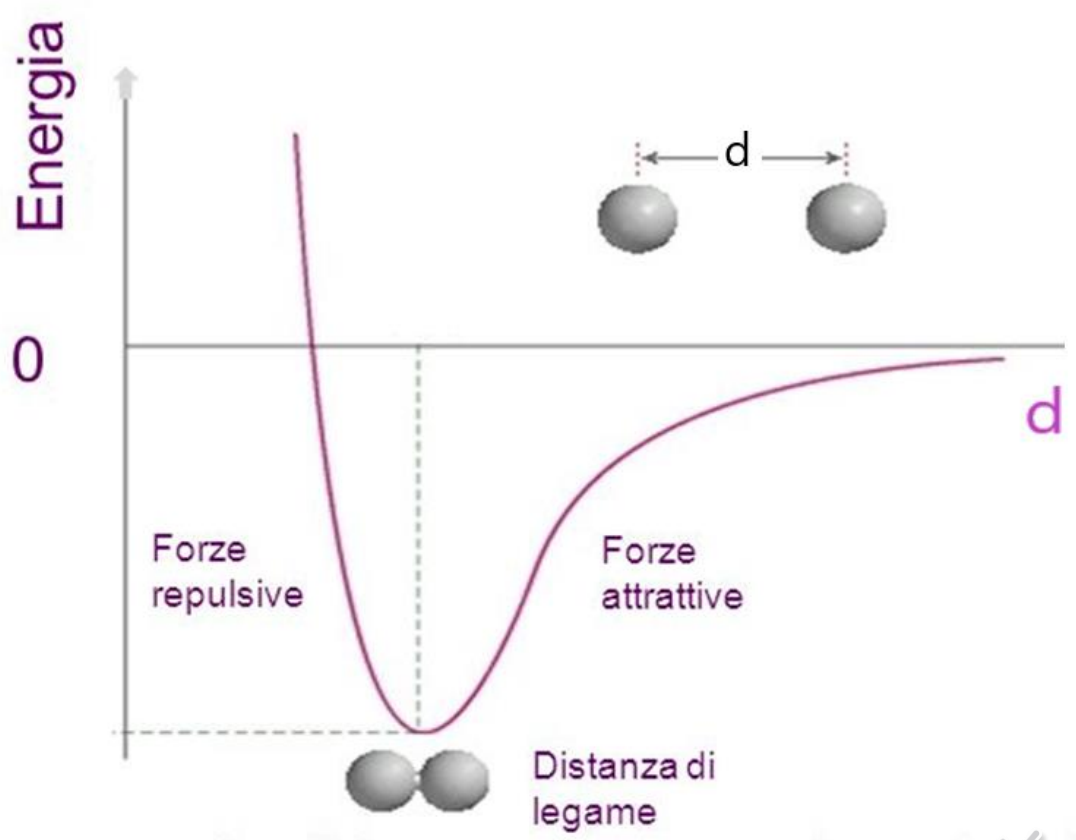
# LEGAME CHIMICO

ATOMI → MOLECOLE
- FORMULA BRUTA (es. $H_2O$, $C_2H_4$, $H_2SO_4$)
- FORMULA DI STRUTTURA

- LEGAME CHIMICO
  - IONICO
  - COVALENTE
    - OMEOPOLARE
    - POLARE
  - METALLICO
- FORZE INTERMOLECOLARI
  - VAN DER WAALS
  - LEGAME IDROGENO




ENERGIA DI LEGAME
DISTANZA DI LEGAME

# LEGAME IONICO

Ioni positivi e negativi tenuti insieme da interazioni elettrostatiche

Ioni positivi (cationi) → elementi aventi basso I (metalli)

$Na \rightarrow Na^+ + e^-$

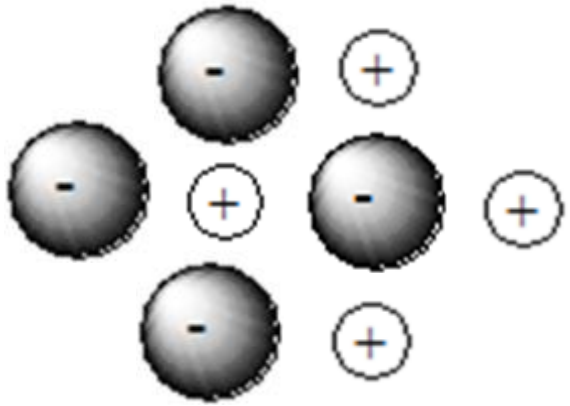
$[Ne]3s^1 \rightarrow [Ne]$

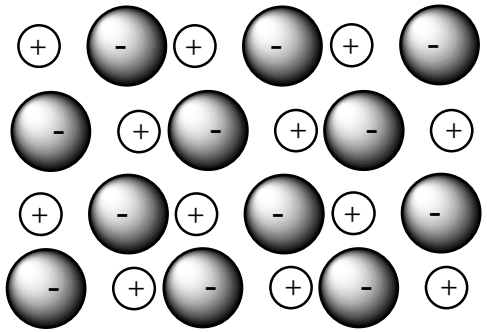
Ioni negativi (anioni) → elementi aventi alta $A_e$ (non metalli)

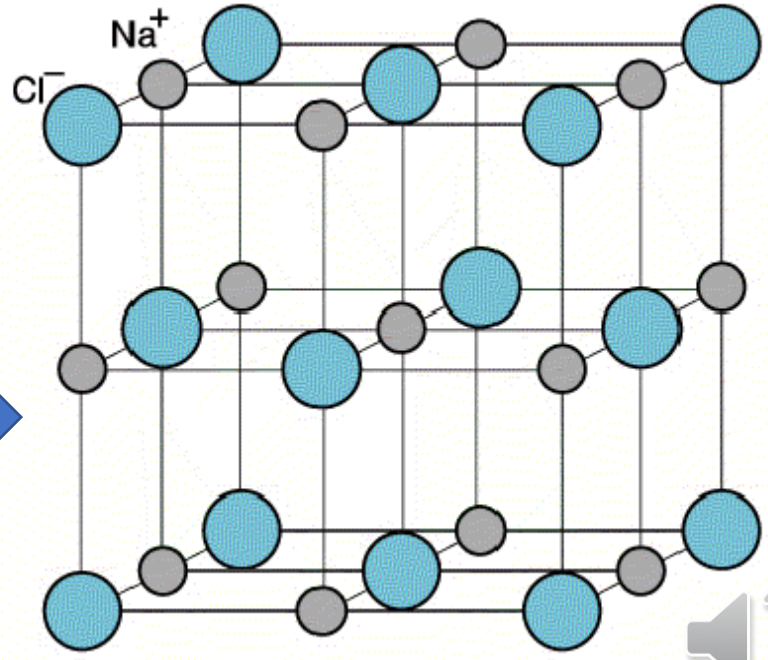
$Cl + e^- \rightarrow Cl^-$

$[Ne]3s^23p^5 \rightarrow [Ne]\ 3s^23p^6 = [Ar]$

$Na^+ + Cl^- \rightarrow Na^+Cl^- = NaCl$





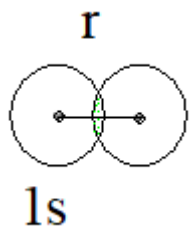


# LEGAME COVALENTE

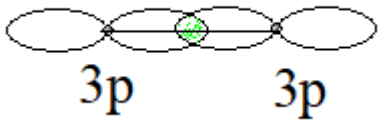
Teoria a coppia di elettroni (Lewis )
Teoria del legame di valenza (VB)

