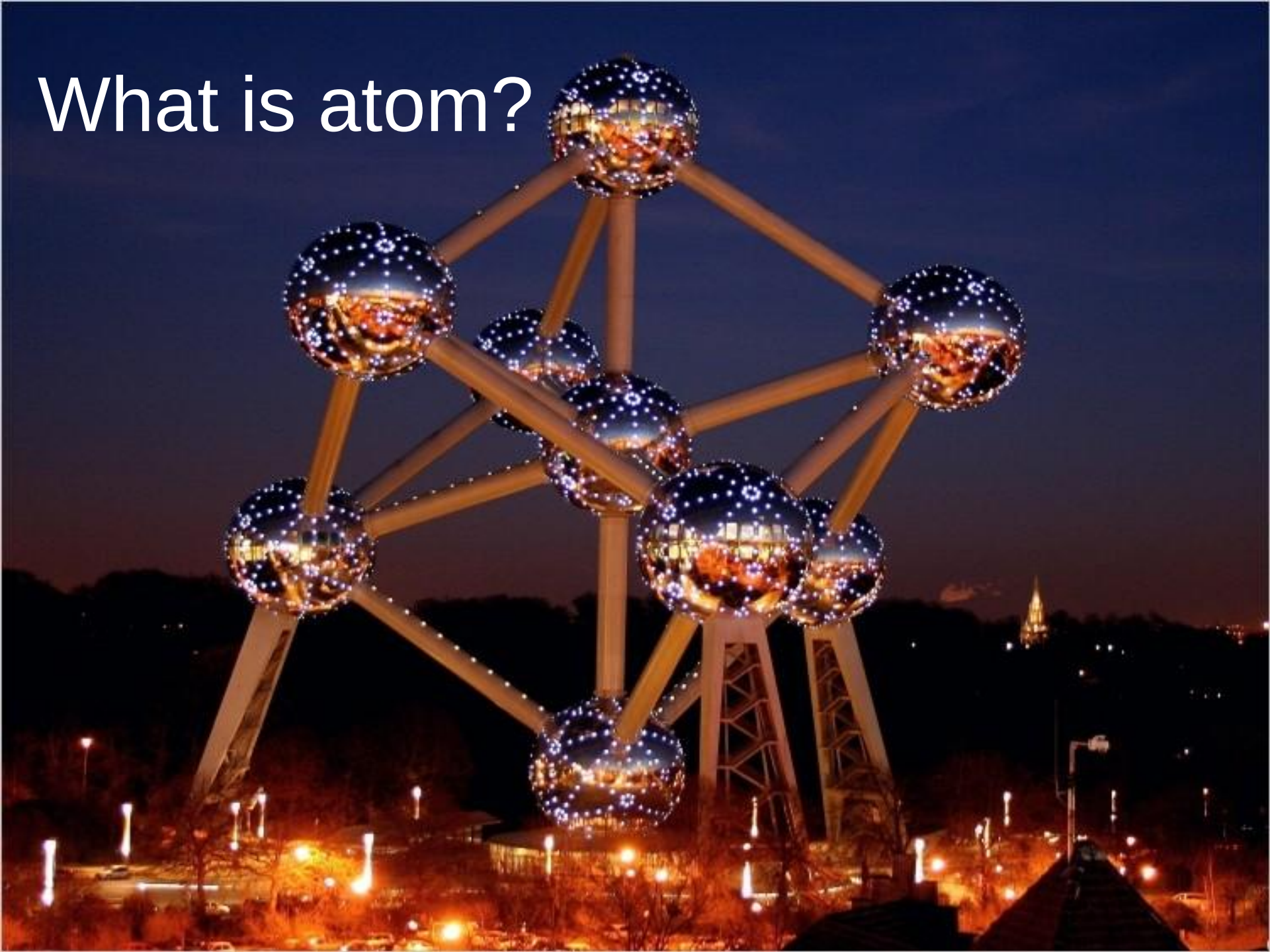
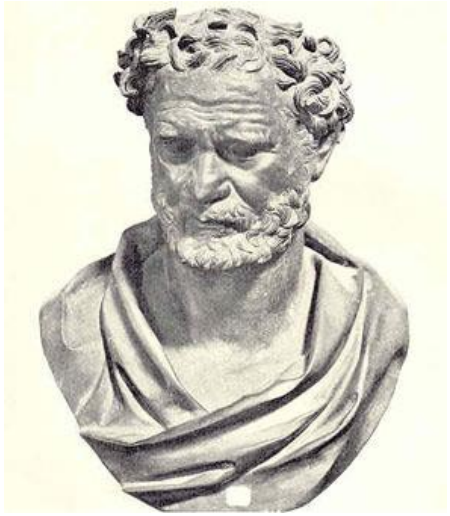
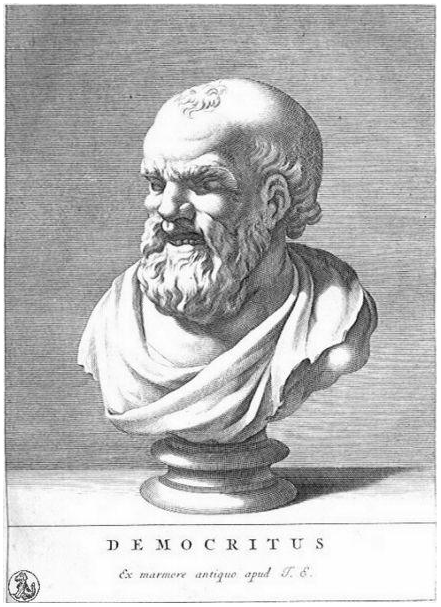
What is atom?



Atomic theory

- LEUCCIPUS and DEMOCRITUS (5th century BC) – originators of ancient atomism: THE ATOM is indestructible and indivisible element from which everything is made (*atomos* – indivisible)





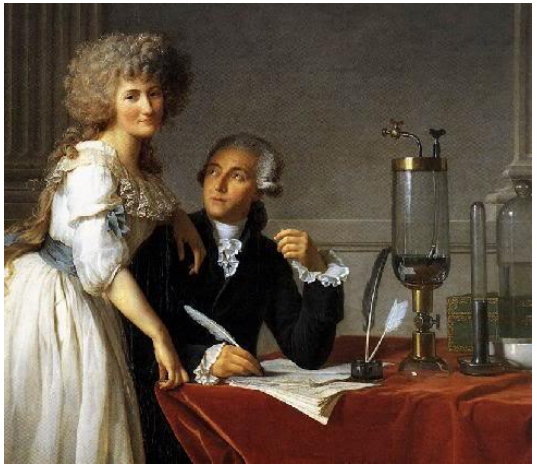
Atomic theory

- DALTON (19th cent.), scientific approach

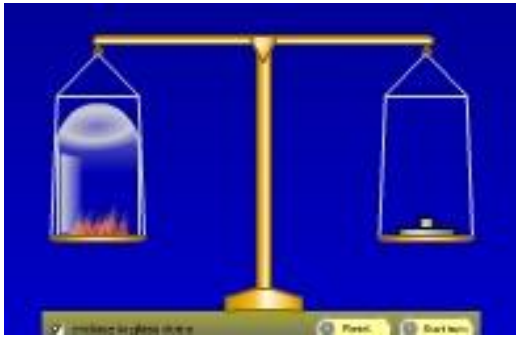
1. The elements are made from small pieces called atoms
2. Atoms of a given element are different from atoms of other elements according to their atomic weights
3. All atoms of a given element are identical
4. Atoms of one element can combine with atoms of other elements, forming chemical compounds; resulting compound always has the same relative number of types of atoms
5. Atom can not be created, divided into smaller portions or destroyed by chemical process; chemical reaction only changes the way the atoms are grouped

Chemical laws

1. The law of conservation of mass, Lavoisier, 1789.



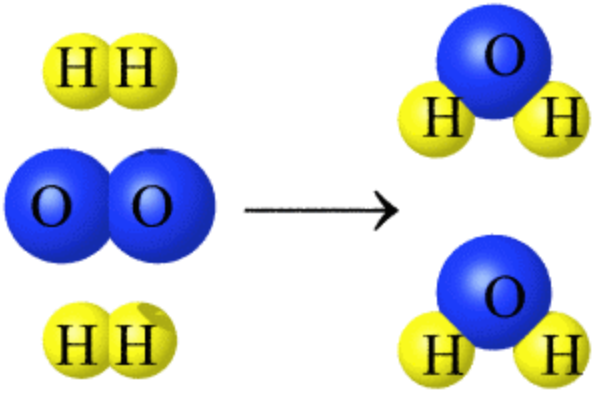
- No changes can be observed in the total mass of all substances involved in a chemical reaction.
- German chemist Landolt confirmed some 100 years after Lavoisier accuracy of this law with very precise measurement of the mass of the reaction vessel with the reaction system before and after the chemical reaction. The weight change of only 10^{-6} g could be observed.



