Structure of atoms: Brief review

The bonding mechanisms between atoms are closely related to the structure of the atoms themselves.

Atoms = nucleus (protons and neutrons) + electrons

Charges:

Electrons and protons have negative and positive charges of the same magnitude, 1.6×10^{-19} Coulombs.

Neutrons are electrically neutral.

Masses:

Protons and Neutrons have the same mass, 1.67×10^{-27} kg.

Mass of an electron is much smaller, 9.11×10^{-31} kg and can be neglected in calculation of atomic mass.

protons gives chemical identification of the element

 # protons = atomic number (Z)

neutrons defines isotope number

The atomic mass (A) = mass of protons + mass of neutrons

Atomic mass units. Atomic weight.

The atomic mass unit (amu) is often used to express atomic weight.

1 amu is defined as 1/12 of the atomic mass

of the most common isotope of carbon atom that has 6 protons (Z=6) and six neutrons (N=6).

$\mathbf{M}_{proton} \approx \mathbf{M}_{neutron} = 1.66 \text{ x } 10^{-24}$ g = 1 amu.

The atomic mass of the 12C atom is 12 amu.

The atomic weight of an element = weighted average of the atomic masses of the atoms naturally occurring isotopes.

Atomic weight of carbon is 12.011 amu.

The atomic weight is often specified in mass per mole.

A mole is the amount of matter that has a mass in grams equal to the atomic mass in amu of the atoms (A mole of carbon has a mass of 12 grams).

The number of atoms in a mole is called the Avogadro number, Nav = 6.023×10^{23}.

1 amu/atom = 1 gram/mol

<u>Example:</u>

Atomic weight of iron = 55.85 amu/atom = 55.85 g/mol

The number of atoms per cm3, n, for material of density ***d*** (g/cm3) and atomic mass M (g/mol):

$$n = Nav \times d / M$$

- Graphite (carbon): d = 2.3 g/cm3, M = 12 g/mol

n = 6×10^{23} atoms/mol × 2.3 g/cm3 / 12 g/mol = 11.5×10^{22} atoms/cm3

- Diamond (carbon): d = 3.5 g/cm3, M = 12 g/mol

n = 6×10^{23} atoms/mol × 3.5 g/cm3 / 12 g/mol = 17.5×10^{22} atoms/cm3

- Water (H_2O) d = 1 g/cm3, M = 18 g/mol

n = 6×10^{23} molecules/mol × 1 g/cm3 / 18 g/mol = 3.3 × 1022 molecules/cm3

For material with n = 6×10^{22} atoms/cm3 we can calculate mean distance between atoms L = (1/n)1/3 = 0.25 nm.

The scale of atomic structures in solids – a fraction of 1 nm or a few A .

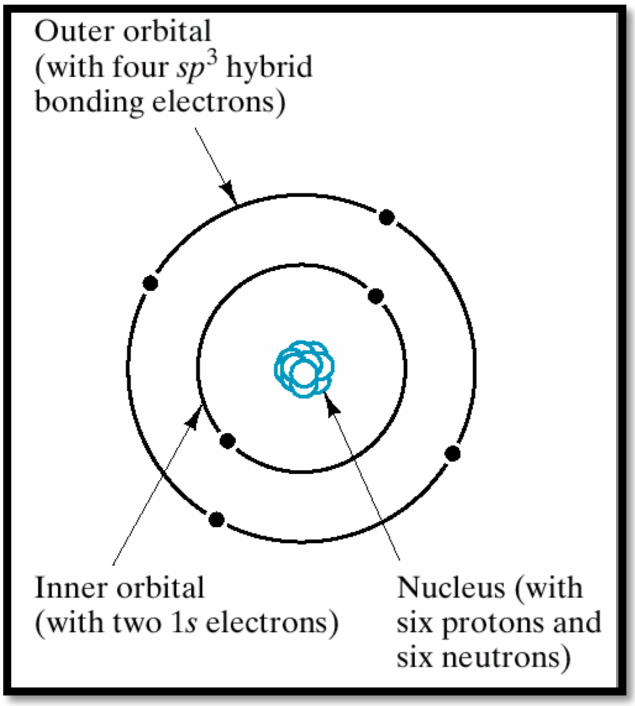
Electrons in Atoms

Electrons move not in circular orbits, but in 'fuzzy‘ orbits.

Actually, we cannot tell how it moves, but only can say what is the probability of finding it at some distance from the nucleus.

Only certain “orbits” or shells of electron probability densities are allowed.

- The shells are identified by a **principal quantum number n**, which can be related to the size of the shell, n = 1 is the smallest; n = 2, 3 .. are larger.
- **The second quantum number l,** defines subshells within each shell.
- **Two more quantum numbers** characterize states within the subshells.
- **Pauli Exclusion Principle**: only one electron can have a given set of the four quantum numbers.