## MOLECOLE BIATOMICHE OMONUCLEARI:

$H_2$ H 1s H · · H → H-H



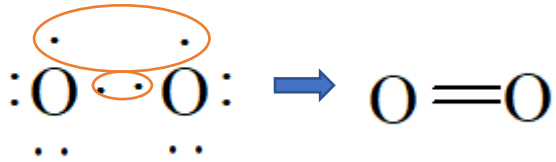

$Cl_2$ Cl $3s^2$ $3p^5$ : Cl · · Cl : → Cl-Cl

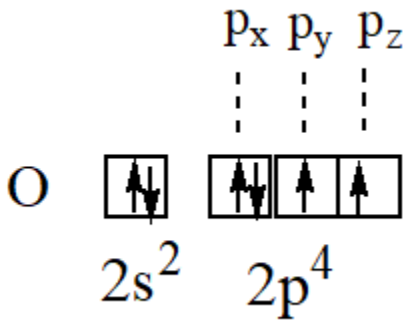


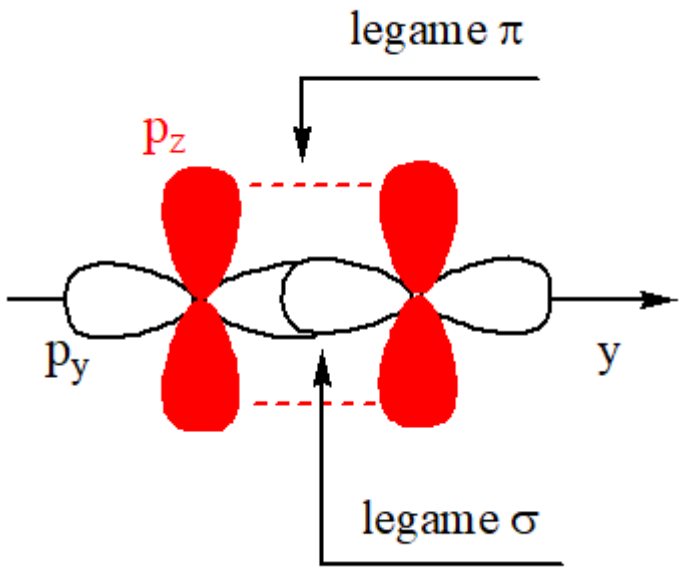

Valenza→ capacità di un atomo di formare legami

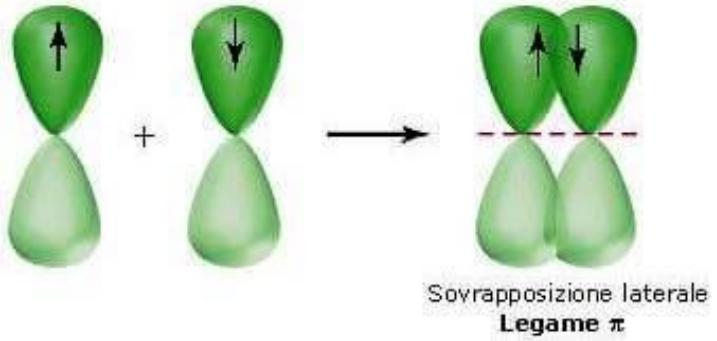
# Legami multipli

$O_2$






O ═ O

$E_\sigma > E_\pi$

σ + π

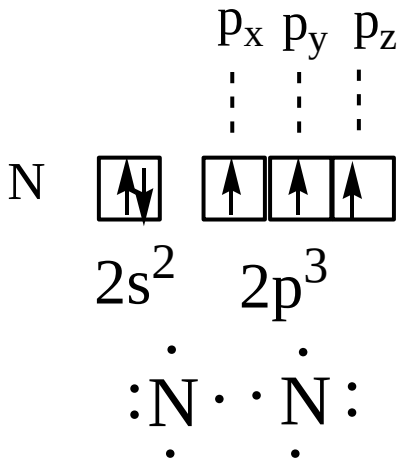
Legame singolo → σ

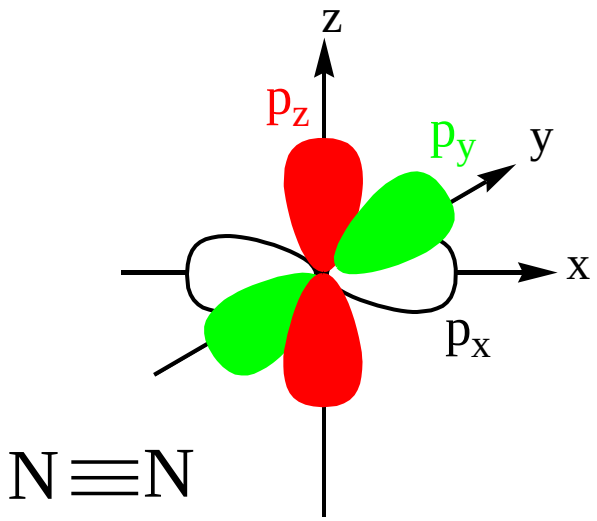
Legame doppio → σ + π

$E_{doppio} > E_{singolo}$

Orbitali s → σ

Orbitali p → σ, π



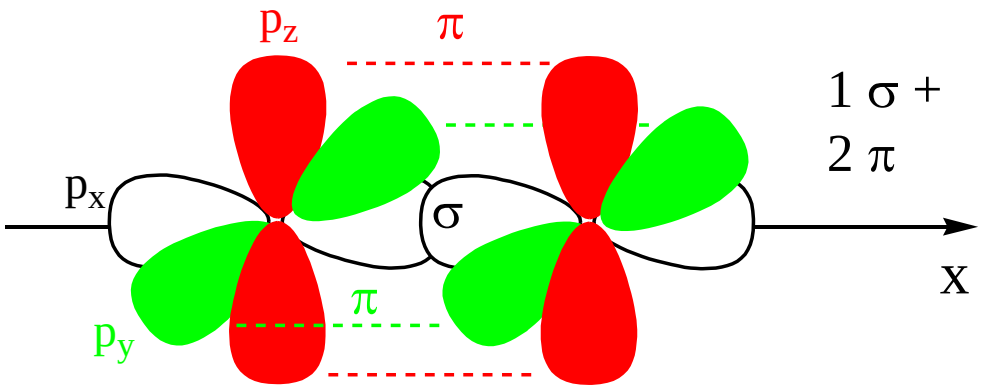



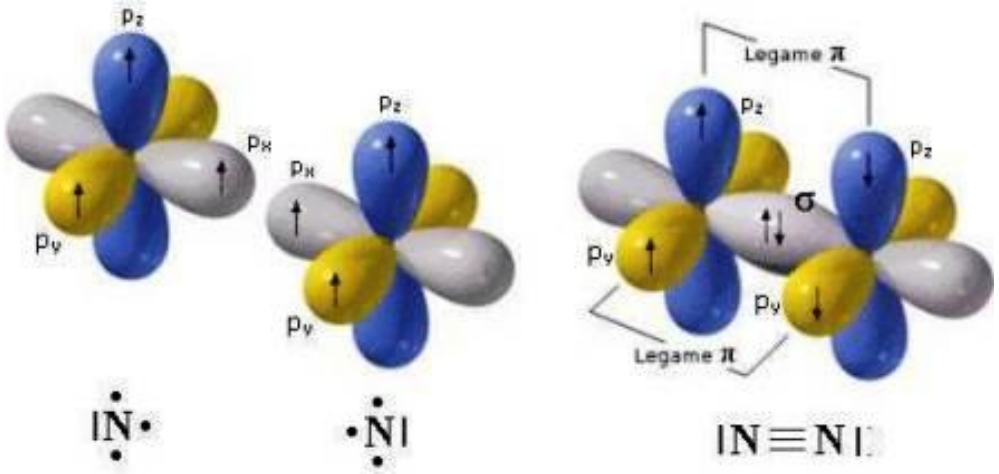

$N \equiv N$

Legame singolo → σ
Legame doppio → σ + π
Legame triplo → σ + 2 π

$E_{triplo} > E_{doppio} > E_{singolo}$

$d_{triplo} < d_{doppio} < d_{singolo}$



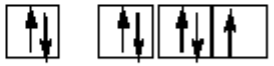



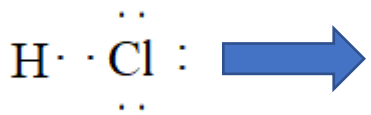
# MOLECOLE BIATOMICHE ETERONUCLEARI

## LEGAME COVALENTE POLARE

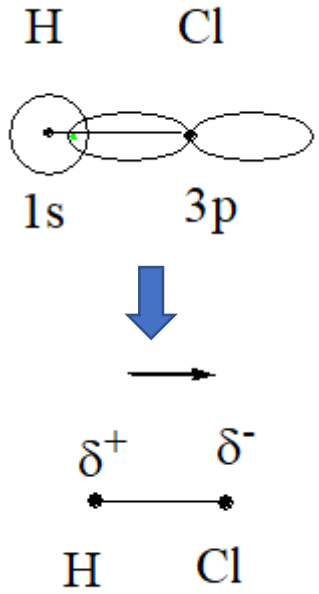
HCl

H  1s

Cl  $3s^2$ $3p^5$




H-Cl




Momento di dipolo $\mu = q \times d$

ELETTRONEGATIVITA’ → Tendenza di un atomo ad attrarre su di sé gli elettroni di legame

Differenza di elettronegatività

$\Delta E > 2 \rightarrow$ legame ionico

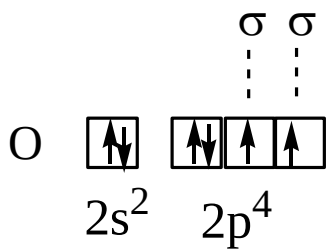
$0 < \Delta E < 2 \rightarrow$ legame covalente polare (eteropolare)

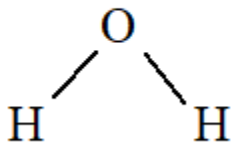
$\Delta E = 0 \rightarrow$ legame covalente puro o omeopolare

