Organic Electronics

Electronic devices fabricated by means of organic molecules

Molecules containing C and H

Sometimes other elements could be present (O, N, P, S e alogens)

In the late 1977 a group of researchers led by Shirikawa, Heeger e MacDiarmid demontrated that by proper doping some polymers as polyacetylene with AsF_5 its conductivity could be increased by orders of magnitude

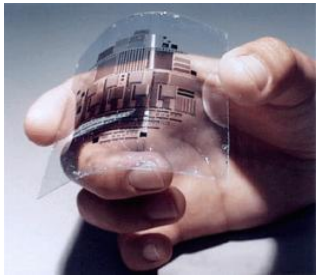
Plastics:

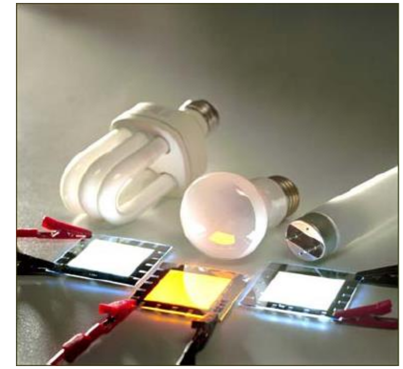
Insulators

Semiconductors

Conductors

Organic Electronics





OFET
(**O**rganic **F**ield-**E**ffect **T**ransistors)

Solar Cells

OLED
(**O**rganic **L**ight **E**mitting **D**iode)

Applicazioni:
Smart wearable electronics
Solar Energy
Flexible Displays
Electronic paper

Organic Electronics

Vantaggi:

- ✓ thin films, flexible, large areas
- ✓ Low Temperature
- ✓ Low cost technology (inkjet printing etc.)
- ✓ Suitable for transparent applications
- ✓ Tunable electrical properties

Svantaggi:

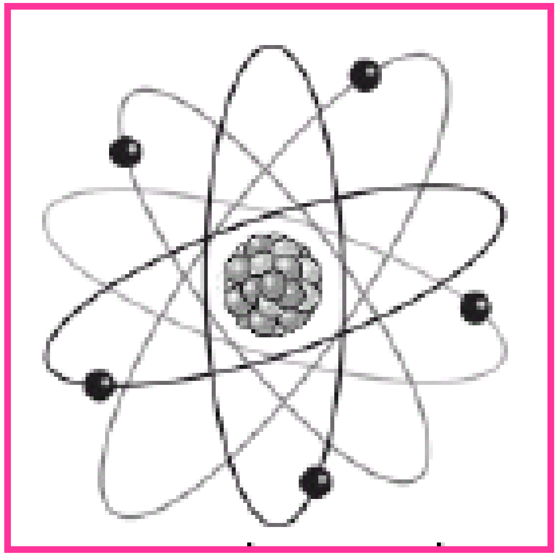
- ✓ Less reliable and reproducible
- ✓ Lower mobility → slower devices
- ✓ Aging effects

A little bit of Chemistry

The Atom

An atom is made out of a massive and dense core, positively charged, where protons and neutros are placed, which is called nucleus (average dimensions 10^{-15} m)

A cloud of electrons with dimensions around 10^{-10} m generally travelling at a speed around 10^{11} m/s.



The Periodic Table of Elements

Valence Electrons the electrons which are placed in the outer shell of an atom, and determine the properties of that element

Number of electrons in the outer shell → valence of the element

The periodic table is characterized by 7 rows.

Each row starts with an element having 1 valence electron and ends up with an element having its outer shell full

Hydrogen has only one electron, whereas Elium has two electrons.