Chemical laws

2. Law of definite proportions, Proust, 1799.

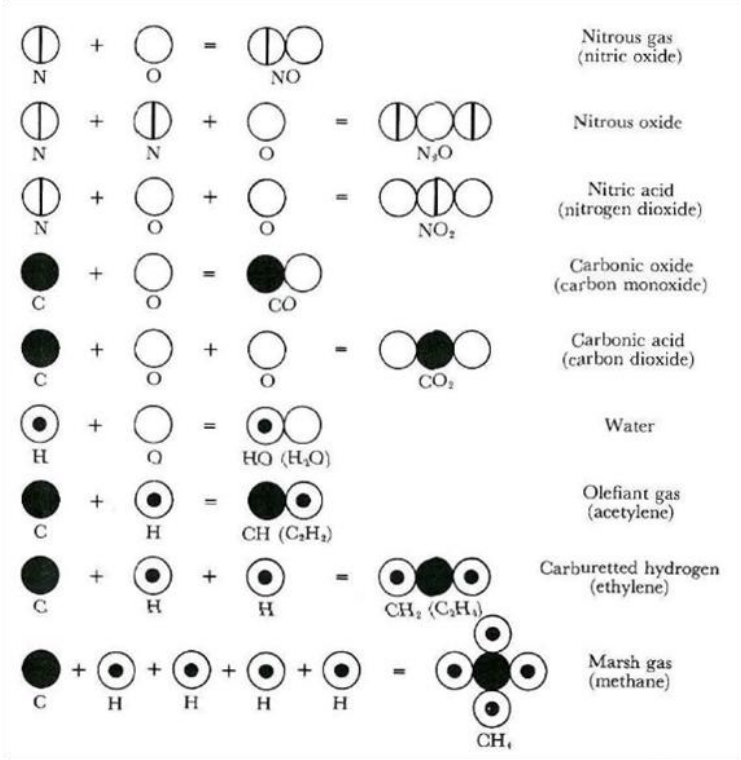
- Some particular chemical compound always contains exactly the same proportion of chemical elements by mass
- Water: composed of oxygen and hydrogen. Oxygen makes up about 88,81% of the mass of <u>any sample of pure water</u>, while hydrogen makes up the remaining 11,19% of the mass



Chemical laws

3. Law of multiple proportions, Dalton, 1803.

- If two elements form more than one compound between them, then the ratios of the masses of the second element which combine with a fixed mass of the first element will be ratios of small whole numbers (1:2:3 etc.)
- The masses of elementary substances with which they enter into mutual chemical reactions are called equivalent weights.

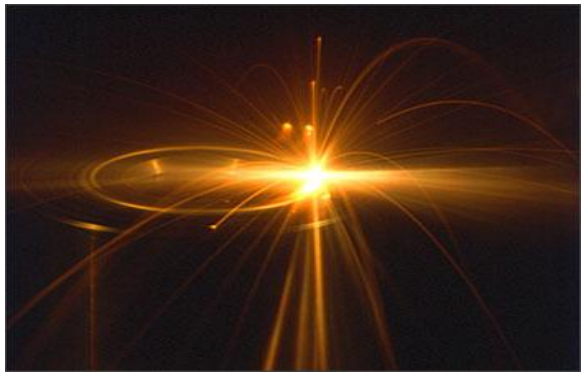


Chemical laws

4. Law of definite proportions (stoichiometry), Richter, 1789.

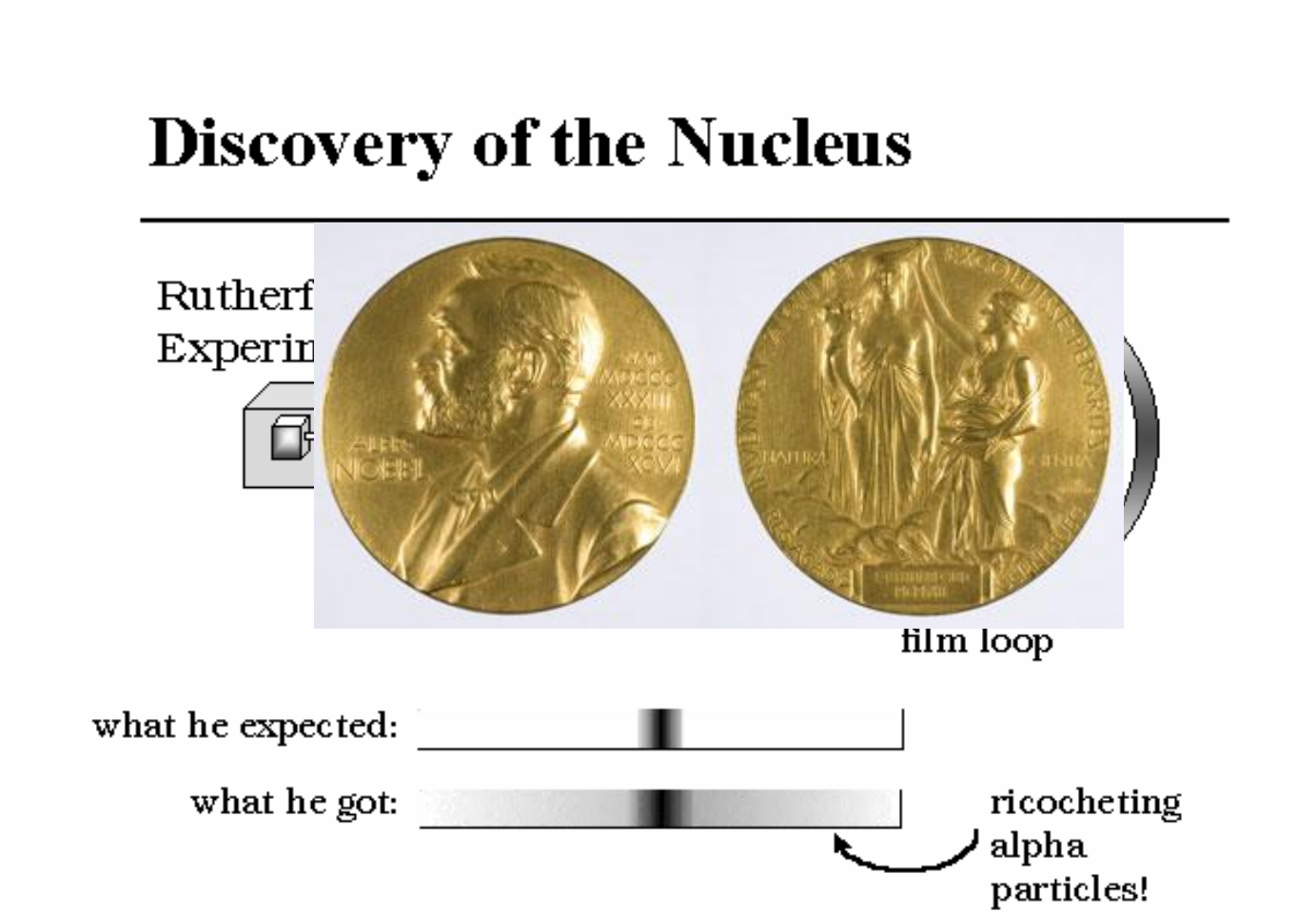
- The ratio by weight of the compounds consumed in a chemical reaction is always the same
- Introduced the term stoichiometry, which he defined as the *art of chemical measurements, which has to deal with the laws according to which substances unite to form chemical compounds*.