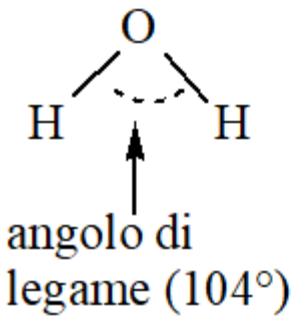
# MOLECOLE POLIATOMICHE

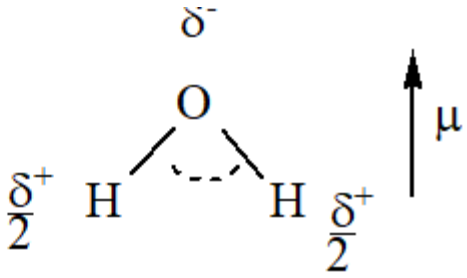
Formula di struttura

$H_2O$

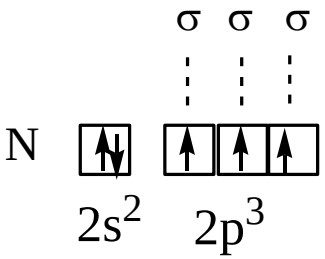


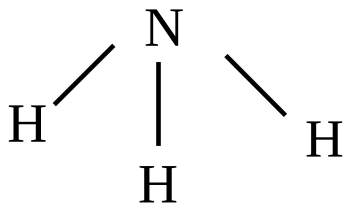




$NH_3$




Angolo di legame 106°

# ORBITALI IBRIDI

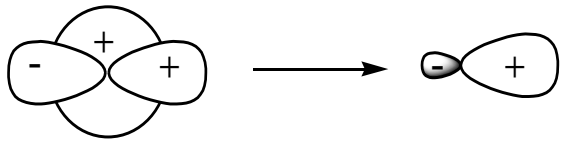
C 

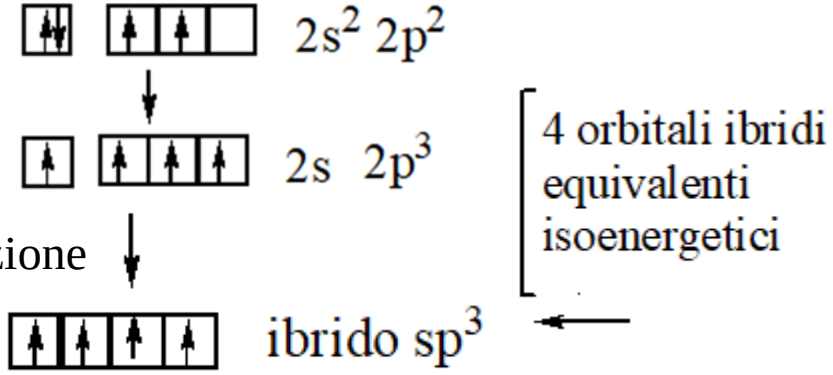
$2s^2$ $2p^2$

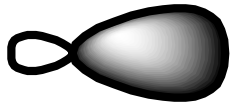
Divalente → no! TETRAVALENTE

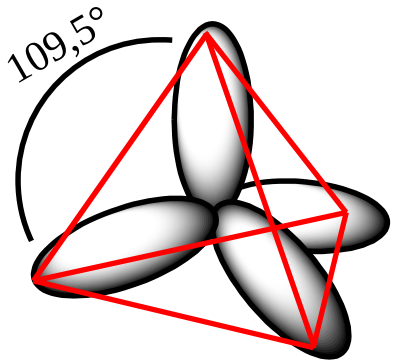
$CH_4$ 4 legami equivalenti

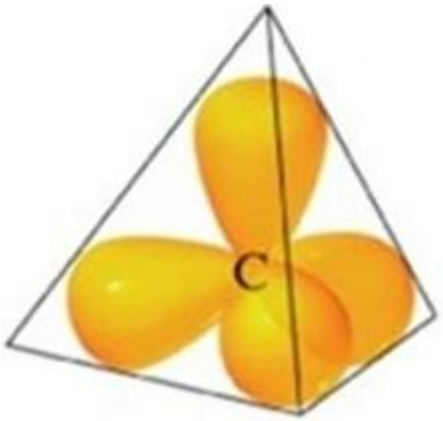
$\Psi_{sp^3} = N (\Psi_{2s} + 3\Psi_{2p})$

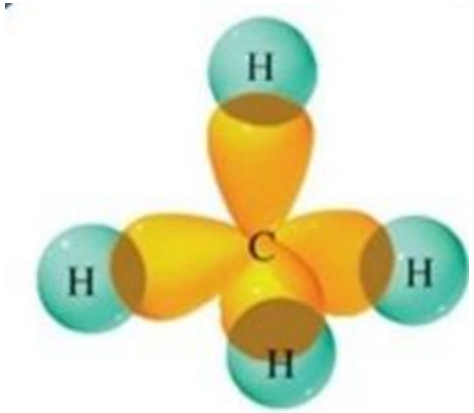


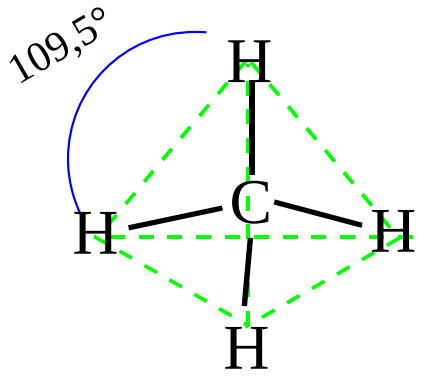



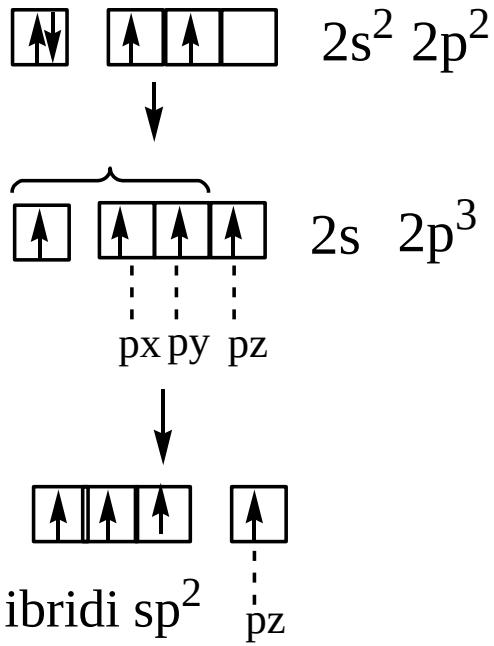





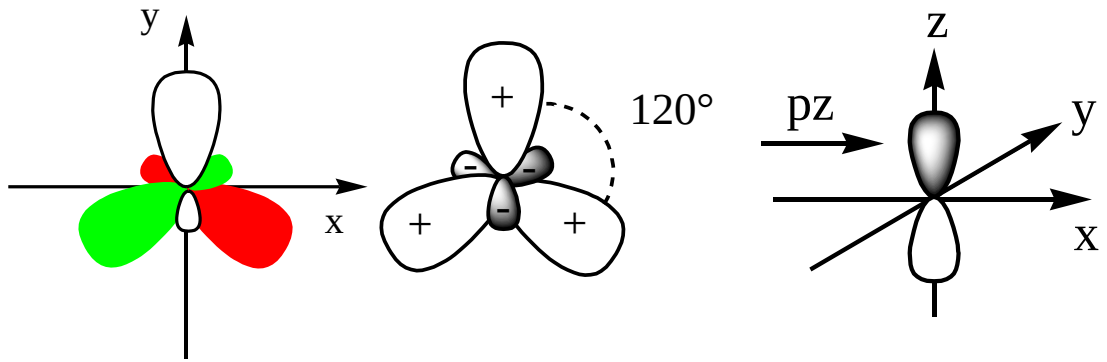






$$\Psi_{sp^2} = N\,(\Psi_{2s} + \Psi_{2p_x} + \Psi_{2p_y})$$

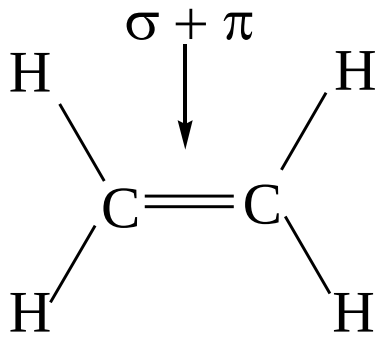


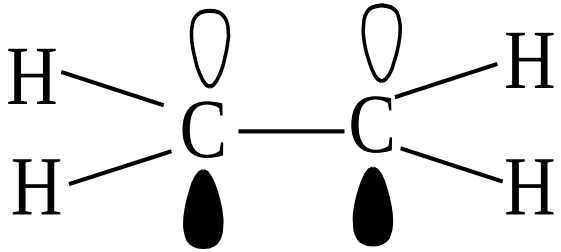

L'orbitale pz non ibridizzato rimane lungo l'asse z
⊥ al piano degli orbitali ibridi

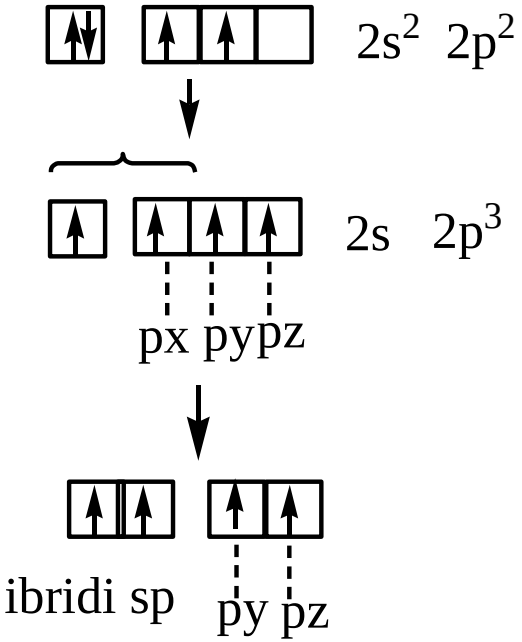
Orbitali ibridi: legami σ
Orbitale non ibrido: legame π

3 legami σ + 1 legame π

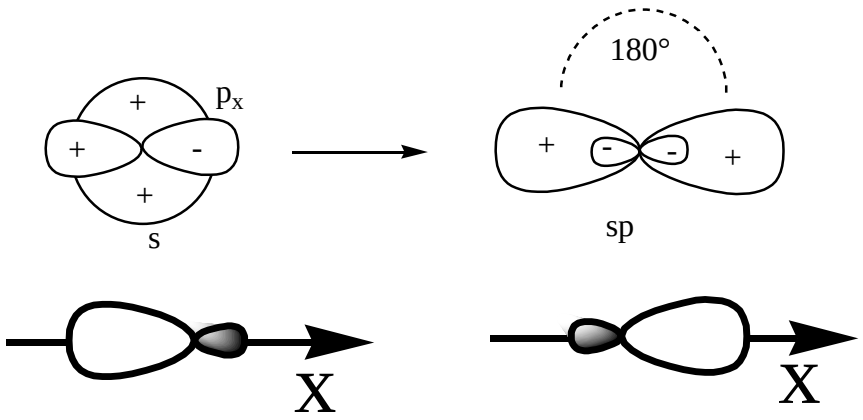
Un legame doppio (σ+π)
Due legami semplici (σ)






