

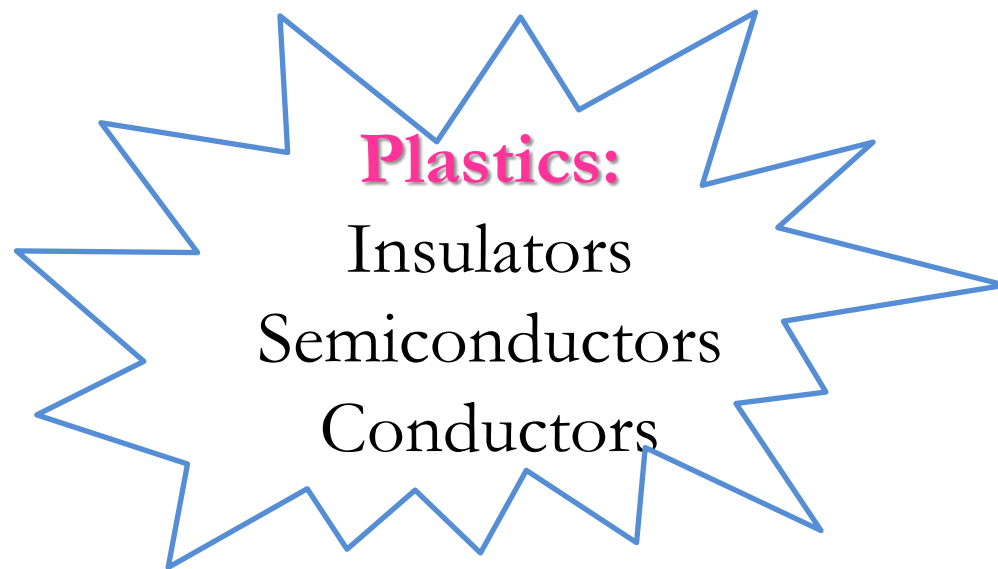
# Organic Electronics

Electronic devices fabricated by means of organic molecules

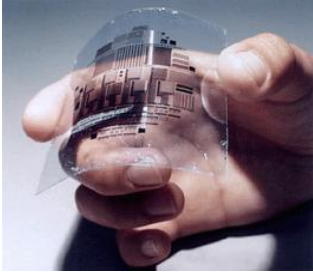
## Molecules containing C and H

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



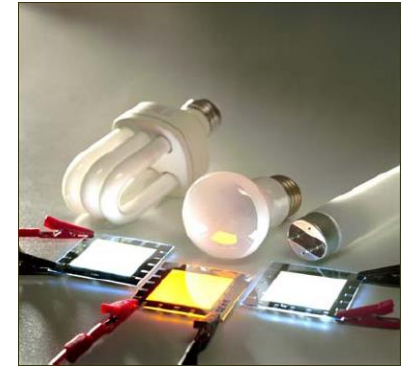
# Organic Electronics



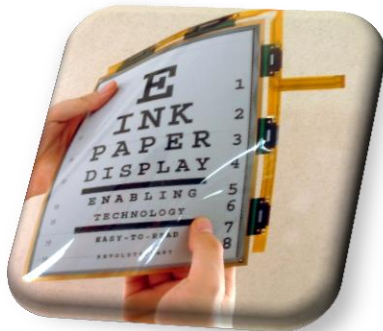
**OFET**  
(Organic Field-Effect Transistors)



**Solar Cells**



**OLED**  
(Organic Light Emitting Diode)



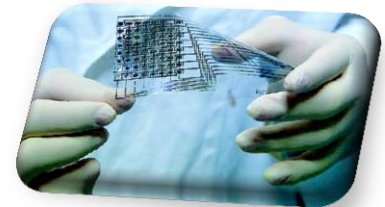
**Applicazioni:**  
Smart wearable electronics  
Solar Energy  
Flexible Displays  
Electronic paper