Electron



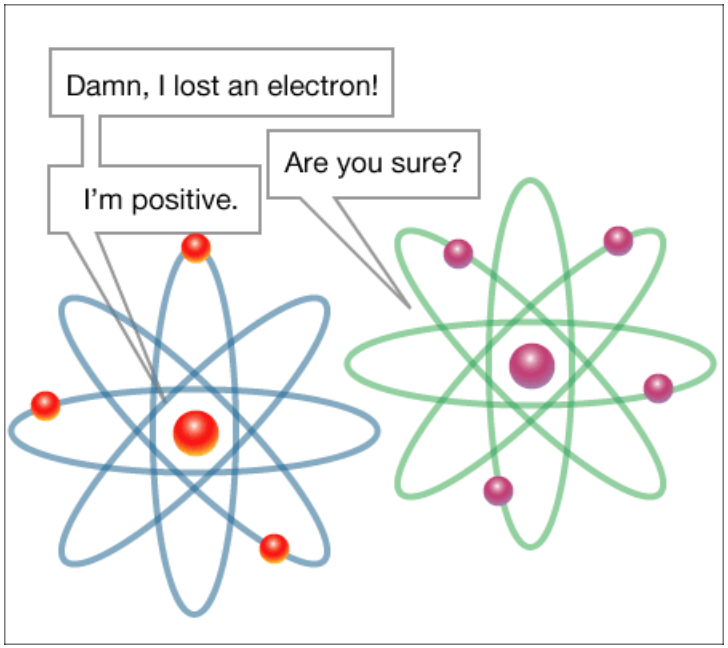
- Discovery of the first electron Thomson 1897.
- Dalton: “Atom is indivisible particle!” 
- Negative particle with charge $-1{,}6 \cdot 10^{-19}$ C
- Negligible mass
- It has a spin - rotation about its own axis, creating a magnetic field

Atomic nucleus



Atomic nucleus

- PROTONs (+, p); charge = $+1{,}6 \cdot 10^{-19}$ C
- NEUTRONs (0, n); charge = 0 C
- Mass of proton = mass of neutron ≈ 1840 x electron mass
- Number of protons = number of neutrons



- ATOMIC NUMBER, Z: number of protons or electrons
- MASS NUMBER, A: number of protons+neutrons, i.e. the number of nucleons

Mass number → A

Atomic number → Z

X

- ISOTOPE: same number of protons, different number of neutrons
- elements occur in nature as mixtures of isotopes
- i.e. Sn has 10 isotopes

$^{1}_{1}H$ protium

$^{2}_{1}H$ deuterium

$^{3}_{1}H$ tritium

Atomic mass

- very small, determined by mass spectrometry
- more significant relationship of atomic mass to another atom
- RELATIVE ATOMIC (MOLECULAR) MASS, Ar (Mr)

$$Ar(X) = \frac{\overline{m}_a(X)}{\frac{m_a(^{12}C)}{12}}$$

- $\overline{m}_a(X)$ average mass of atom X
- $\frac{m_a(^{12}C)}{12} = m_u = 1{,}66 \cdot 10^{-27}\,kg$ unified atomic mass unit

Mole

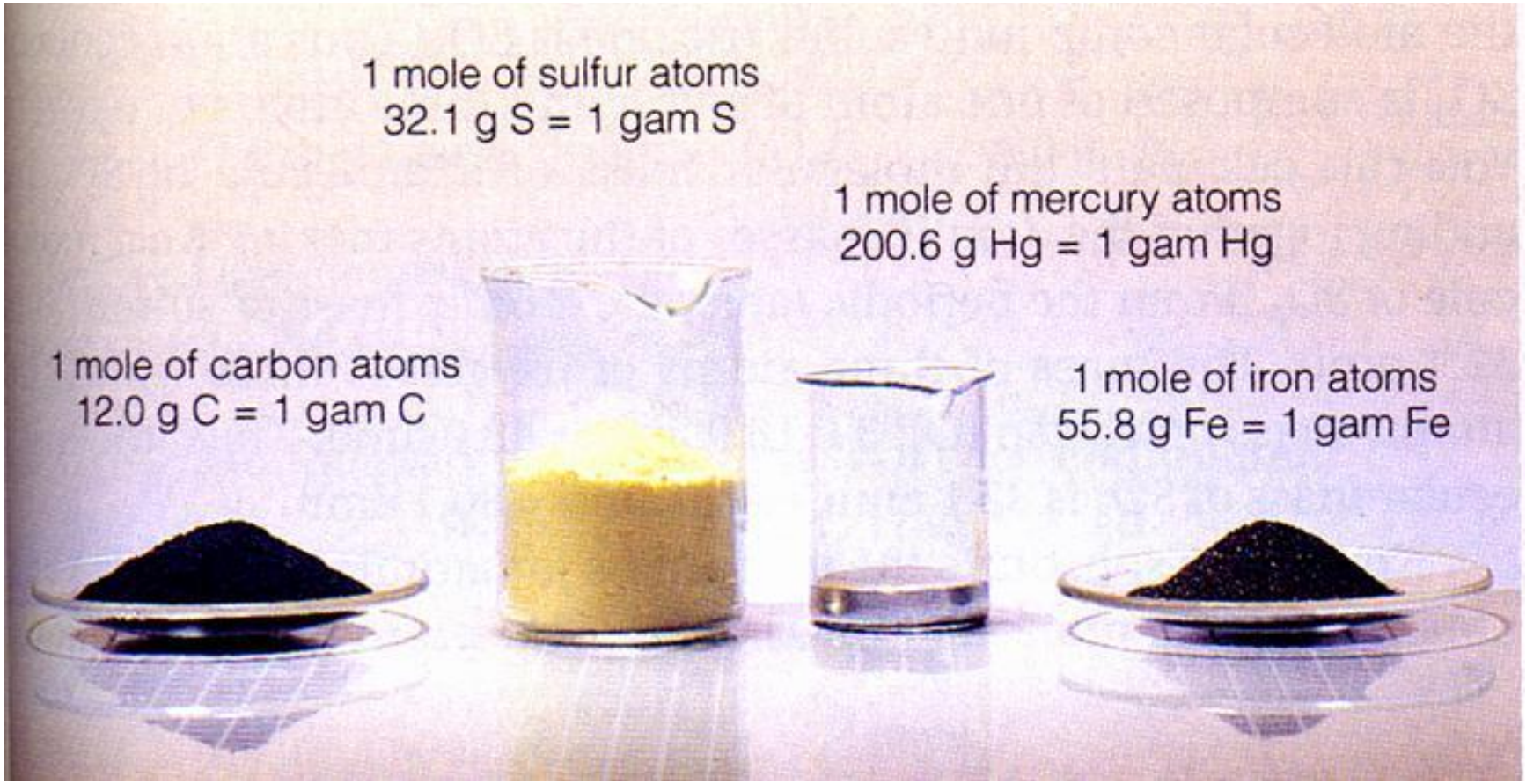
- MOLE, n = amount of a substance that contains as many elementary entities as there are atoms in 12 g of pure carbon-12 (^{12}C)
- elementary entity – atoms, molecules, ions, electrons, photon.....