$\Psi_{sp} = N (\Psi_{2s} + \Psi_{2p_x})$




Orbitali ibridi: 2 legami σ
Orbitali non ibridi: 2 legame π

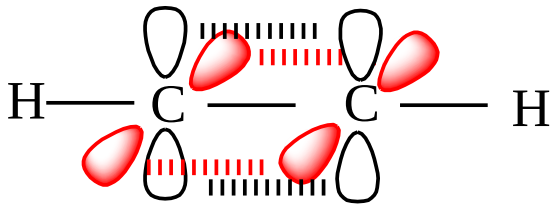
orbitali py e pz non ibridizzati
⊥ tra loro e alla direzione degli orbitali ibridi

$C_2H_2$ H-C≡C-H

↑

σ+2π

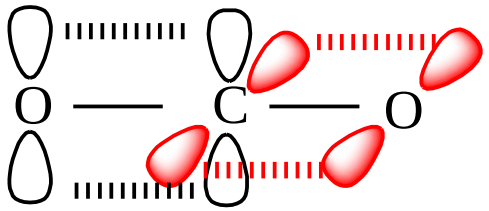
1 legame singolo
+ 1 legame triplo




$CO_2$ O = C = O

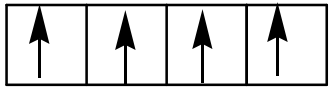
↑ ↑

σ+π σ+π




2 doppi legami

# SOMMARIO



$sp^3$

Ibridazione $sp^3 \rightarrow$ tetraedrica
angoli di 109°
4 orbitali ibridi $\rightarrow$ 4 legami $\sigma$ $\rightarrow$ 4 legami singoli

$sp^2$ p

Ibridazione $sp^2 \rightarrow$ trigonale planare
angoli di 120°
3 orbitali ibridi $\rightarrow$ 3 legami $\sigma$
1 orbitale p non ibridato $\perp$ al piano $\rightarrow$ 1 legame $\pi$
2 legami singoli + un legame doppio

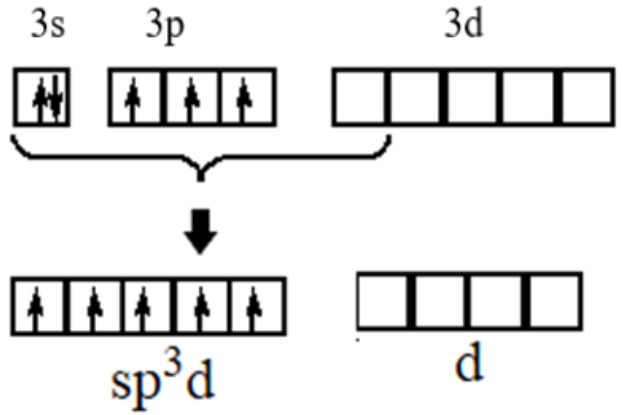
sp p

Ibridazione sp $\rightarrow$ lineare
angoli di 180°
2 orbitali ibridi $\rightarrow$ 2 legami $\sigma$
2 orbitali p non ibridati $\rightarrow$ 2 legami $\pi$

1 legame triplo +
1 legame singolo

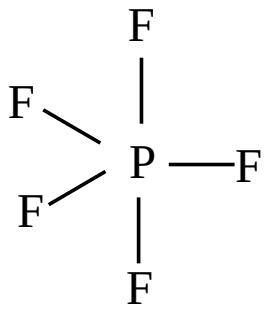
2 doppi legami

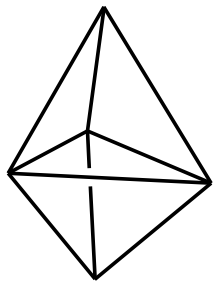
$PF_5$



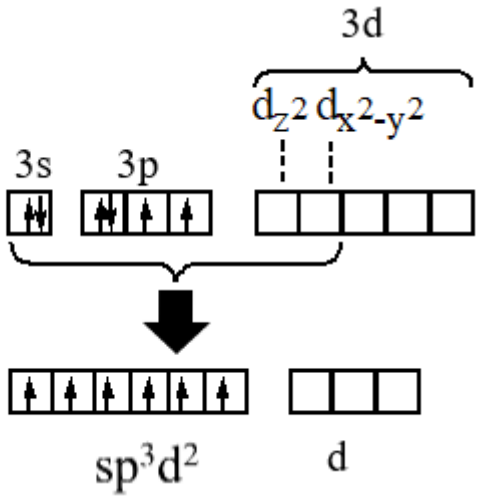

5 legami σ

n c = 5



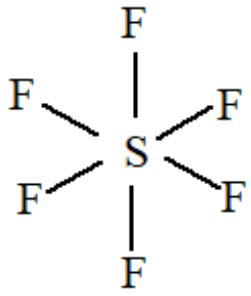



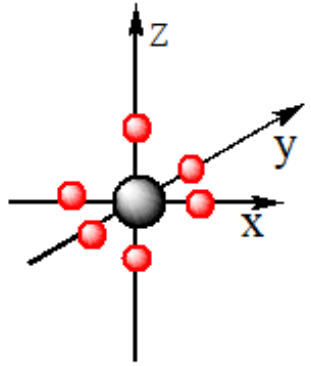
$SF_6$

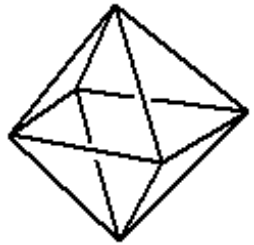


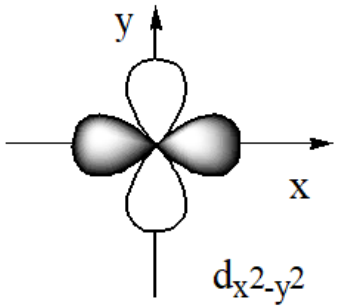

6 legami σ

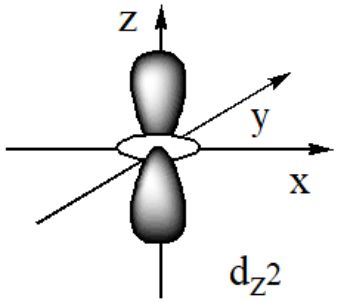
nc = 6



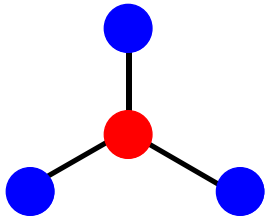





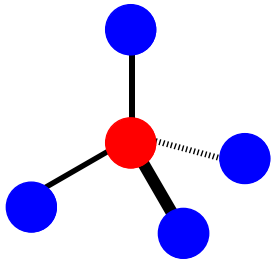



# VALENCE SHELL ELECTRON PAIRS REPULSION (VSEPR)

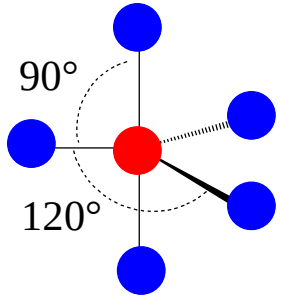
nc=2 180°
lineare
sp



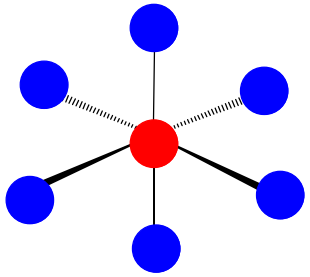
nc=3 120°
trigonale
planare
$sp^2$



nc=4 109,5°
tetraedrica
$sp^3$

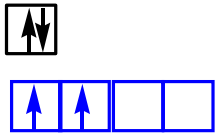



nc=5
bipiramide
trigonale
$sp^3d$



nc=6 90°
ottraedrica
$sp^3d^2$

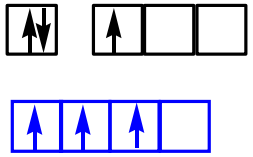
nc = 2

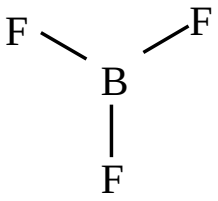
Be 

H-Be-H

$2\sigma$ 180°

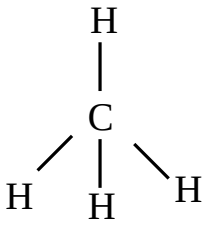
nc = 3

B 



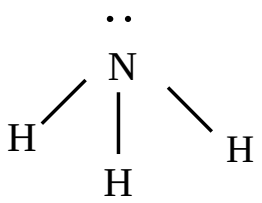

$3\sigma$ 120°

nc =4 C 



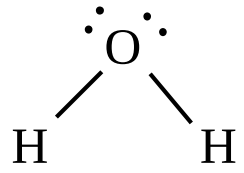

4σ
109,5°

N 




3σ +1 lp
106°

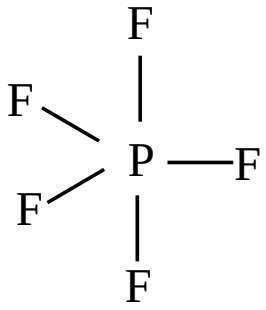
O 

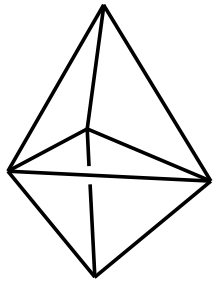



2σ + 2lp
104°

5 legami σ

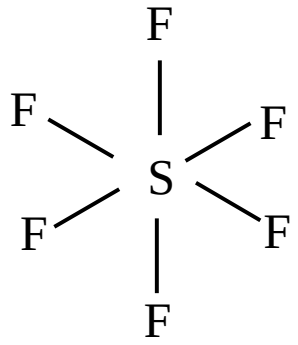
n c = 5

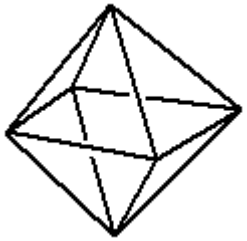


nc = 6

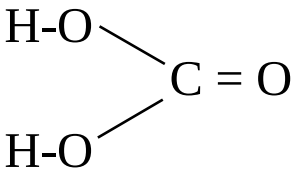
$SF_6$ 6 legami σ



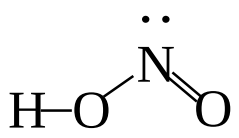



E se ci sono legami π?