# 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

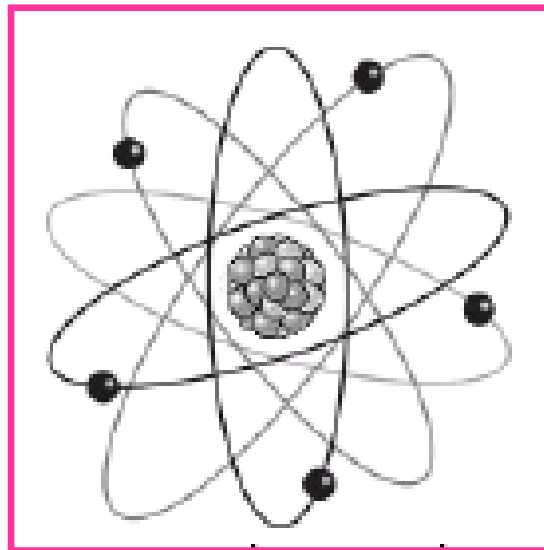


# **A little bit of Chemistry**

# The Atom

An atom is made out of a massive and dense core, positively charged, where protons and neutrons 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 Helium 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

1 IA																												18 VIIIA				
1	1,0079 -1 1-1																	4,0026 0														
1	H Idrogeno																	He Elio														
2 IIA																17 VIIA		18 VIIIA														
3	6,941	9,0122																10	20,179													
2	Li Litio	Be Berillio																F Fluoro	Ne Neon													
3	11 22,9898 +1		12 24,305 +2																17 35,453 -1	18 39,948 0												
3	Na Sodio		Mg Magnesio																Cl Cloro	Ar Argon												
3 IIB																		4 IVB	5 VB	6 VIB	7 VIIB	8 VIIIB	9 VIIIB	10 VIIIB	11 IB	12 IIB	13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18 VIIIA
4	19 39,0983 +1	20 40,08 +2	21 44,9559 +3	22 47,9 +4	23 50,9415 +3	24 51,996 +2	25 54,938 +3	26 55,847 +2	27 58,9332 +3	28 58,7 +2	29 63,546 +2	30 65,38 +2	31 69,72 +3	32 72,59 +3	33 74,9216 +3	34 78,96 +4	35 79,904 -1	36 83,8 0														
4	K Potassio	Ca Calcio	Sc Scandio	Ti Titanio	V Vanadio	Cr Cromo	Mn Manganese	Fe Ferro	Co Cobalto	Ni Nikel	Cu Rame	Zn Zinco	Ga Gallio	Ge Germanio	As Arsenico	Se Selenio	Br Bromo	Kr Kripton														
5	37 85,4678 +1	38 87,62 +2	39 88,9059 +3	40 91,22 +4	41 92,9064 +5	42 95,94 +6	43 (98) +7	44 101,07 +8	45 102,9055 +9	46 106,4 +8	47 107,868 +9	48 112,41 +10	49 114,82 +3	50 118,69 +4	51 121,75 +5	52 127,6 +6	53 126,9045 -1	54 131,3 0														
5	Rb Rubidio	Sr Stronzio	Y Ittrio	Zr Zirconio	Nb Niobio	Mo Molibdeno	Tc Tecnezio	Ru Rutenio	Rh Rodio	Pd Palladio	Ag Argento	Cd Cadmio	In Indio	Sn Stagno	Sb Antimonio	Te Tellurio	I Iodio	Xe Xenon														
6	55 132,9054 +1	56 137,33 +2	57 138,9055 +3	72 178,49 +4	73 180,9479 +5	74 183,85 +6	75 186,207 +7	76 190,2 +8	77 192,22 +9	78 195,09 +8	79 196,9665 +9	80 200,59 +2	81 204,37 +3	82 207,2 +4	83 208,9804 +5	84 (209) +4	85 (210) -1	86 (222) 0														
6	Cs Cesio	Ba Bario	La Lantanio	Hf Afnio	Ta Tantalio	W Tungsteno	Re Renio	Os Osmio	Ir Iridio	Pt Platino	Au Oro	Hg Mercurio	Tl Tallio	Pb Piombo	Bi Bismuto	Po Polonio	At Astatio	Rn Radon														
7	87 (223) +1	88 226,025 +2	89 227,028 +3	104 (261) +4	105 (262) +5	106 (266) +6	107 (264) +7	108 (277) +8	109 (268) +9	110 (271) +8	111 (272) +9																					
7	Fr Francio	Ra Radio	Ac Attinio	Rf Rutherfordio	Db Dubnio	Sg Seaborgio	Bh Bohrio	Hs Hassio	Mt Meitnerio	Ds Darmstadio	Rg Roentgenio																					