- In one mol of any substance there is AVOGADRO'S NUMBER of entities, N_A, L

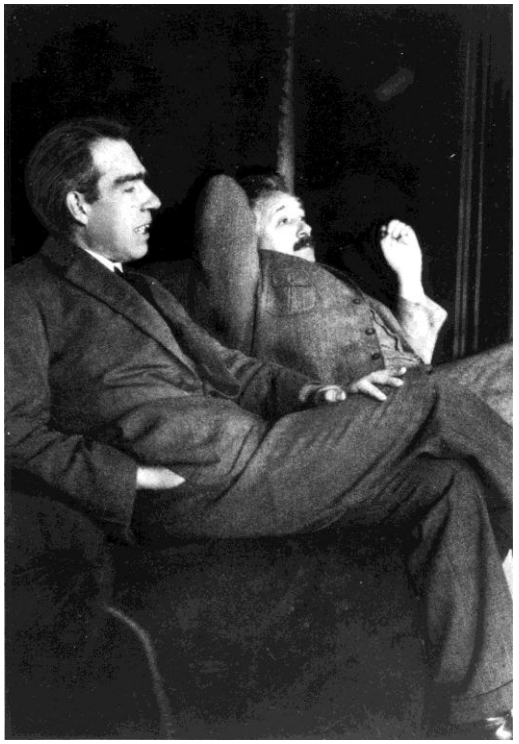
$$N_A = 6{,}022 \cdot 10^{23}\ mol^{-1}$$

- MOLAR MASS, M = numerically equal to Ar or Mr expressed in grams

$$M = \frac{m}{n}$$

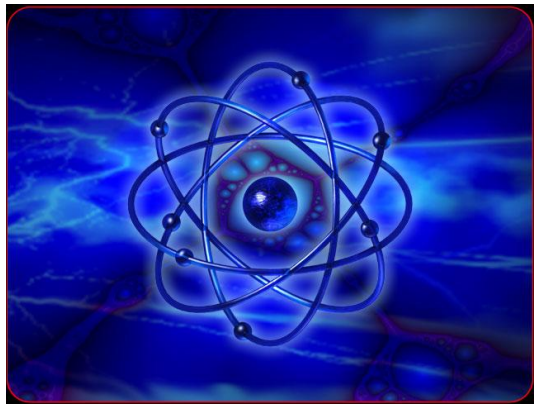

1 mole of sulfur atoms
32.1 g S = 1 gam S
1 mole of mercury atoms
200.6 g Hg = 1 gam Hg
1 mole of carbon atoms
12.0 g C = 1 gam C
1 mole of iron atoms
55.8 g Fe = 1 gam Fe

Arrangement of electrons in atoms



BOHR's MODEL

- Electrons move around nucleus on allowed circular orbits
- Energy of electrons is quantized
- Line spectra can be explained
- This model does not explain the scattering of spectra in the electric and magnetic field



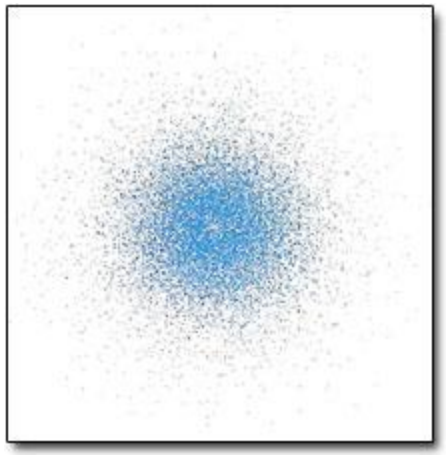
Distribution of electrons in atoms

QUANTUM MECHANICS THEORY

- dual properties of electron: particle or wave
- based on solutions of Schrödinger's equation

$$-\frac{h^2}{8\pi^2 m}\left(\frac{d^2\Psi}{dx^2}\right)+V\Psi=E\Psi$$

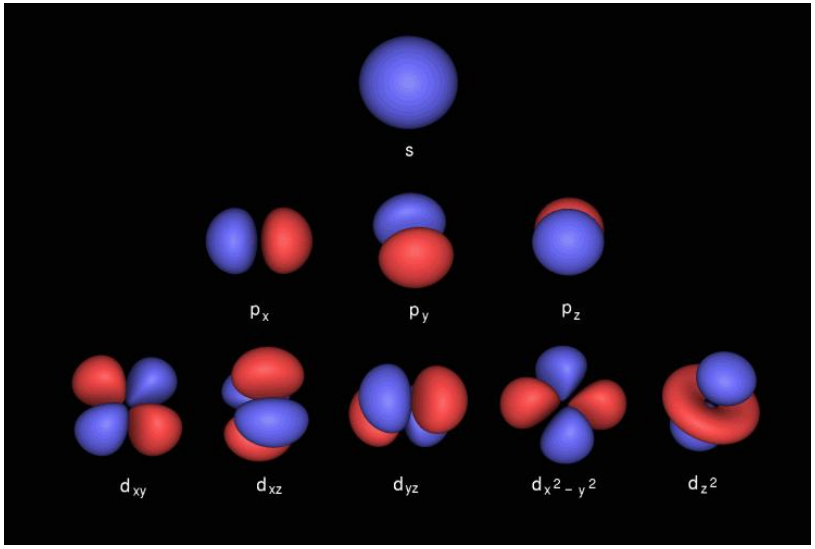
h – Planck constant = $6{,}63\cdot10^{-34}$ Js
V – potential energy of electron
E – total energy of electron
Ψ – wave function or ORBITAL



- solution of Sch. equation only gives the probability of finding an electron in any space around the nucleus.

ATOMIC ORBITAL

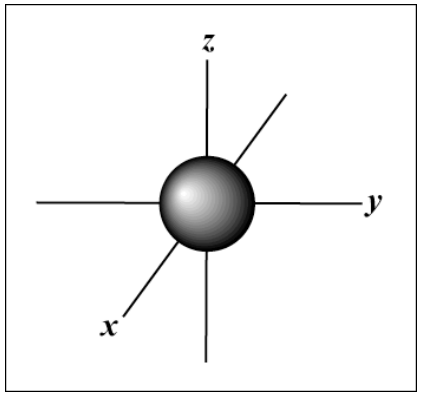
- Mathematical = amplitude of electron wave
- Physically = space in which electron moves wavy with a high probability
- Descriptive = border area in which there are 90-95% of electron density

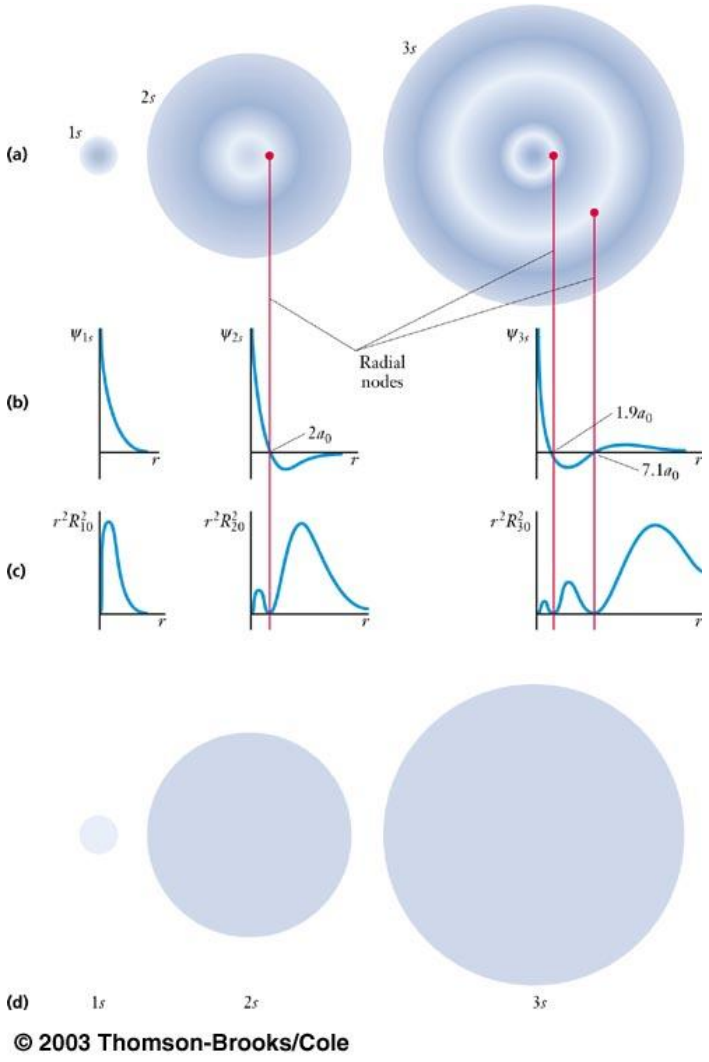


s-orbital

- spherically-symmetric;
- the probability of electron density decreases moving away from the nucleus