Solo legami σ + lone pair determinano la geometria molecolare




3 σ→120°




2 σ + 1 lp→120°

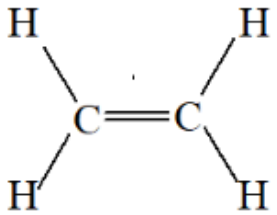
H-C≡N

2σ → 180°

O=C=O

2σ → 180°

E se ci sono legami π?
I legami π seguono la direzione dei legami σ
Solo legami σ + lone pair determinano la geometria molecolare




3 σ → 120°

Ibridazione $sp^2$
3 legami σ + 1 legame π

O=C=O

Ibridazione sp

2 legami σ + 2 legami π

2σ → 180°

H-C≡C-H

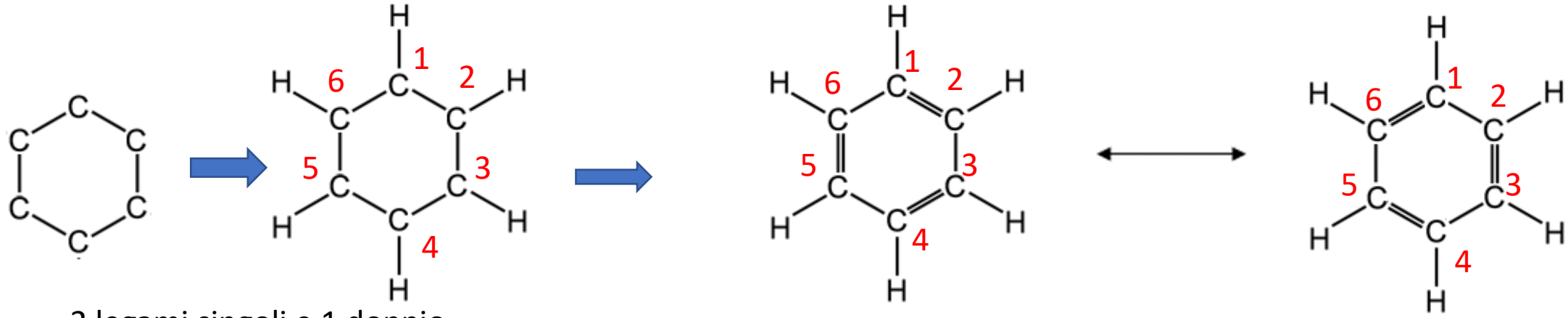
Ibridazione sp

2 legami σ + 2 legami π

2σ → 180°

benzene $C_6H_6$

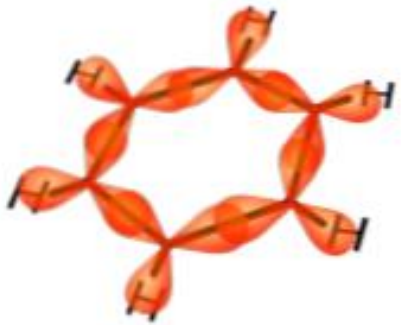
# RISONANZA

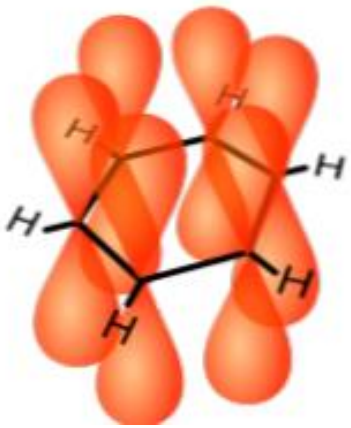


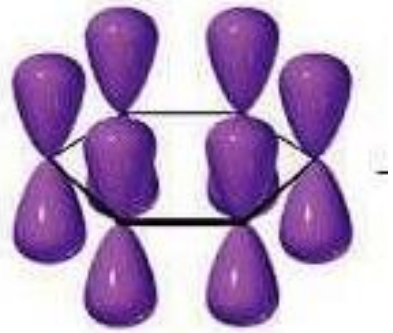

2 legami singoli e 1 doppio
3 σ + 1 π = ibridazione $sp^2$
Trigonale planare

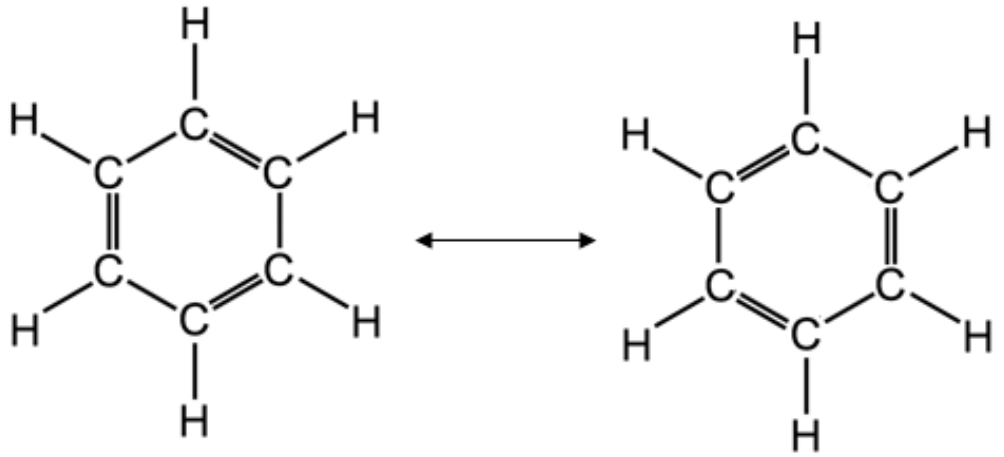
3 C=C e 3 C-C
$E_{C=C} > E_{C-C}$ $d_{C=C} < d_{C-C}$

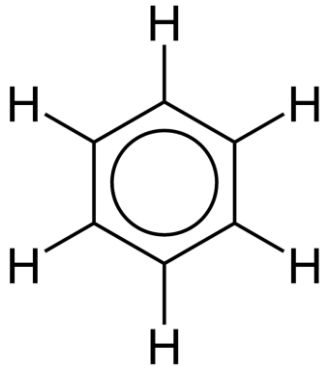
I 6 legami tra gli atomi di carbonio sono uguali tra loro
Stessa energia di legame
Stessa distanza di legame