Metalli Alcalini  
Metalli Alcalino-Terrosi  
Lantanidi  
Attinidi

Elementi di Transizione  
Metalloidi / Non Metalli  
Alogeni  
Gas Nobili

STATI di AGGREGAZIONE a 20 °C

SOLIDI LIQUIDI GASSOSI ARTIFICIALI

Periodo

Gruppo

Numero Atomico  
Peso Atomico  
Valenza  
Densità (g/cm<sup>3</sup>)  
Temp. Fusione (°C)  
Temp. Ebollizione (°C)

Numero di Ossidazione  
Simbolo  
Nome

1 1,0079  
-1  
1-1  
H  
Idrogeno

58 140,12 +4	59 140,9077 +3	60 144,24 +3	61 (145) +3	62 150,4 +3	63 151,96 +3	64 157,25 +3	65 158,9254 +3	66 162,5 +3	67 164,9304 +3	68 167,26 +3	69 168,9342 +3	70 173,04 +3	71 174,967 +3
Ce Cerio	Pr Praseodimio	Nd Neodimio	Pm Promezio	Sm Samario	Eu Europio	Gd Gadolinio	Tb Terbio	Dy Disprozio	Ho Olmio	Er Erbio	Tm Tulio	Yb Itterbio	Lu Lutezio
90 232,0381 +4	91 (209) +4	92 238,029 +4	93 237,048 +4	94 (244) +4	95 (243) +4	96 (247) +4	97 (247) +4	98 (251) +4	99 (252) +4	100 (257) +4	101 (258) +4	102 (259) +4	103 (260) +4
Th Torio	Pa Protoattinio	U Uranio	Np Nettunio	Pu Plutonio	Am Americio	Cm Curio	Bk Berchelio	Cf Californio	Es Einsteinio	Fm Fermio	Md Mendelevio	No Nobelio	Lr Laurenzio

Serie dei Lantanidi  
Serie degli Attinidi



# Flash back Schroedinger

# Hydrogen atom

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

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

We have introduced two integer numbers

- $n = 1, 2, 3, \dots$
- $l = 0, 1, 2, \dots, n - 1$

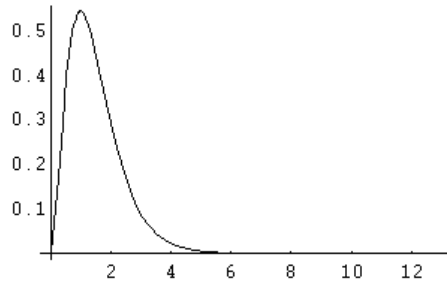
# Hydrogen atom

For the fundamental state ( $n = 1$ ), there will be only one  $l$  value, and the energy will be  $-13.6 \text{ eV}$  (ionization energy for hydrogen)

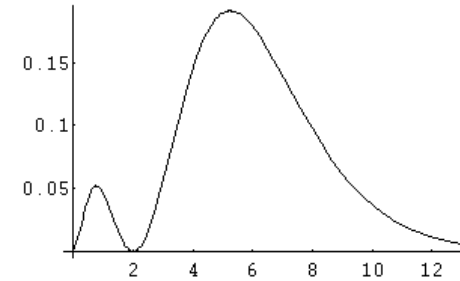
The first excited state ( $n = 2$ ) will give place to two  $l$  values ( $l = 0$  ed  $l = 1$ ), but only one energetic level (in  **$E_n$  depends only on  $n$** )