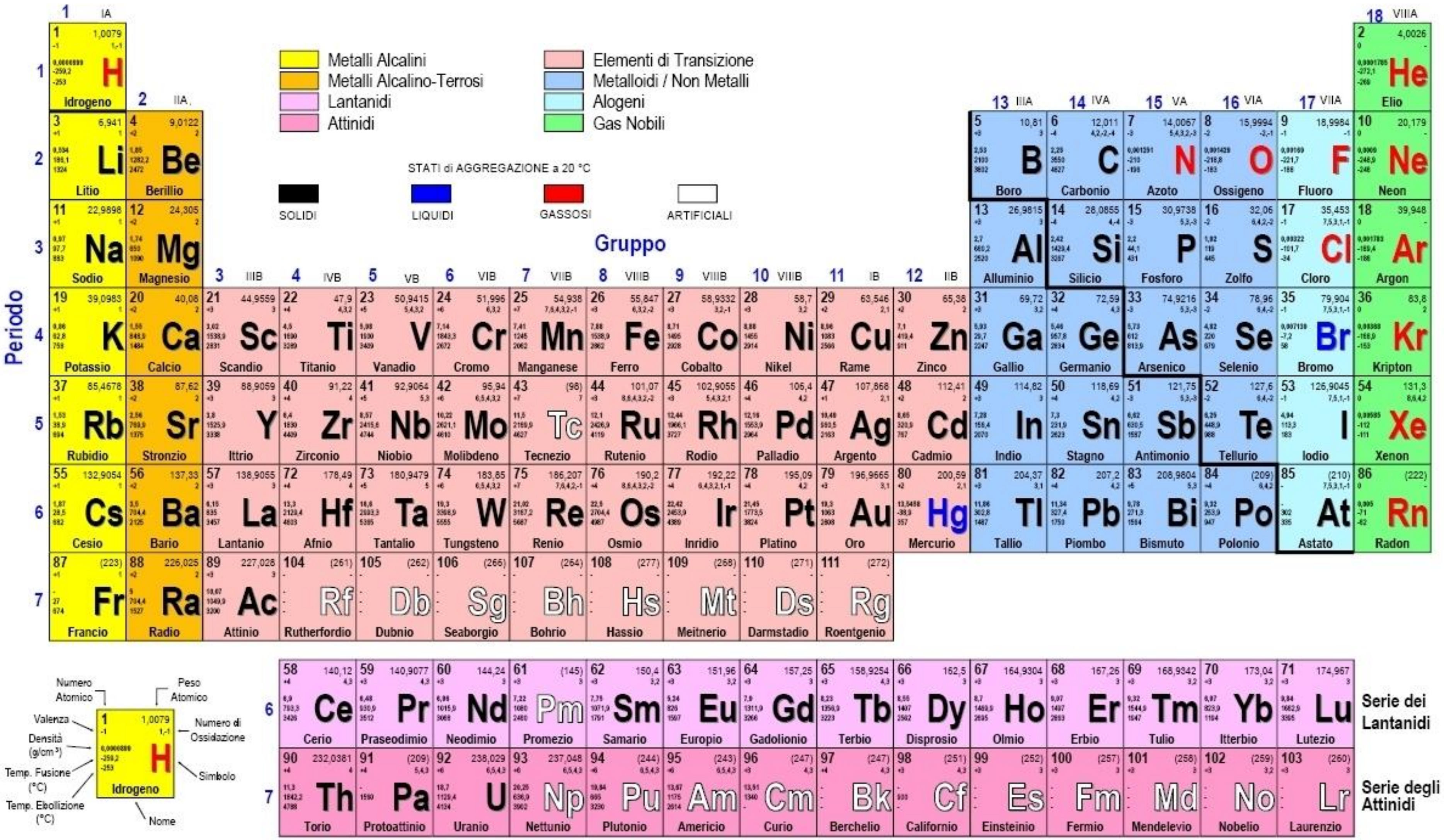
The Periodic Table of Elements

In all chemical reactions an atom tends to acquire or to give electrons in order to give rise to a more stable structure (molecule)

- **Electropositive elements** use to give electrons → **up to 4 valence electrons**

- **Electronegative elements hav from 4 to 8 valence electrons** they want to acquire electrons

The Periodic Table of Elements



Flash back
Schroedinger

Hydrogen atom

The solution of the radial part of the Schroedinger equation for the hidrogen atom allowed us to obtain the possible energies

$$E_n = -\frac{me^4}{8\varepsilon_0^2 h^2}\frac{1}{n^2} \qquad n = 1,2,3,...$$

We have introduced two integer numbers

- n = 1,2,3,…
- l = 0,1,2,…,n – 1

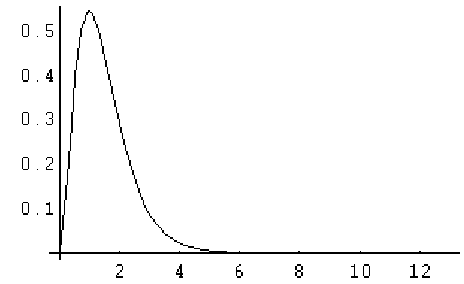
Hydrogen atom

For the fundamental state (n = 1), there will be only one l value, and the energy will be -13. 6 eV (ionization energy for hydrogen)