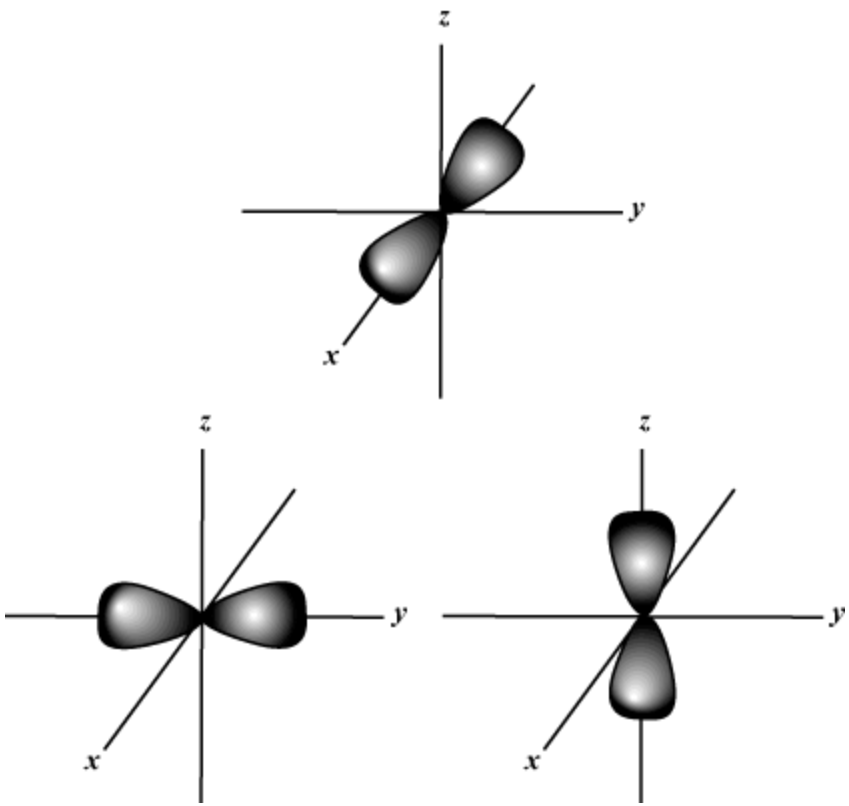
- 1s orbital is closer to the nucleus and has a lower energy than 2s orbital



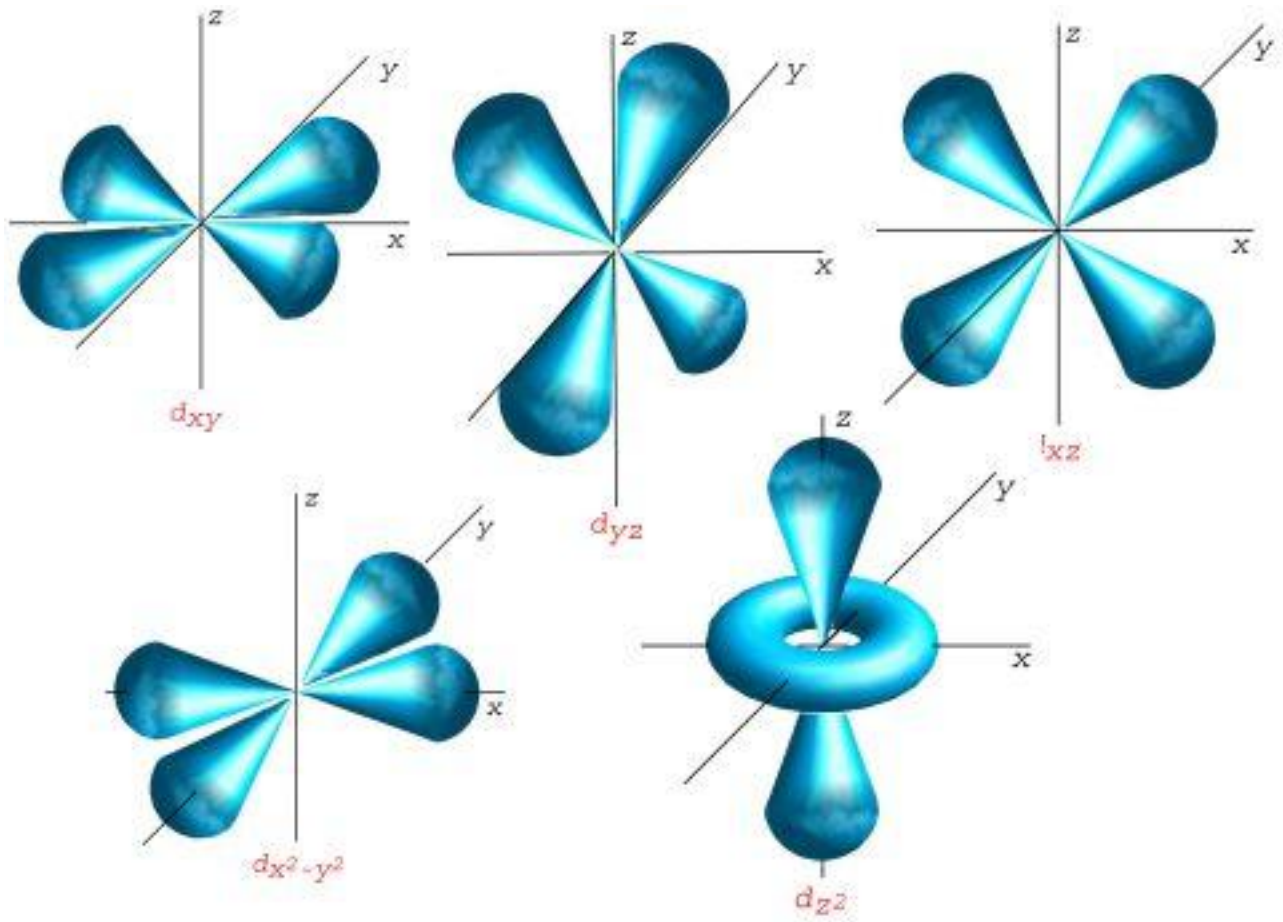


p-orbital

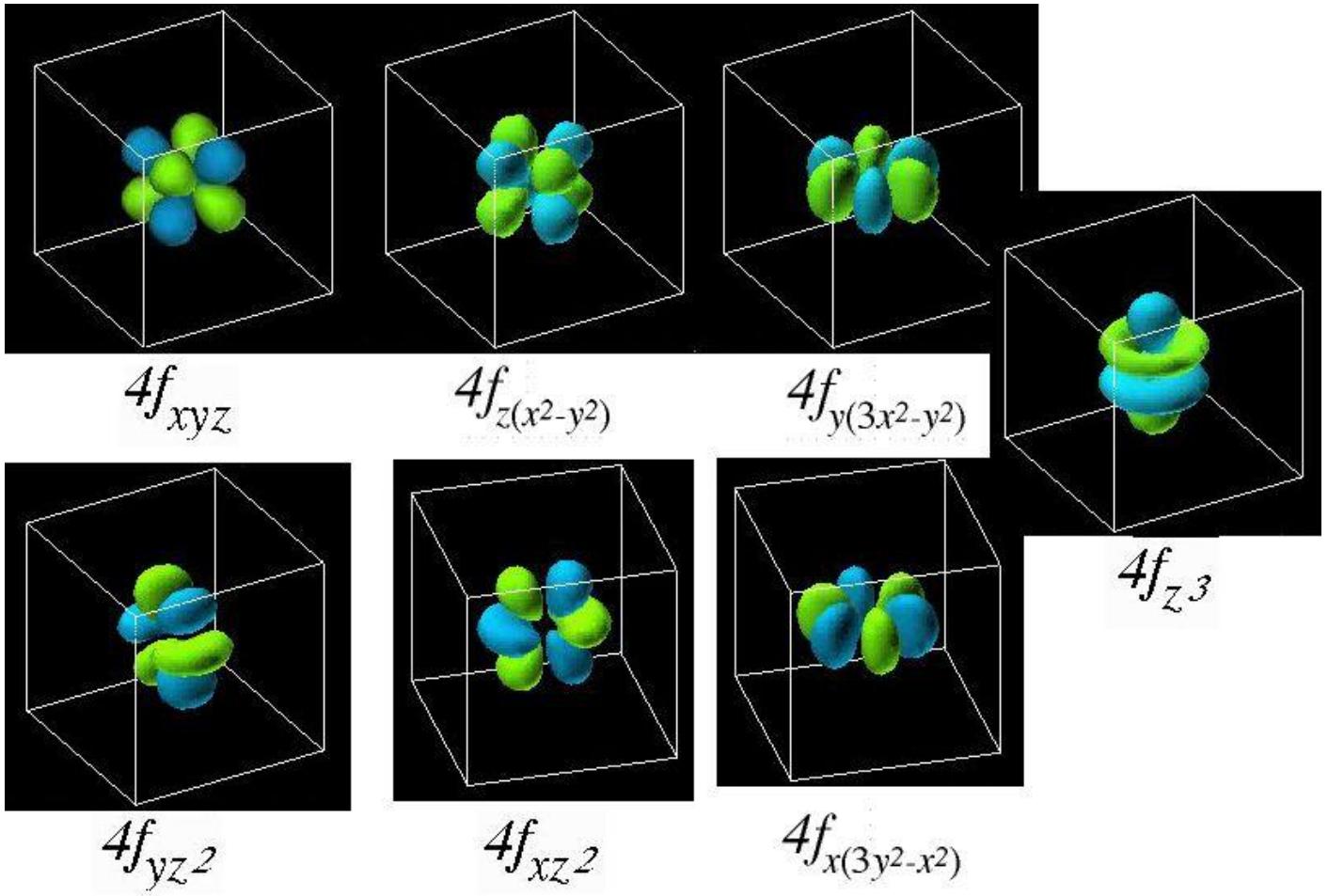
- wave equation has three solutions, i.e. from the second quantum state there are three p-orbitals: x, y and z
- electron density is equal on both sides of the nucleus, that is, there are two lobes