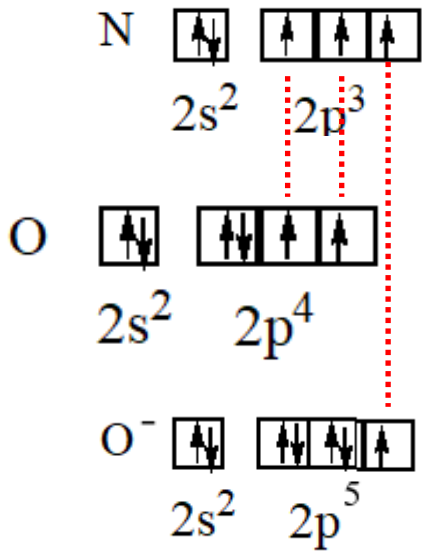


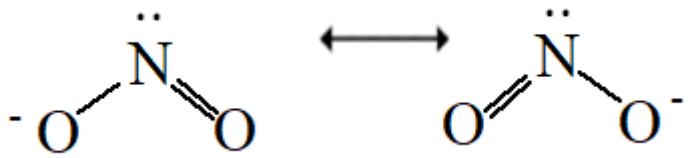






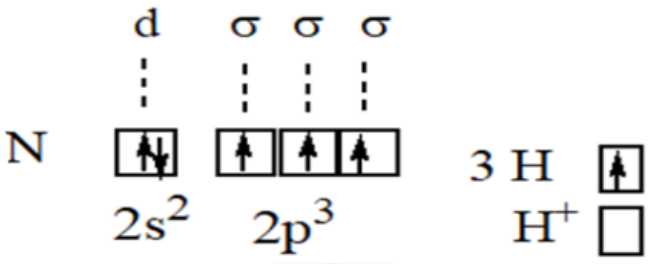
Ione $NO_2^-$

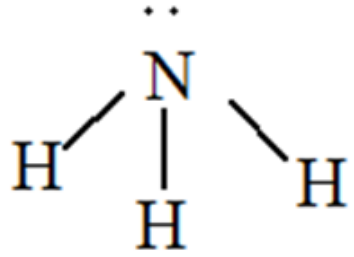


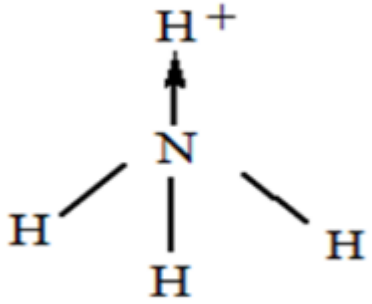



# LEGAME DATIVO

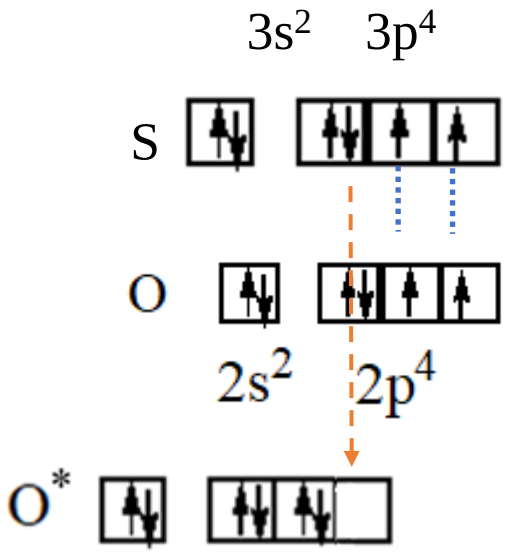
$NH_3 + H^+ \leftrightarrows NH_4^+$

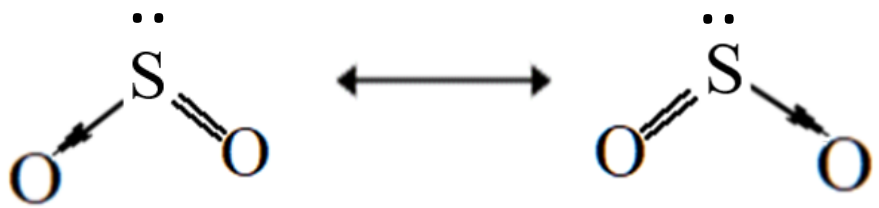


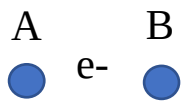




$SO_2$



# Orbitale Molecolare



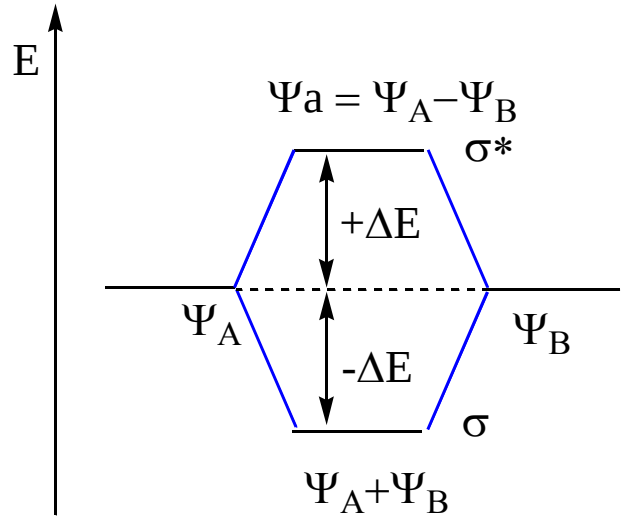

LCAO

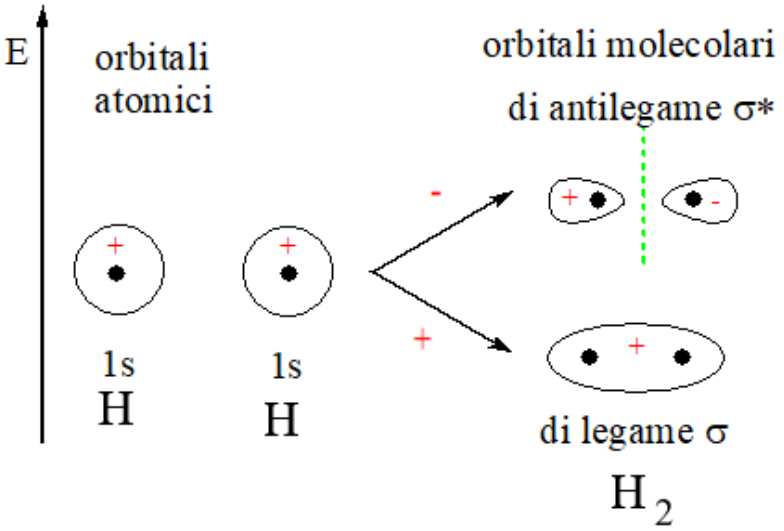
Linear Combination of Atomic Orbitals

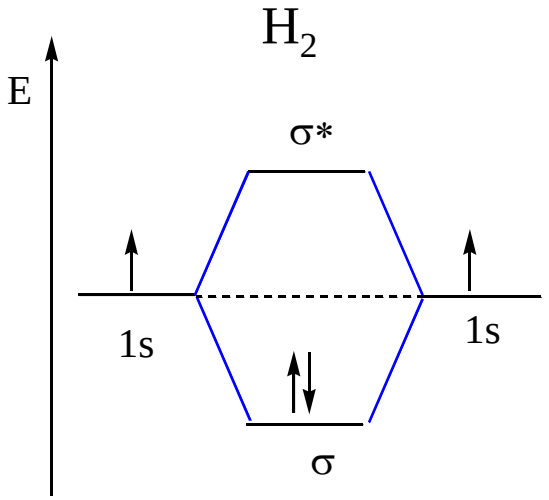
$\Psi_{MO} = \Psi_A \pm \Psi_B$

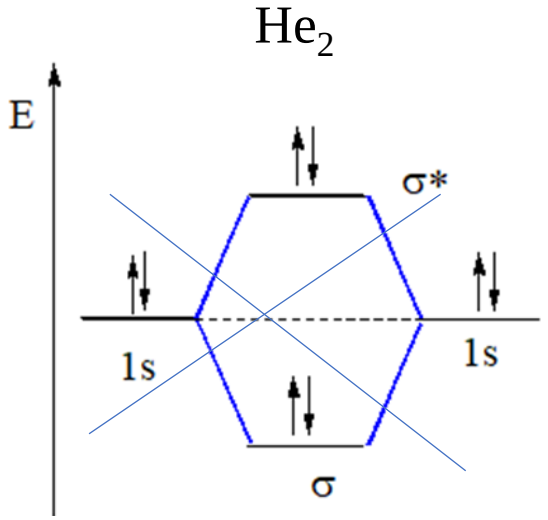
$\Psi_b = \Psi_A + \Psi_B$ Orbitale di legame

$\Psi_a = \Psi_A - \Psi_B$ Orbitale di antilegame



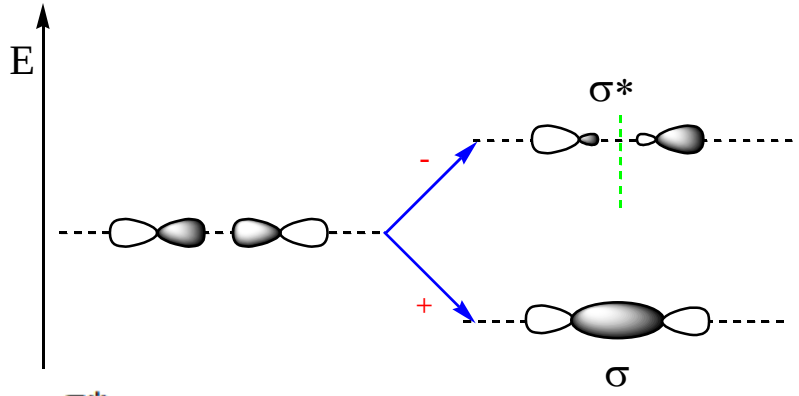



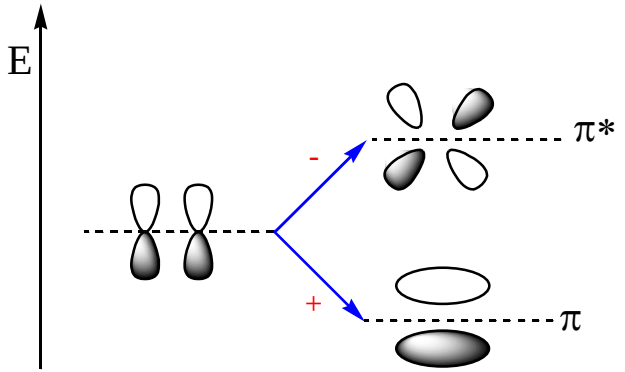



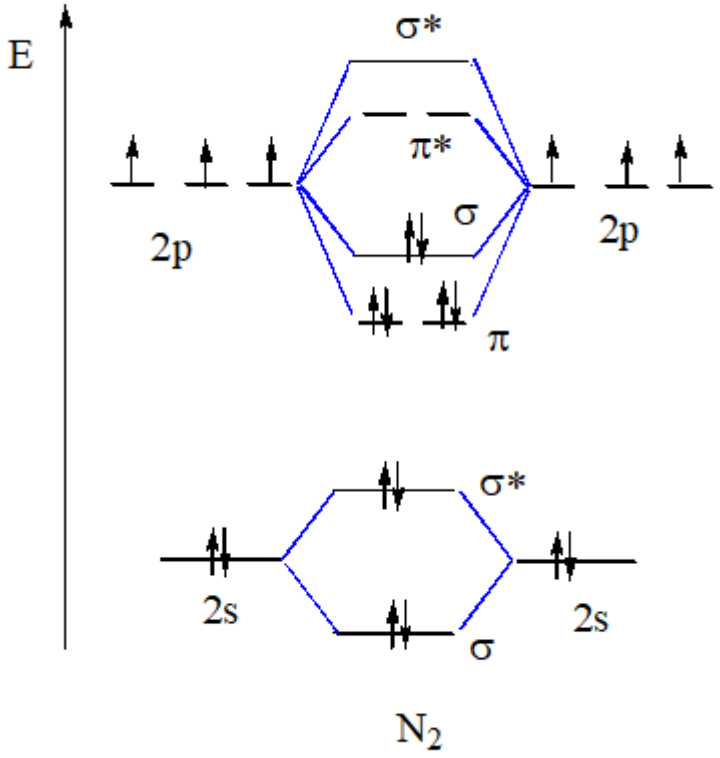




Ordine di Legame = n.coppie$_{legame}$ -n. coppie$_{antilegame}$

LCAO Si combinano orbitali di pari: a) Energia, b)Simmetria (σ o π)