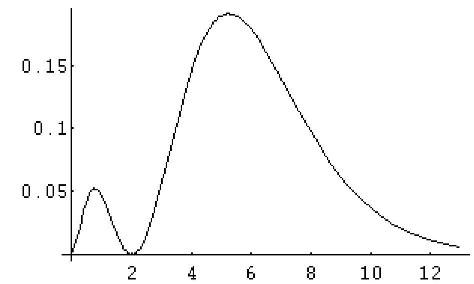
The first excited state (**n = 2**) will give place to two l values (l = 0 ed l = 1), but only one energetic level (in **E_n depends only on n**)

Degenere energy levels, same energy but **different wave functions!**

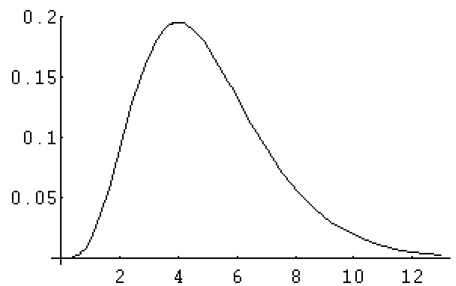
Hydrogen atom



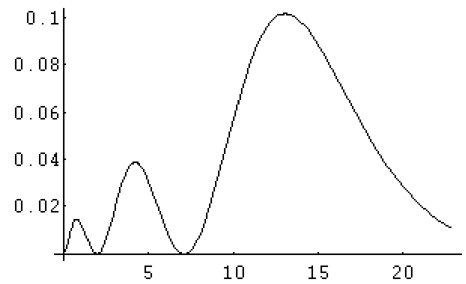
State 1s,
n=1, l=0



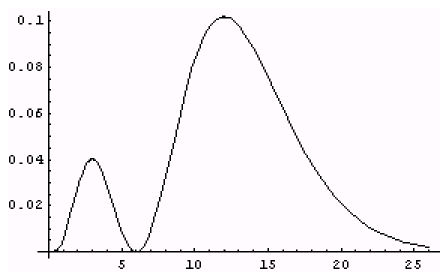
State 2s,
n=2, l=0



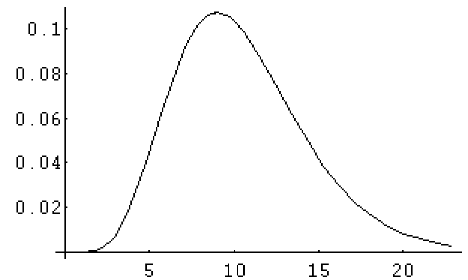
State 2p,
n=2, l=1



State 3s,
n=3, l=0



State 3p,
n=3, l=1



State 3d,
n=3, l=2

Hydrogen atom

The angolar part solution of Scroedinger equation led us to a third quantic number called m = -l, -l+1,..0,..l-1, l (magnetic momentum number).

Therefore:

Given a certain n, there will be a single energetic level, but n different l values and 2l+1 different m values

Moreover we also have the spin number that can acquire only two values +1/2 e -1/2.

Hydrogen atom

Orbital wave functions

l=0 → s states (m=2l+1=1)	number of s type orbitals
l=1 → p states → m= 3	number of p type orbitals
l=2 → d states → m= 5	number of d type orbitals
l=3 → f states → m= 7	number of f type orbitals

Hydrogen atom

Summarizing:

- n defines the energy (shell)
- l defines the geometry of the orbital (s, p, d, f)
- m defines its spatial position: only one s orbital, 3 different p orbitals, 5 d orbitals and 7 f orbitals
- s defines the spin momentum

Towards the electronic configuration

1° Livello energetico
1 orbitale s (**1s**) capienza max: 2 elettroni

2° Livello energetico
1 orbitale s (**2s**) capienza max: 2 elettroni
3 orbitali p (**2p**) capienza max: 6 elettroni

3° Livello energetico
1 orbitale s (**3s**) capienza max: 2 elettroni
3 orbitali p (**3p**) capienza max: 6 elettroni
5 orbitali d (**3d**) capienza max: 10 elettroni

4° Livello energetico
1 orbitale s (**4s**) capienza max: 2 elettroni
3 orbitali p (**4p**) capienza max: 6 elettroni
5 orbitali d (**4d**) capienza max: 10 elettroni
7 orbitali f (**4f**) capienza max: 14 elettroni

I livelli successivi presentano al massimo la struttura orbitalica del quarto livello.