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

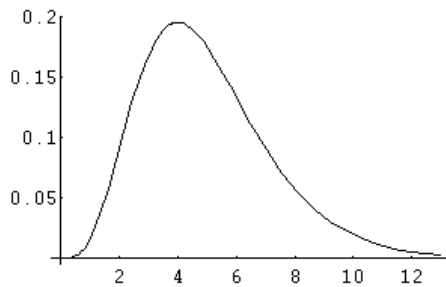
# Hydrogen atom



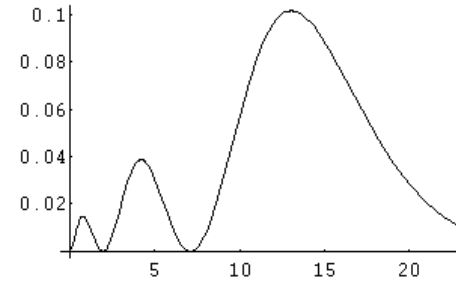
State 1s,  
 $n=1, l=0$



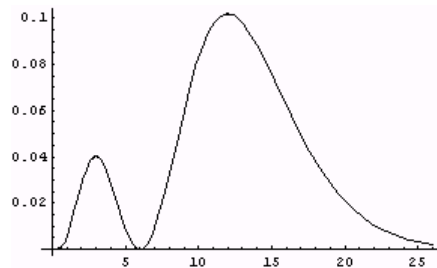
State 2s,  
 $n=2, l=0$



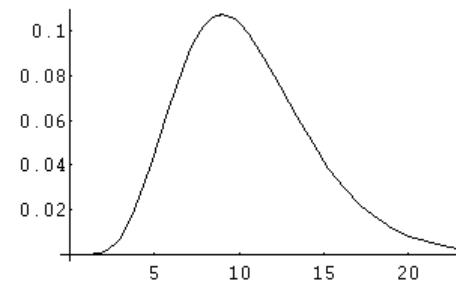
State 2p,  
 $n=2, l=1$



State 3s,  
 $n=3, l=0$



State 3p,  
 $n=3, l=1$



State 3d,  
 $n=3, l=2$

# Hydrogen atom

The angular part solution of Schrödinger equation led us to a third quantum number called  $m = -l, -(l-1), \dots, 0, \dots, (l-1), l$  (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

$l=0 \rightarrow$  s states ( $m=2l+1=1$ )

number of s type orbitals

$l=1 \rightarrow$  p states  $\rightarrow m=3$

number of p type orbitals

$l=2 \rightarrow$  d states  $\rightarrow m=5$

number of d type orbitals

$l=3 \rightarrow$  f states  $\rightarrow m=7$

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				Capienza 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 electrons wih antiparallel spin momentum

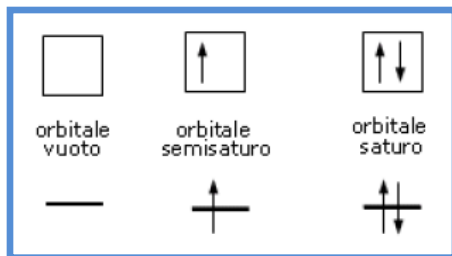
One electron can have only two different spin momenta

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

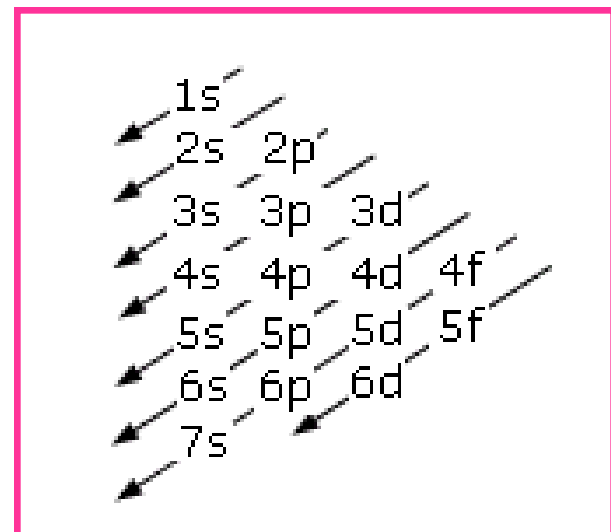
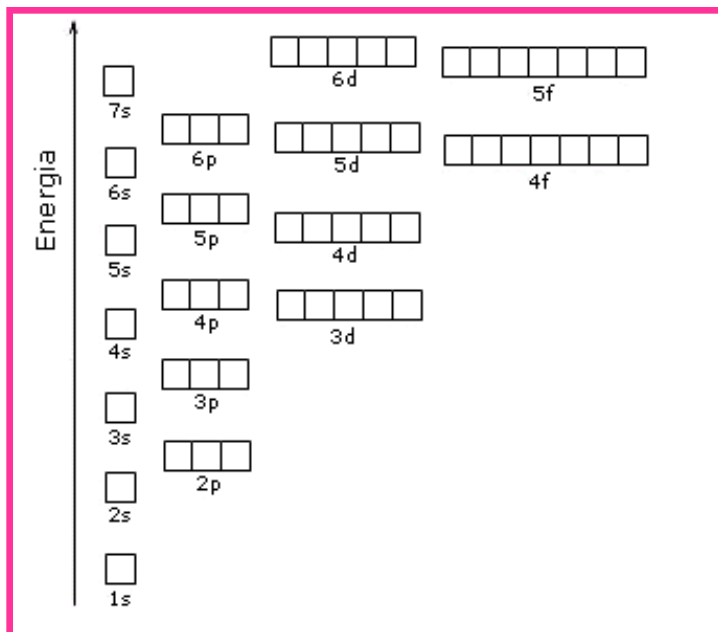
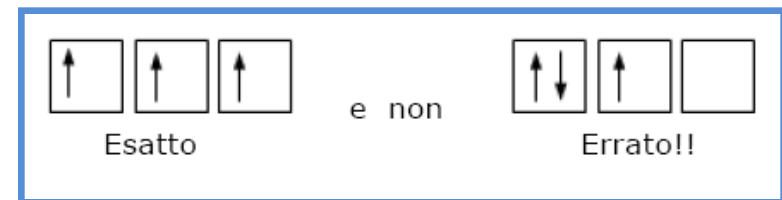
# Electron configuration