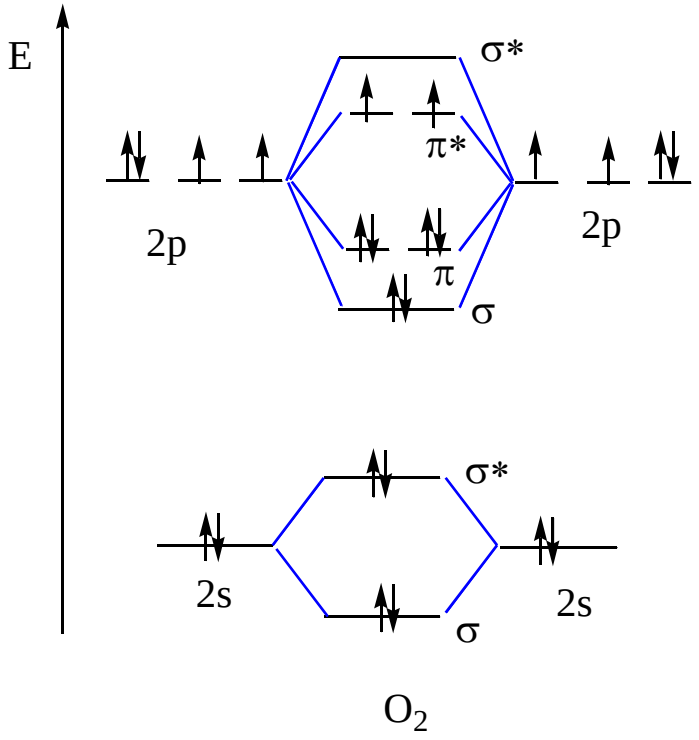


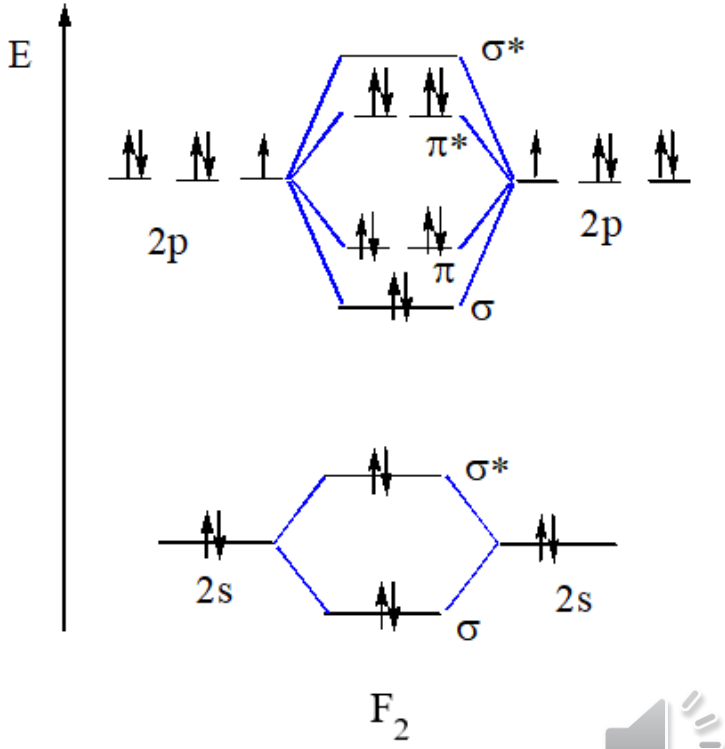

$N_2$

O.L. = 3 N≡N



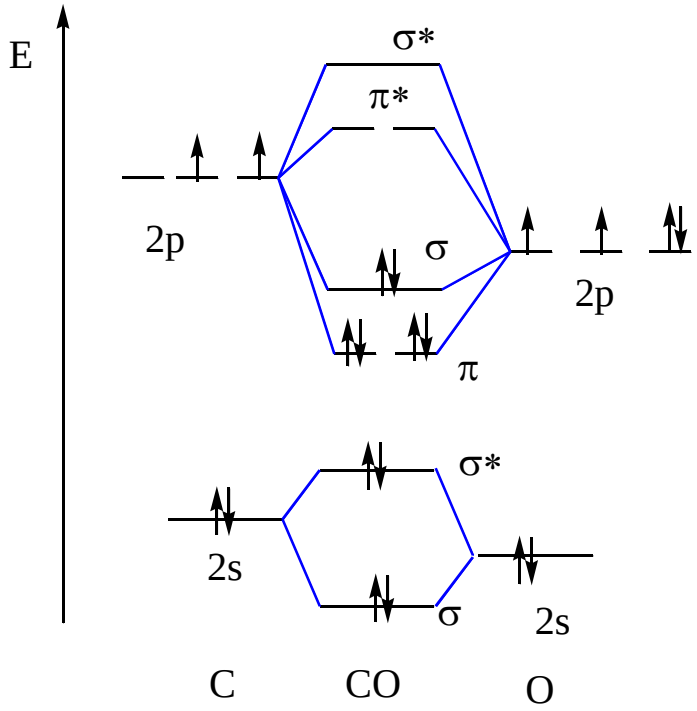

$O_2$

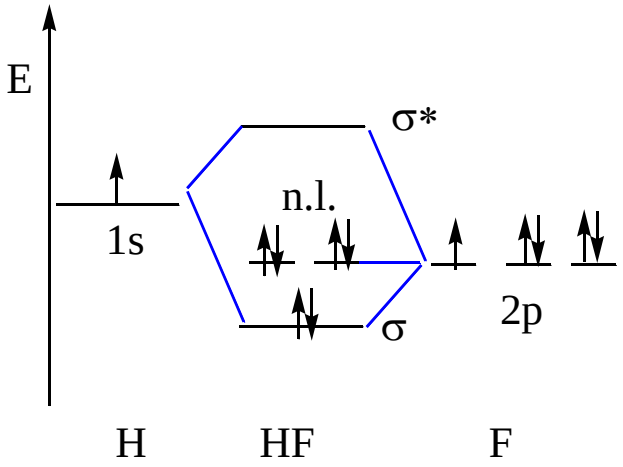
O.L. = 3-2(1/2)=2 O=O

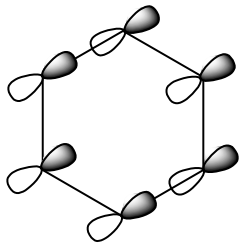


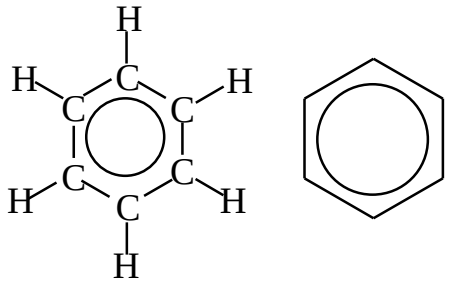

$F_2$

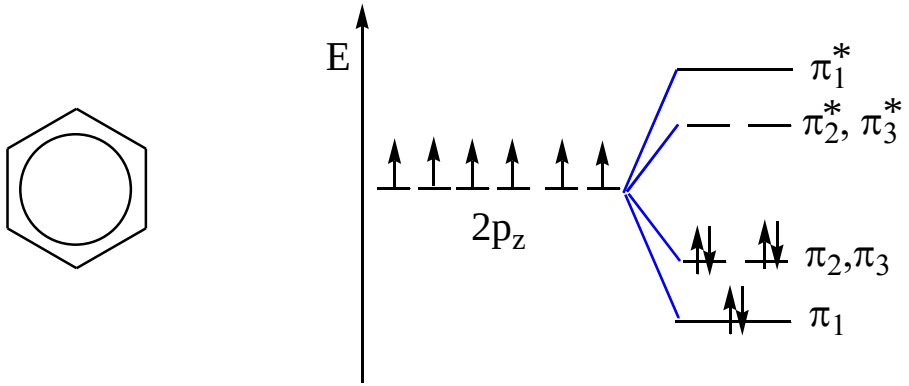
O.L. = 3-2=1 F-F


E
σ*
π*
2p
σ
2p
π
σ*
2s
σ
2s
C
CO
O


E
σ*
n.l.
1s
2p
σ
H
HF
F



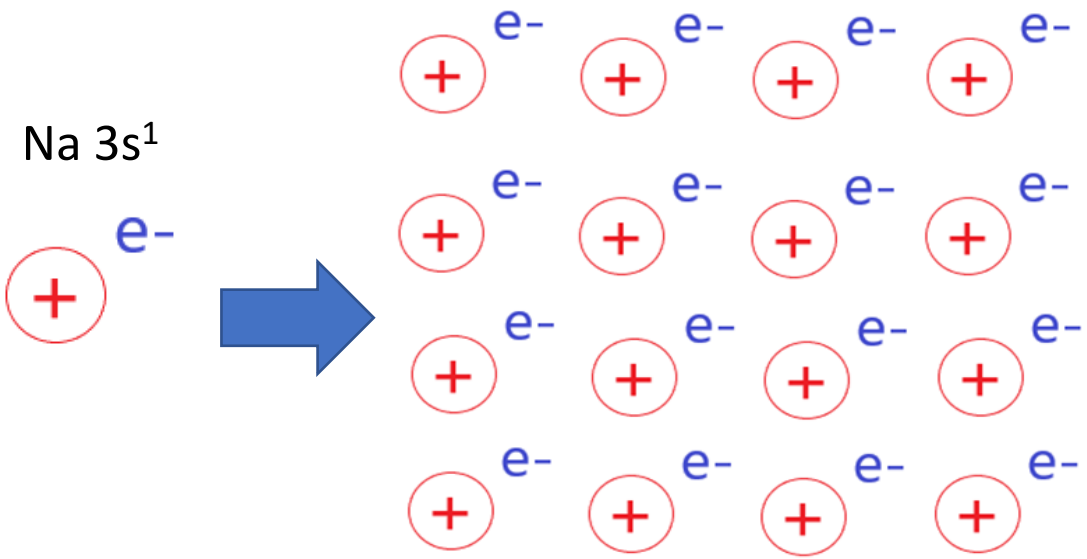

H
H
C
H
C
C
C
H
C
H
H

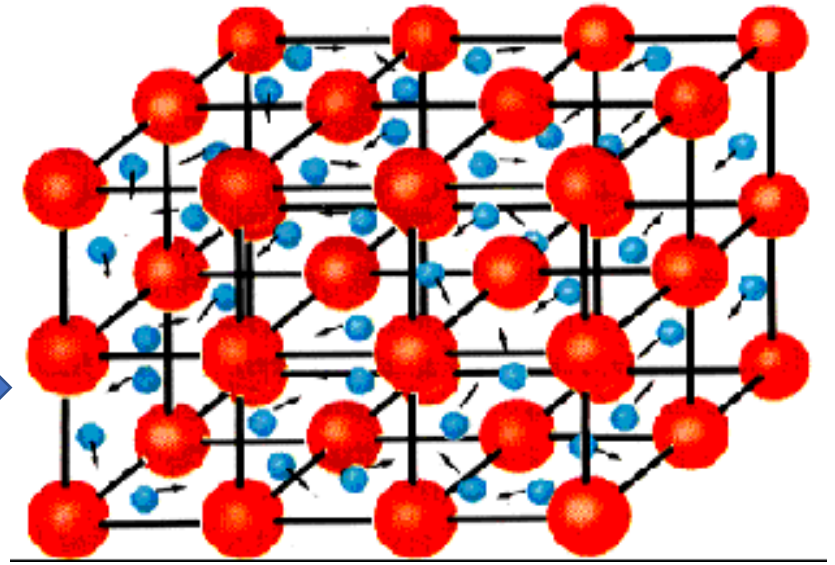

E
$\pi_1^*$
$\pi_2^*, \pi_3^*$
$2p_z$
$\pi_2,\pi_3$
$\pi_1$

# LEGAME METALLICO

Metalli→ Basso I