Gli atomi più pesanti, come l'Uranio, hanno elettroni a sufficienza per occupare 7 livelli energetici, senza tuttavia riuscire a riempirli completamente.

Livello	Orbitali consentiti				Campienza elettronica
1°	*1s*				2
2°	*2s*	*2p*			2+6=**8**
3°	*3s*	*3p*	*3d*		2+6+10=**18**
4°	*4s*	*4p*	*4d*	*4f*	2+6+10+14=**32**
5°	*5s*	*5p*	*5d*	*5f*	"
6°	*6s*	*6p*	*6d*		"
7°	*7s*				"

Electron configuration

Aufbau rules

1) Principle of minimum energy

Electrons tends to occupy a free orbital with the lowest energy

2) Pauli exclusion principle

Each orbital ca be occupied by only two elecrons wih antiparallel spin momentum

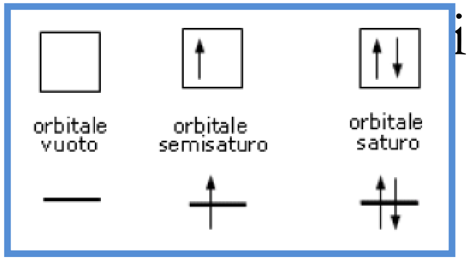
One electron can have only two different spin momenta

The spin momentum is represented by an aroow, facing upwards or downwards

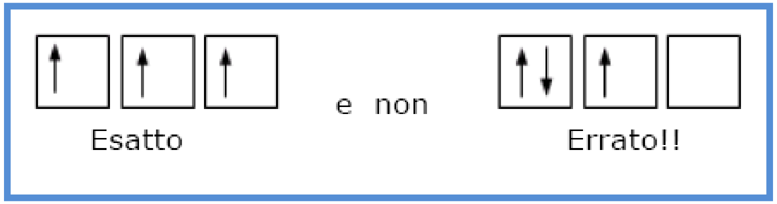
Electron configuration

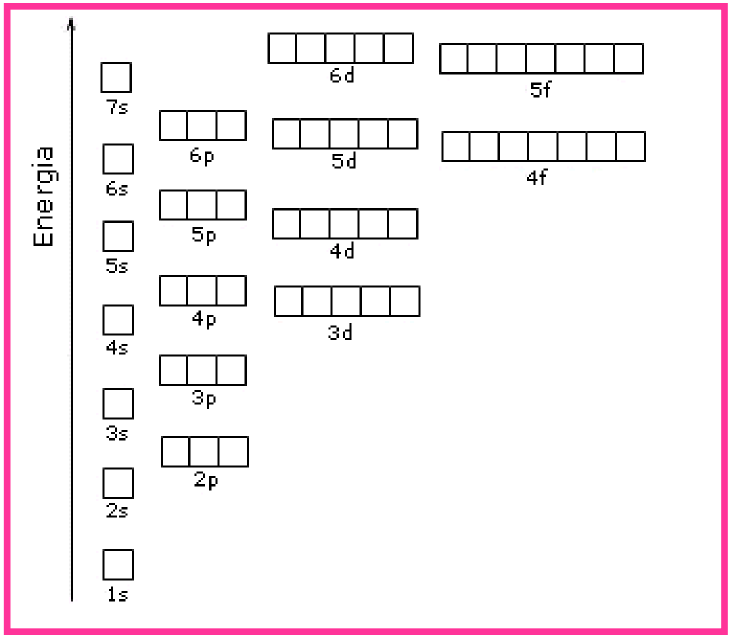
3) Hund's principle of multiplicity

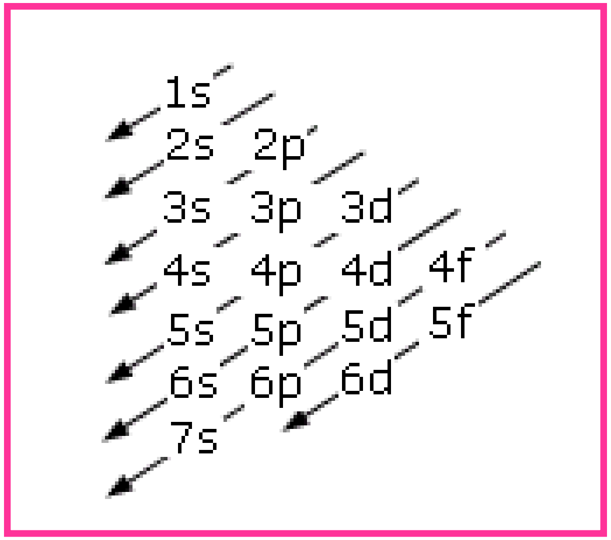
If there are more than one orbitalsith the same energy (degener orbitals) the electrons will try to occupie them separately with parallel spin momentum until all the degeer orbitals have been partially filled