## 3) Hund's principle of multiplicity

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



We have 3 electrons and three degenerate 2p orbitals



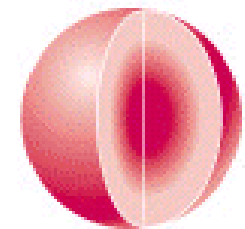
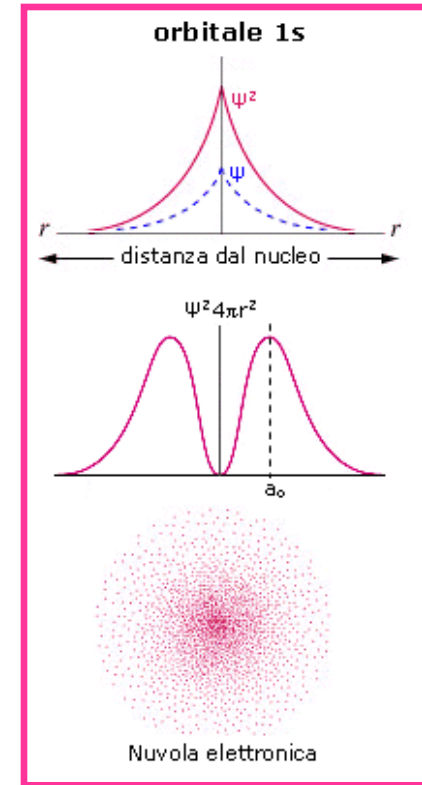
# Atomic orbitals: s type

The s wave functions  $\Psi(s)$  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, its squared modulus gives the probability to find an electron in the space

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

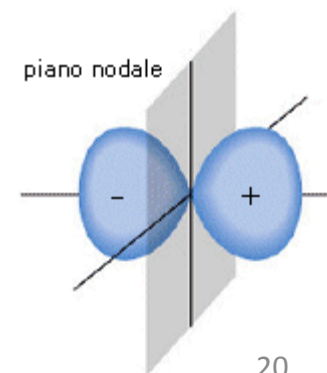
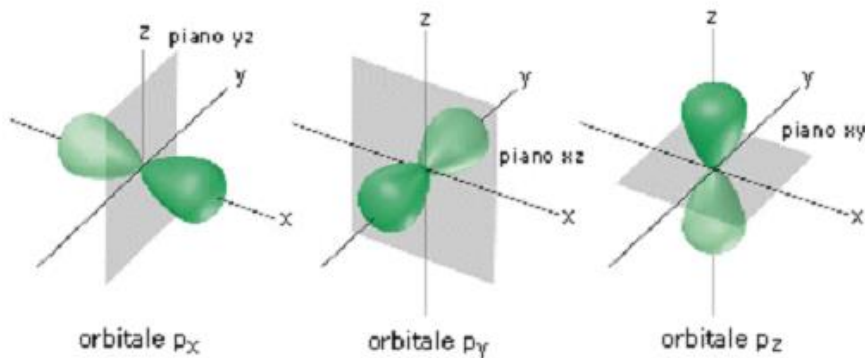
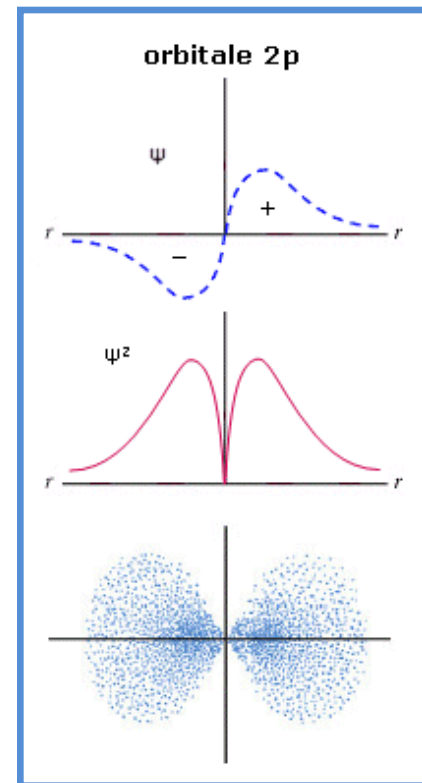