d-orbital

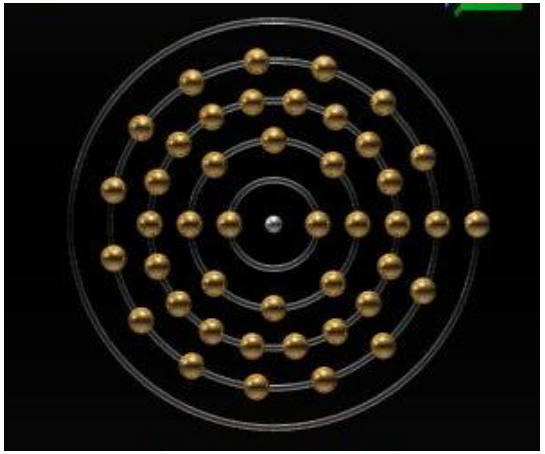


f-orbital



Electron configuration

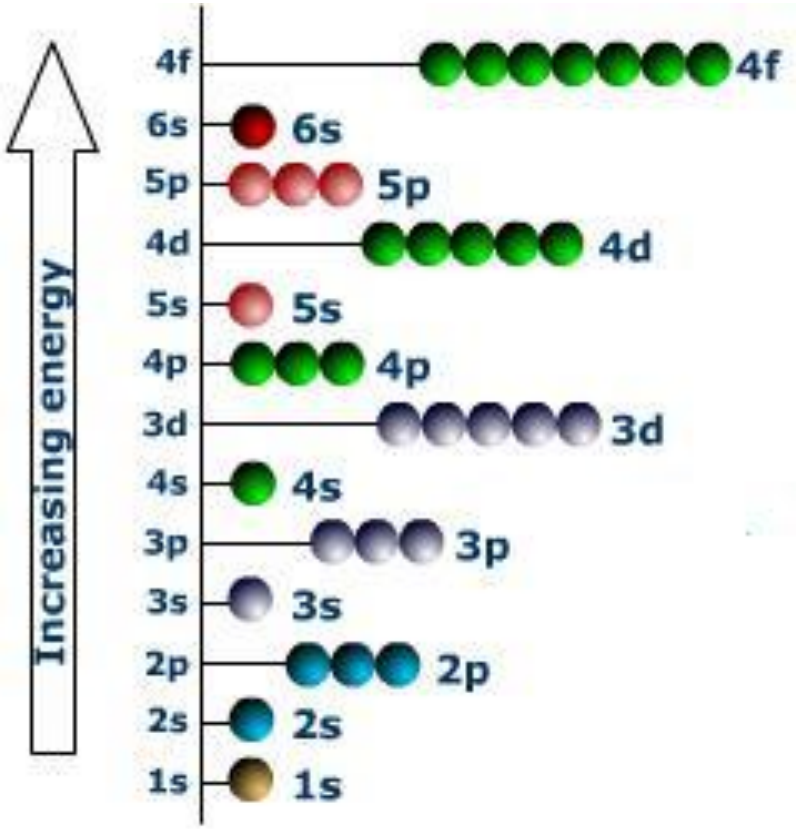
- the size of orbital depends on the charge of nucleus: a higher charge → volume lower
- in one orbital one can find two electrons of opposite spin
- ELECTRON CONFIGURATION – the distribution of electrons in atom or molecule
- electrons fill orbitals of the low energy to a higher
- in identical orbitals electrons are arranged so that the number of unpaired electrons is the maximum



Energy of orbital

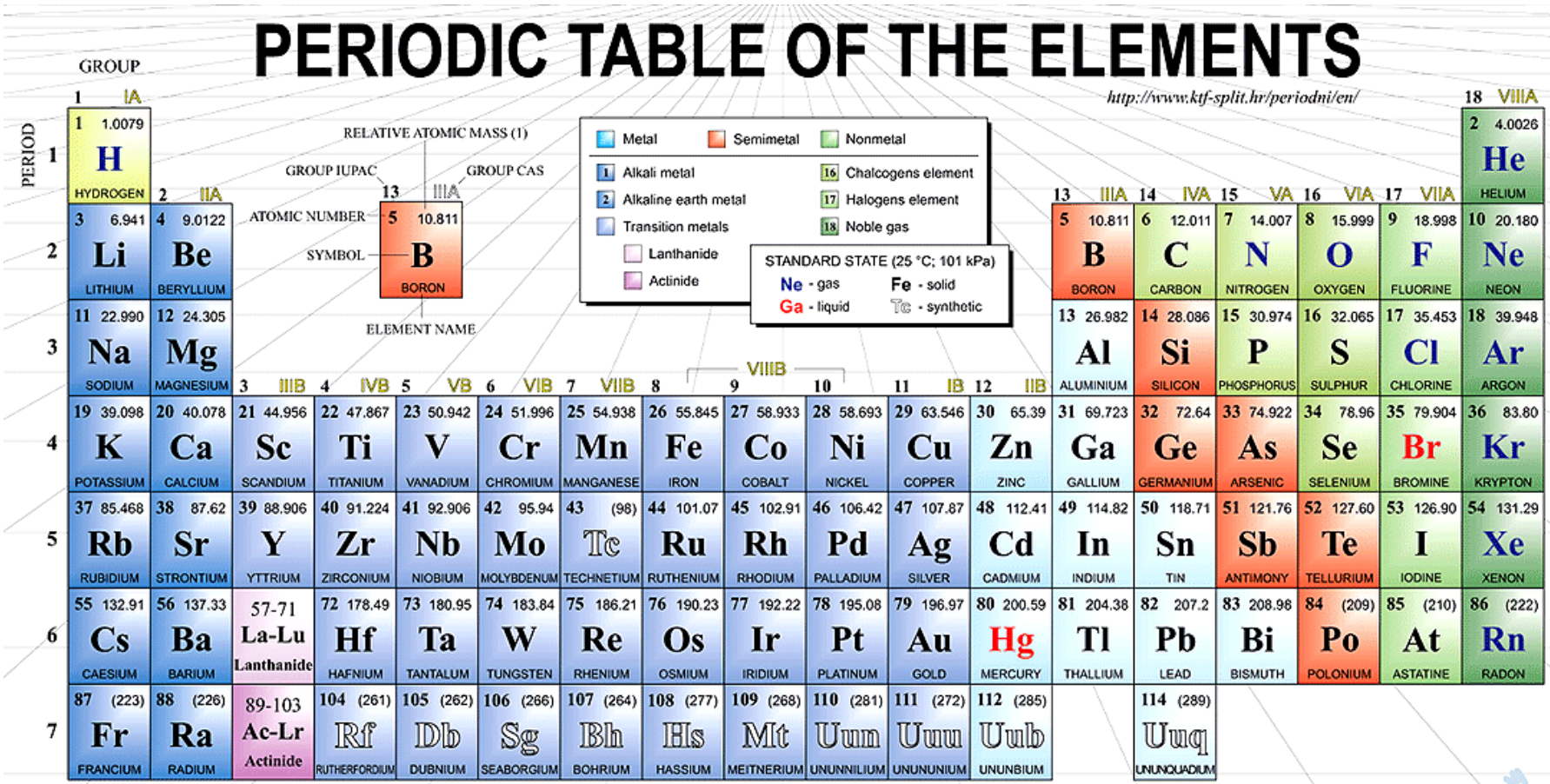
- in the same quantum state s, p and d orbitals have different energy
- i.e. E(3p) < E(3d)
- reason: different penetration to the nucleus
- also: E(4s) < E(3d)