We have 3 electrons and three degenere 2p orbitals



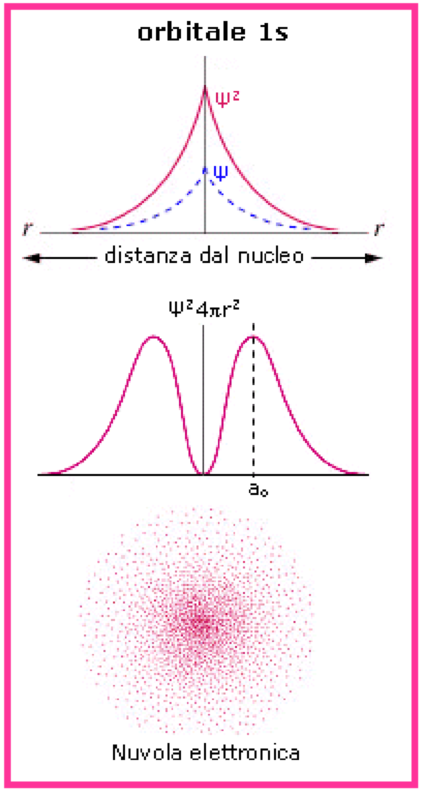




Atomic orbitals: s type

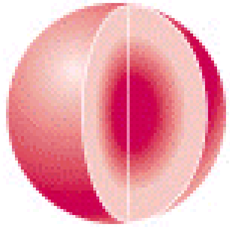
The s wave funtions Ψ(s) are spheric

The probability of finding one electron is equal in every direction, but gets smaller with the distance



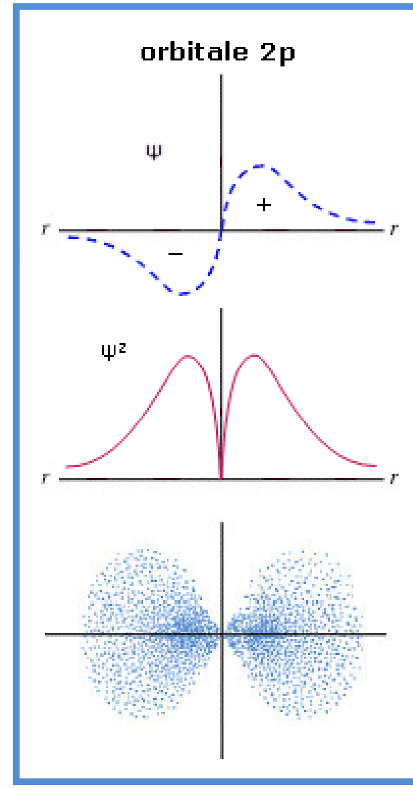
The s orbital, as every orbital is infinite, it squared modulus gives the probability to find an electron in the space