# Atomic orbitals: p type

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:

$p_x$ ,  $p_y$ ,  $p_z$





# Covalent bonds

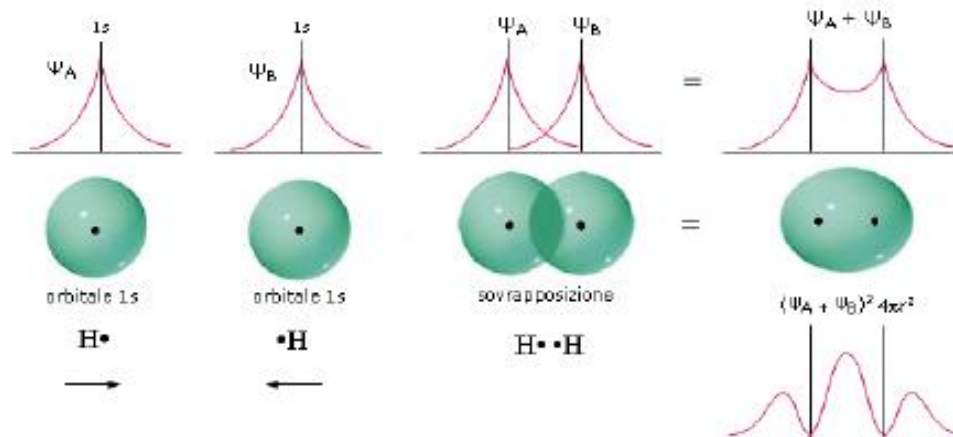
## Valence Bond Theory(VB)

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

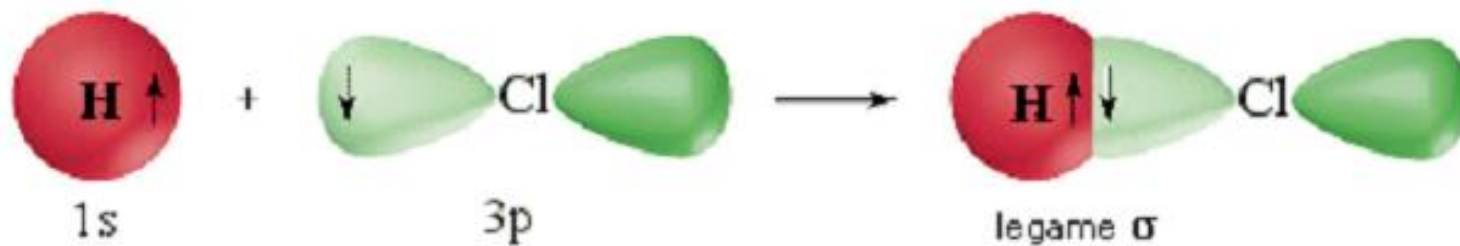
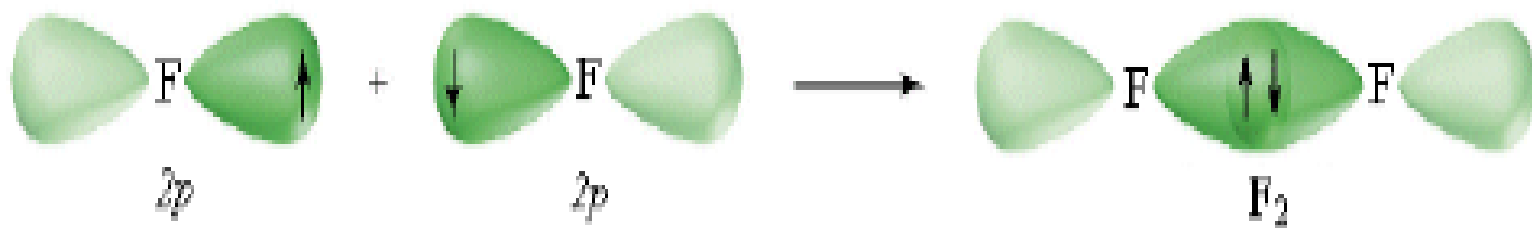
The two wave functions combines together in order to have a new wave function, a new orbital, where the two electron can move.