  E(6s) < E(4f)



PERIODIC TABLE OF THE ELEMENTS

http://www.ktf-split.hr/periodni/en/



LANTHANIDE

57	58	59	60	61	62	63	64	65	66	67	68	69	70	71
138.91	140.12	140.91	144.24	(145)	150.36	151.96	157.25	158.93	162.50	164.93	167.26	168.93	173.04	174.97
La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
LANTHANUM	CERIUM	PRASEODYMIUM	NEODYMIUM	PROMETHIUM	SAMARIUM	EUROPIUM	GADOLINIUM	TERBIUM	DYSPROSIUM	HOLMIUM	ERBIUM	THULIUM	YTTERBIUM	LUTETIUM

ACTINIDE

89	90	91	92	93	94	95	96	97	98	99	100	101	102	103
(227)	232.04	231.04	238.03	(237)	(244)	(243)	(247)	(247)	(251)	(252)	(257)	(258)	(259)	(262)
Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr
ACTINIUM	THORIUM	PROTACTINIUM	URANIUM	NEPTUNIUM	PLUTONIUM	AMERICIUM	CURIUM	BERKELIUM	CALIFORNIUM	EINSTEINIUM	FERMIUM	MENDELEVIUM	NOBELIUM	LAWRENCIUM

(1) Pure Appl. Chem., 73, No. 4, 667-683 (2001)

Relative atomic mass is shown with five significant figures. For elements have no stable nuclides, the value enclosed in brackets indicates the mass number of the longest-lived isotope of the element.

However three such elements (Th, Pa, and U) do have a characteristic terrestrial isotopic composition, and for these an atomic weight is tabulated.

Editor: Aditya Vardhan (adivar@nettlinx.com)

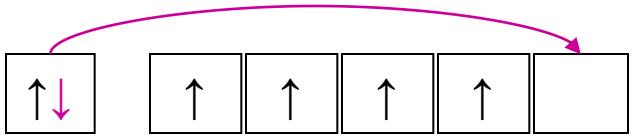
Filling of orbital with electrons

H	$1s^1$	He	$1s^2$
Li	$1s^2\ 2s^1$		
Be	$1s^2\ 2s^2 \rightarrow$ extremely stable configuration!		
B	$1s^2\ 2s^2\ 2p^1$		
C	$1s^2\ 2s^2\ 2p^2 \rightarrow 2p^1_x\ 2p^1_y$		
N	$1s^2\ 2s^2\ 2p^3 \rightarrow$ very stable configuration!		
Ne	$1s^2\ 2s^2\ 2p^6 \rightarrow$ closed shell configuration		
Na	$1s^2\ 2p^2\ 2p^6\ 3s^1$		
.....			
K	4s is filled, not 3d		
....			
Sc	all transition elements fill 3d orbital		
Lanthanides	4f orbital		

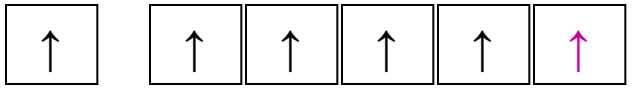
- Periodically repeating of el.configuration explains periodicity of chemical properties of elements

Filling of orbital with electrons

- Cr (atomic number 24)



$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ \cancel{4s^2}\ \cancel{3d^4}$



$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^1\ 3d^5$

much more stable configuration!

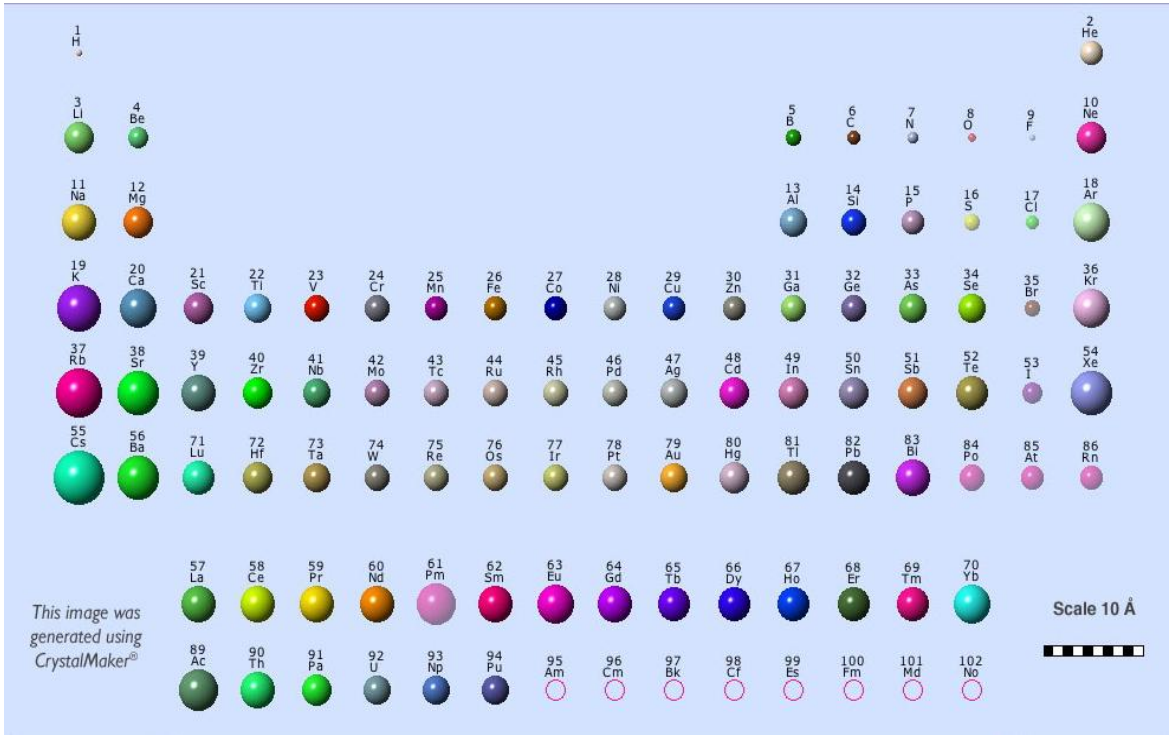
- configuration of noble gasses (closed shell) – the most stable → hardly make bonds with other elements
- next most stable configuration – half-filled orbitals (Mo, W...)