$\Psi(s)^2$ maximum at the center



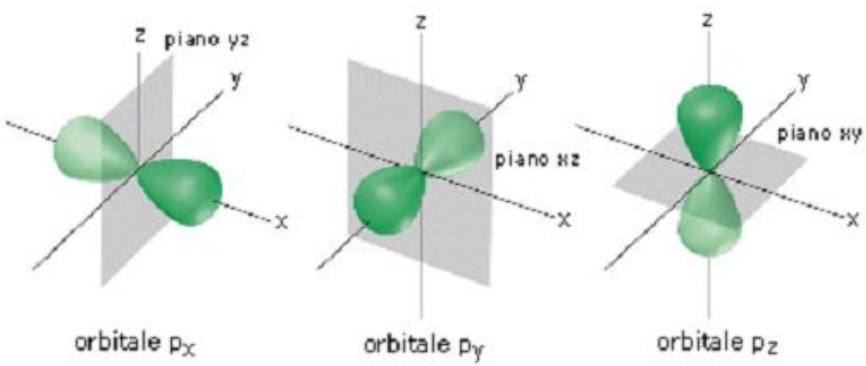
Atomic orbitals: p type

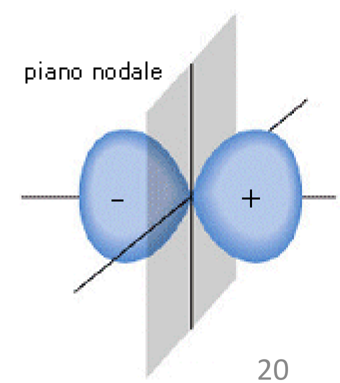
The p orbitals are cylindrical, there is a preferential direction.



There are three p orbitals for each energetic level and they are perpendicularly oriented into the three axes:

px, py, pz





Covalent bonds

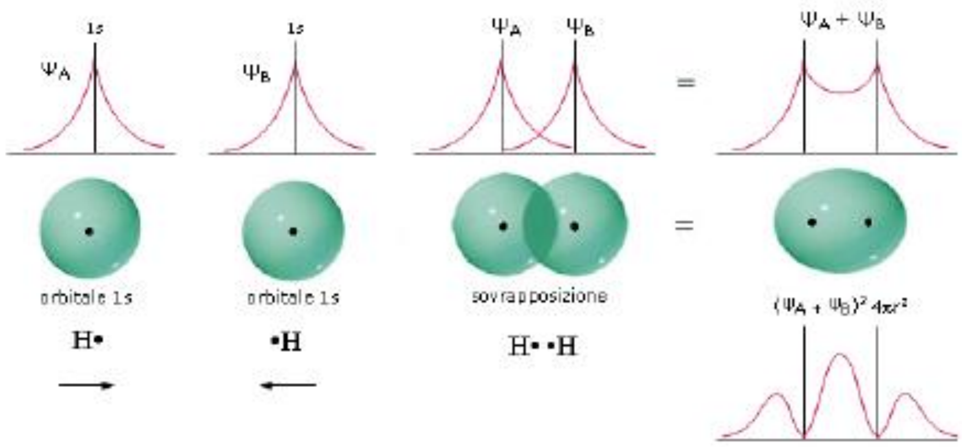
Valence Bond Theory(VB)

Overlapping of atomic orbitals. Each orbital has one electron, the two orbitals share their electron in order to have a pair

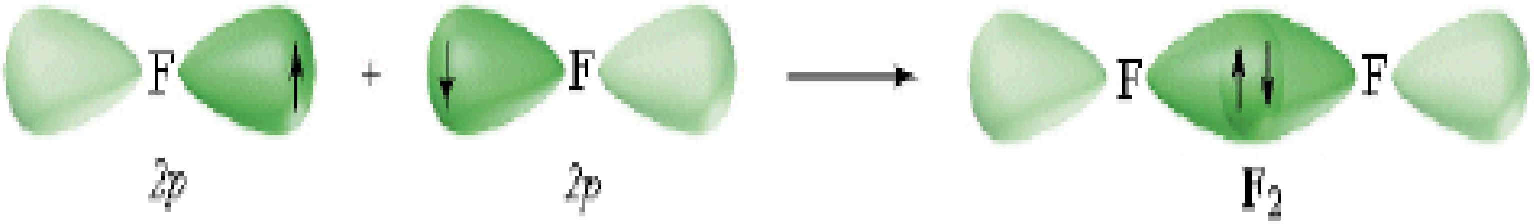
The two wave functions combines together in order to have a new wave function, a new orbital, where the two electron can move.

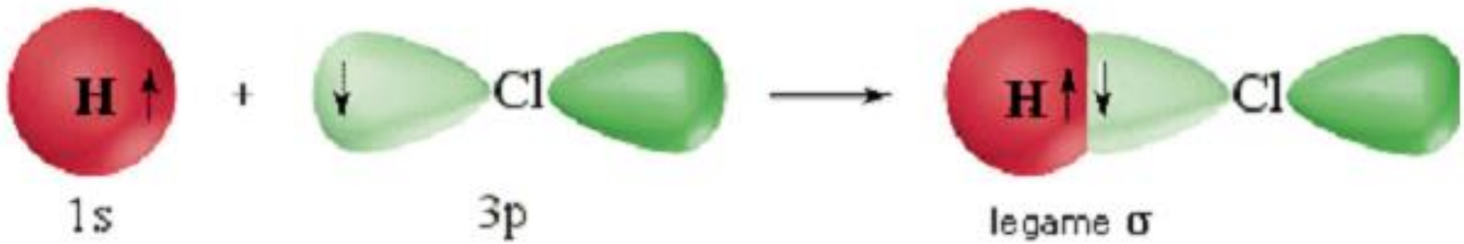
The new orbital is shared by the two oms and hosts the two electrons with antiparallel spin momentum.