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

legame  $\sigma$

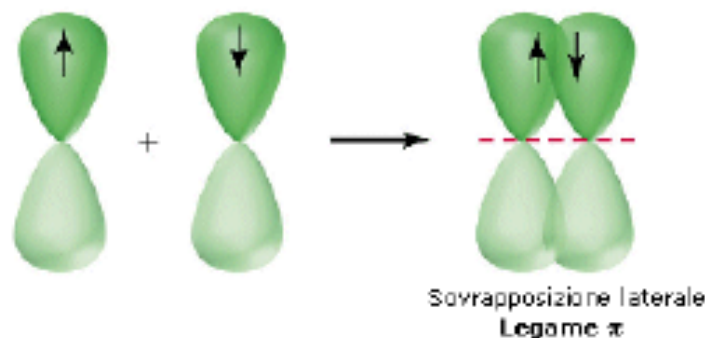


# Covalent bonds: $\sigma$ bonds



# Covalent bonds: $\pi$ 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  $\sigma$  bond, **can overlap laterally** (along the smaller axes).  
This bond is called  **$\pi$  bond** and its is **energetically less stable**, due to the **lower overlapping** between the two involved orbitals.

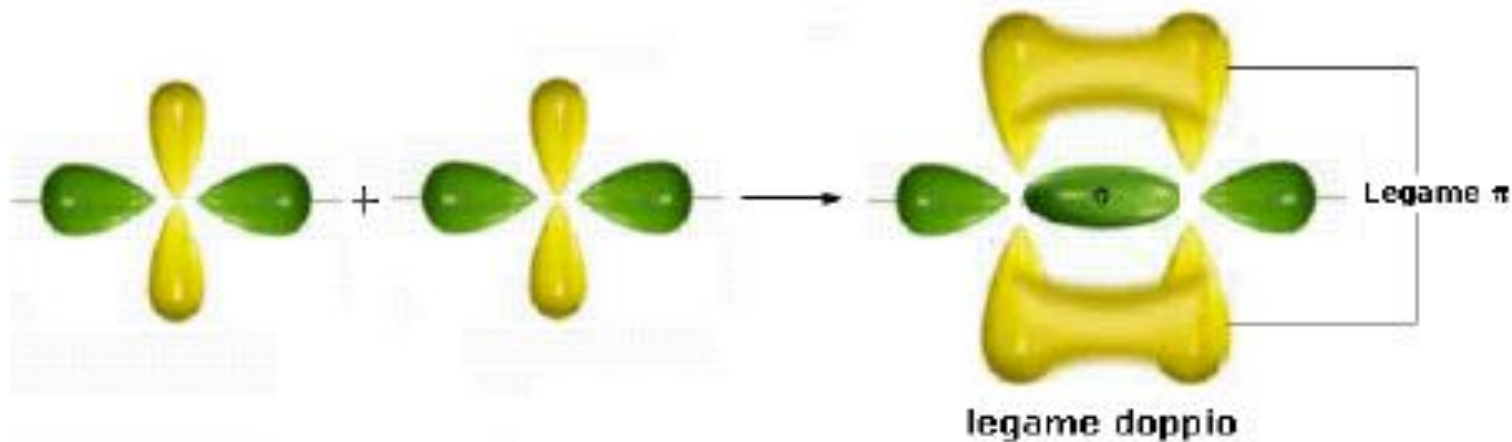


legame  $\pi$

Internuclear axis  $\rightarrow \sigma$  bond

Out of axis  $\rightarrow \pi$  bond

# Covalent bonds: double bonds



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