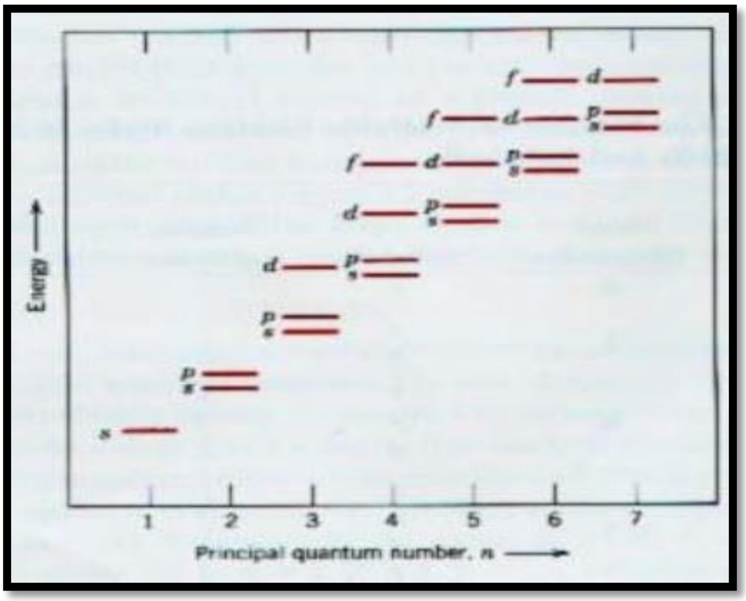


The number of available states in electron shells & subshells

Principal Q. N., n		Subshells	Number of States	Number of Electrons Per Subshell	Number of Electrons Per Shell
1 (l=0)	*K-shell*	s	1	2	2
2 (l=0)	*L-shell*	s	1	2	8
2 (l=1)		p	3	6	
3 (l=0)	*M-shell*	s	1	2	18
3 (l=1)		p	3	6	
3 (l=2)		d	5	10	
4 (l=0)	*N-shell*	s	1	2	32
4 (l=1)		p	3	6	
4 (l=2)		d	5	10	
4 (l=3)		f	7	14	

Each "orbit" or shell can accommodate only a maximum number of electrons, which is determined by quantum mechanics.

- In brief, the most inner *K-shell* can accommodate only two electrons, called *s-electrons*;
- the next *L-shell* two *s-electrons* and six *p-electrons*;
- the *M-shell* can host two *s-electrons*, six *pelectrons*, and ten *d-electrons*; and so on.



Subshells by energy: 1s,2s,2p,3s,3p,4s,3d,4s,4p,5s,4d,5p,6s,4f,…

- Electrons that occupy the outermost filled shell – **the valence electrons** – they are responsible for bonding.
- Electrons fill quantum levels in order of increasing energy (only n, l make a significant difference).

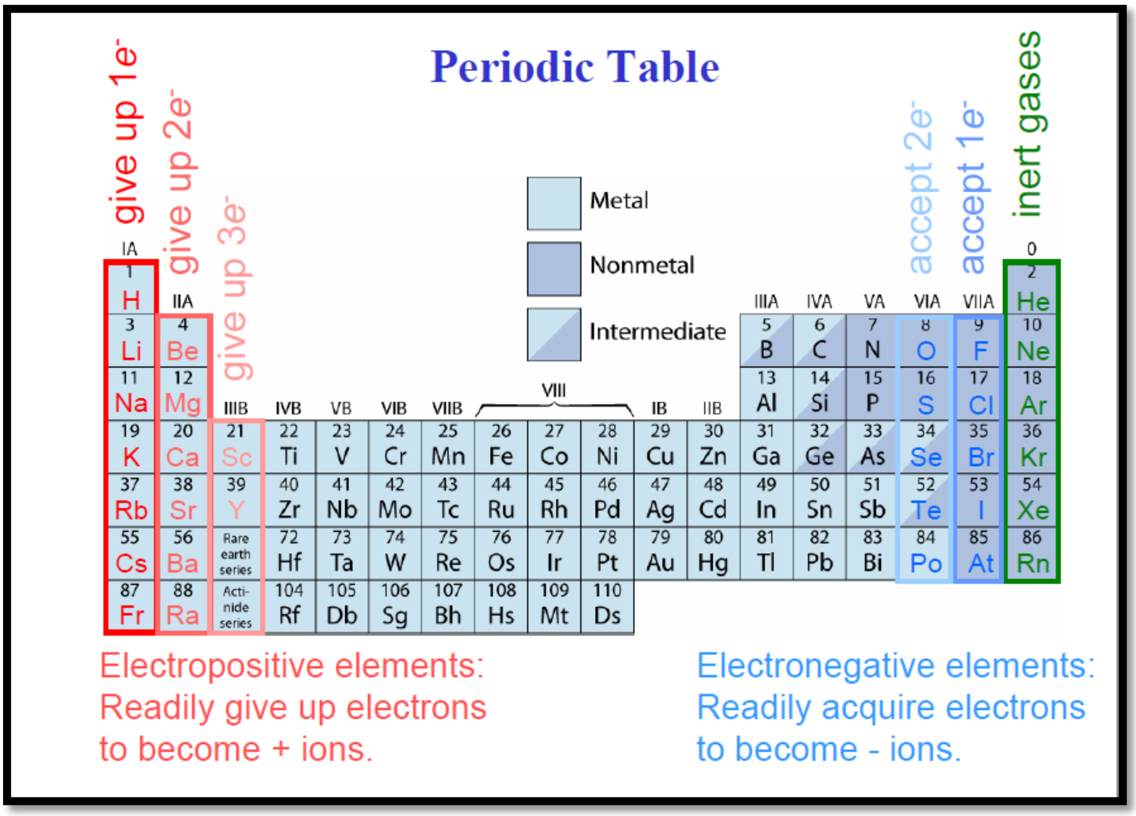
Examples:

Argon, Z = 18: 1s22s22p63s23p6

Iron, Z = 26: 1s22s22p63s23p63d64s2

<u>Periodic Table</u>

All elements in the periodic table have been classified **according to the electron configuration**.



1-Elements in the same column (Elemental Group) share similar properties. Group number indicates the number of electrons available for bonding.

2- 0: Inert gases (He, Ne, Ar...) have filled subshells: chem. inactive

3- IA: Alkali metals (Li, Na, K…) have one electron in outermost occupied s subshell - eager to give up electron – chem. active

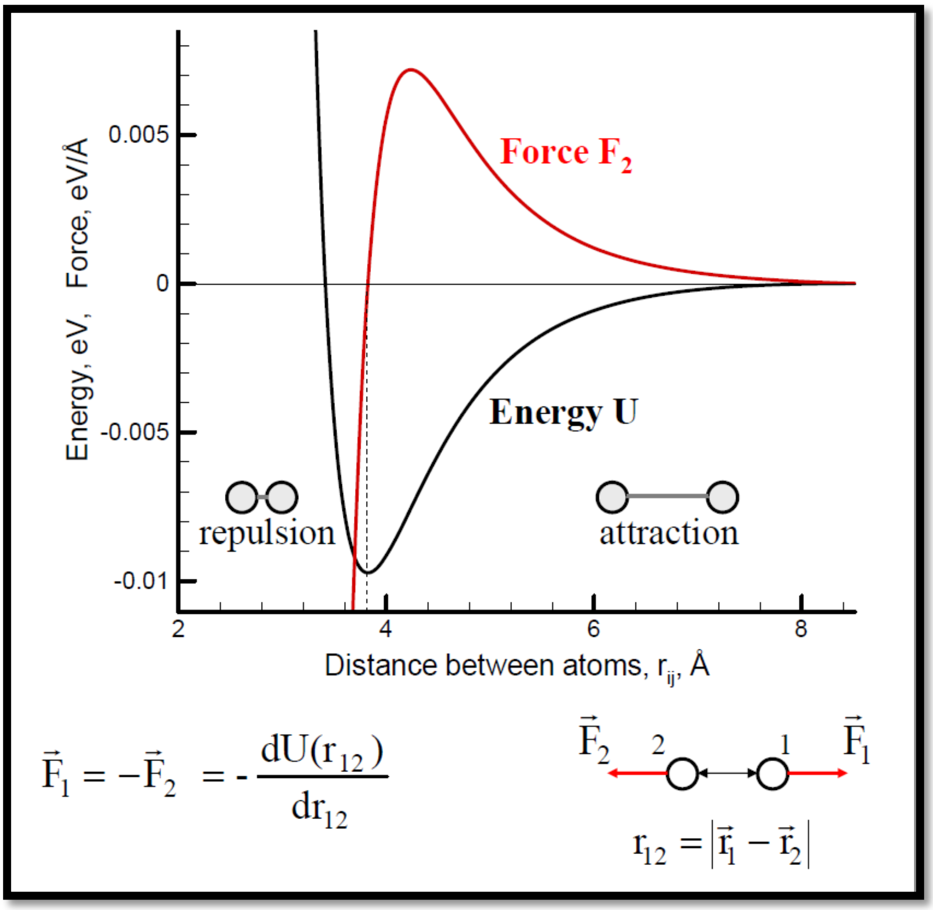
4-VIIA: Halogens (F, Br, Cl...) missing one electron in outermost occupied p shell - want to gain electron - chem. active

Electronegativity - a measure of how willing atoms are to accept electrons Subshells with one electron → low electronegativity Subshells with one missing electron → high electronegativity.

Electronegativity increases from left to right Metals are electropositive – they can give up their few valence electrons to become positively charged ions.

Bonding Energies and Forces

Forces can be calculated from the potential energy of interatomic interaction. For example, for a system of two atoms (e.g. a diatomic molecule), the potential depends only on the distance between the two atoms U(*r12*) .



The electron volt (eV)–energy unit convenient for description of atomic bonding.

Electron volt - the energy lost / gained by an electron when it is taken through a potential difference of one volt.

$$\mathbf{E = q \times V}$$

for q = 1.6 x 10-19 Coulombs and V = 1 volt

1 eV = 1.6 x 10-19 J