legame σ



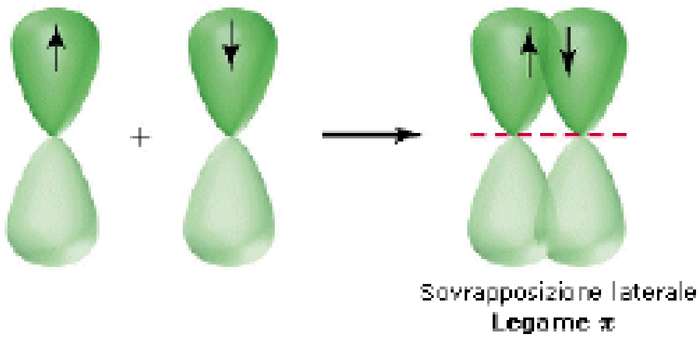
Covalent bonds: σ bonds





Covalent bonds: π bonds

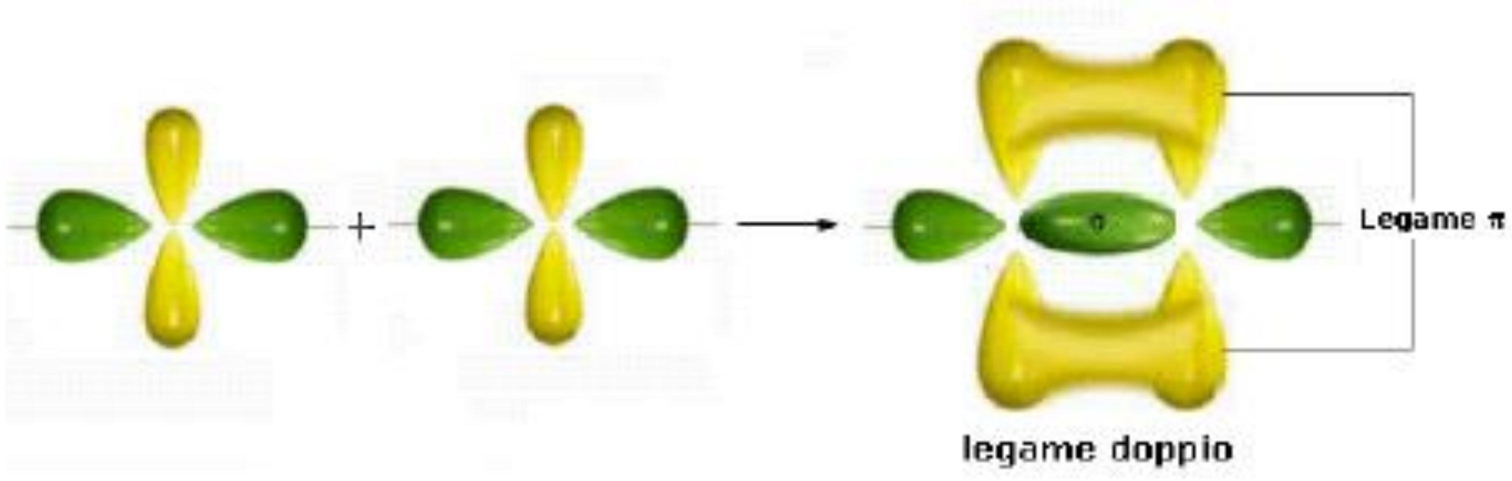
Sometimes double or triple bonds are required,
It could happen that **p orbitals** which are perpendicularly oriented, with respect of the first two which have already formed a σ bond, **can overlap laterally** (along the smaller axes).
This bond is called **π bond** and its is **energetically less stable,** due to the **lower overlapping** between the two involved orbitals.



legame π

Internuclear axis →**σ** bond
Out of axis → **π bond**

Covalent bonds: double bonds



When a covalent double bond takes place there will be a first **σ bond in the direction between the two nuclei, and a second π bond that will take place above and below the previous one and will be much less stable**