Periodicity of chemical properties of elements

- MAIN ELEMENTS – fill s and p orbitals
- TRANSITION ELEMENTS – fill d orbitals
- INNER-TRANSITION ELEMENTS (actinides and lanthanides) – fill f orbitals
- 7 periods – correspond to shells
- 18 groups – outer shell of the main elements have the same configuration
- ATOMIC RADIUS, IONIZATION ENERGY, ELECTRON AFFINITY

Atomic radius

- Increases downward because the number of shells increases
- decreases from left to right in each period because the force of nucleus attraction and the number of electrons that come into the same shell increase



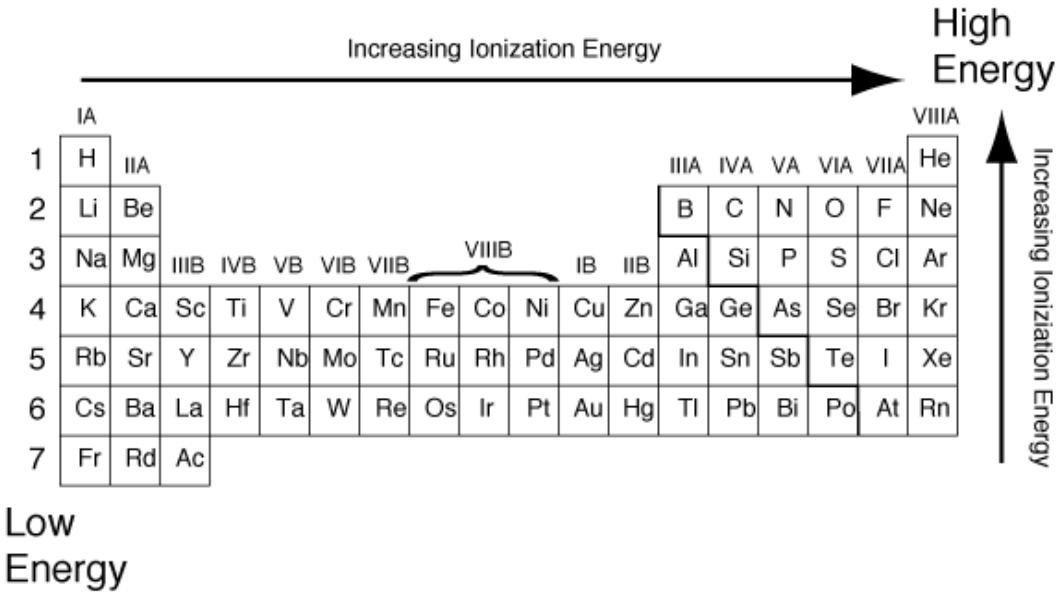
Ionization energy, E_i

- the energy it takes to remove an electron from an atom

$$\begin{array}{ll} A_{(g)} \rightarrow A^{+}_{(g)} + e & + E_{i,1} \\ A^{+}_{(g)} \rightarrow A^{2+}_{(g)} + e & + E_{i,2} \end{array} \Big\}+$$

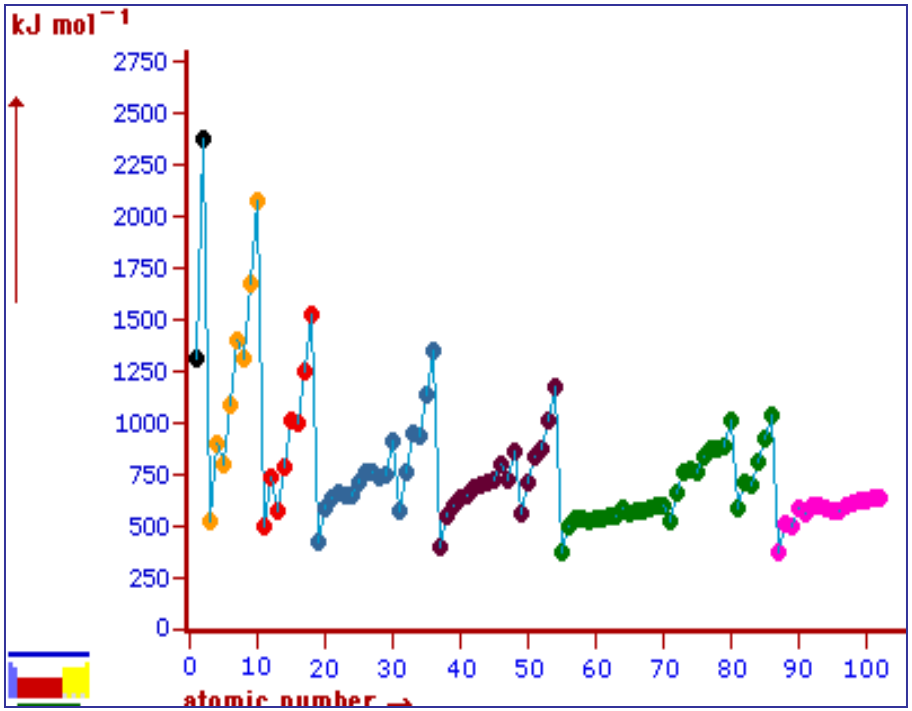
$$\overline{A_{(g)} \rightarrow A^{2+}_{(g)} + 2e} \qquad \overline{E_{i,1} + E_{i,2}}$$

$$E_{i,1} < E_{i,2}$$



- in group E_i decreases downward because radius increases and nucleus attraction force weak
- in period E_i increases from left to right because radius decreases

- exception because the stable configuration so it takes more energy to release electrons
- i.e. Be, N...



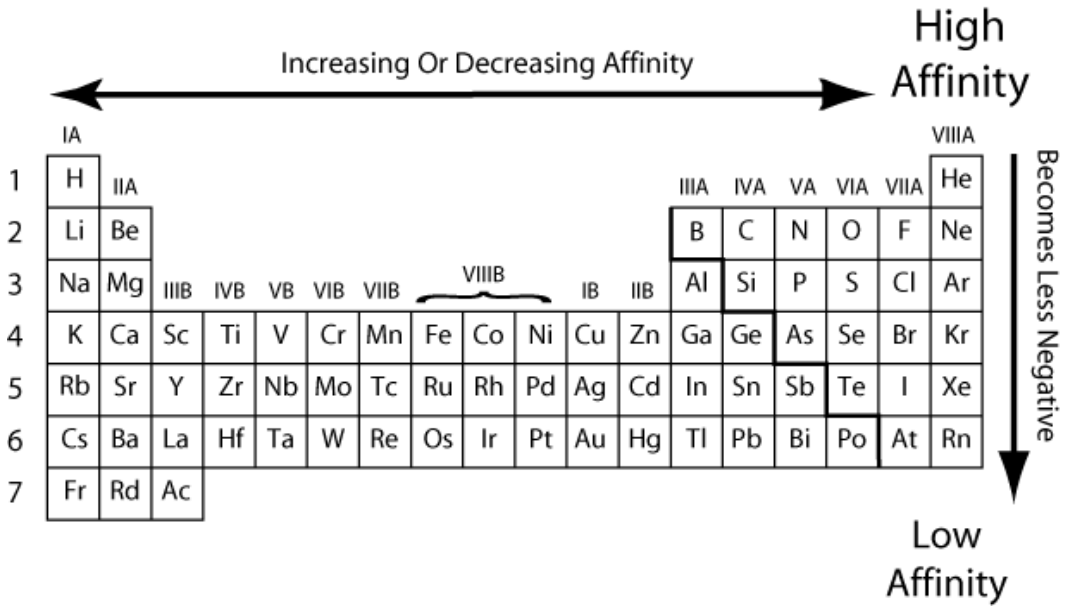
Electron affinity, E_a

- the amount of energy *released* or taken when an electron is added to a neutral atom or molecule to form a negative ion

$$\left.\begin{array}{l} A_{(g)} + e \rightarrow A^-_{(g)} \\ A^-_{(g)} + e \rightarrow A^{2-}_{(g)} \end{array}\right\}+ \qquad \begin{array}{l} \pm E_{a,1} \\ + E_{a,2} \end{array}$$

$$A_{(g)} + 2e \rightarrow A^{2-}_{(g)} \qquad E_{a,1} + E_{a,2}$$

$$\left.\begin{array}{ll} O_{(g)} + e \rightarrow O^-_{(g)} & E_{a,1} = -1{,}47 eV \\ O^-_{(g)} + e \rightarrow O^{2-}_{(g)} & E_{a,2} = +8{,}10 eV \end{array}\right\}+$$



- in group E_a decreases downward and becomes less negative
- in period E_a increases or decreases from left to right

- exception because the stable configuration so it takes more energy to release electrons
- i.e. noble gasses