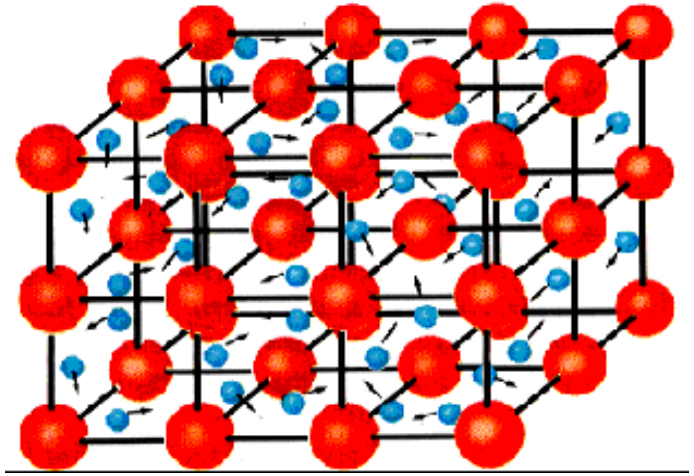
Na $3s^1$



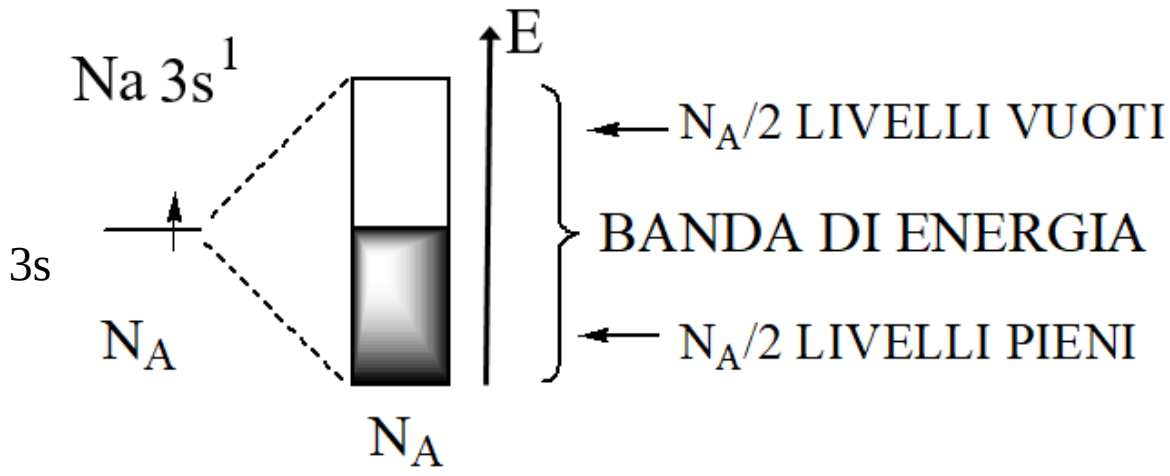
RETICOLO CRISTALLINO
→ IONI METALLICI

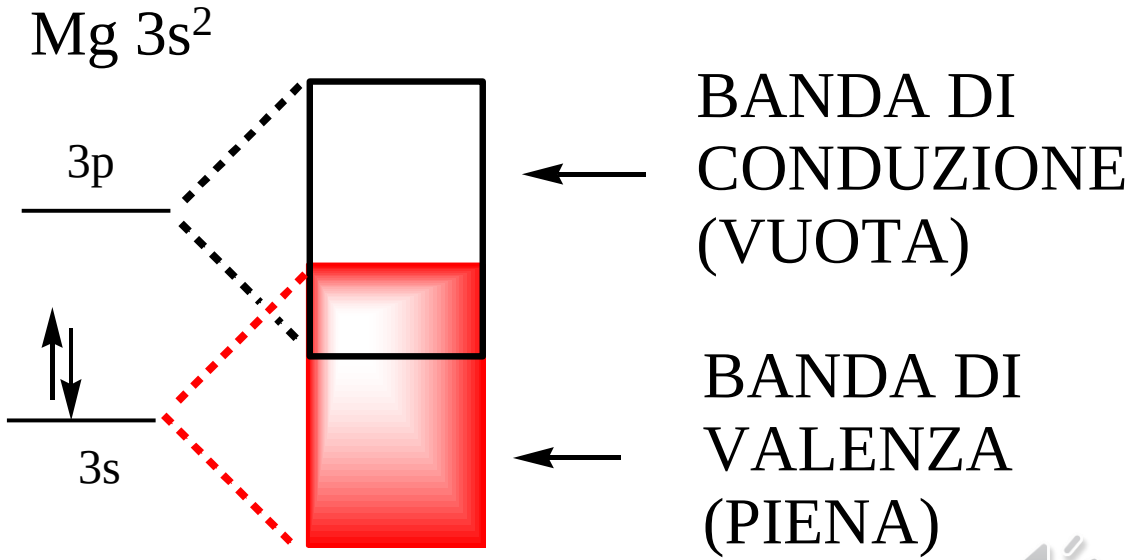
ELETTRONI DI VALENZA
→MARE DI FERMI



CONDUCIBILITA
-ELETTRICA
-TERMICA

MALLEABILITA',
DUTTILITA'



# FORZE INTERMOLECOLARI

| | Energia |
|---|---|
| Legami covalenti | 100-1000 KJ/mole |
| Forze intermolecolari | 0,1-10 KJ/mole |

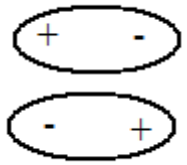
- van der Waals
  - dipolo-dipolo
  - dipolo-dipolo indotto
  - dipolo istantaneo-dipolo indotto
- legame idrogeno

Solidi > liquidi >> gas ≈ 0
Gas reali> gas ideali = 0

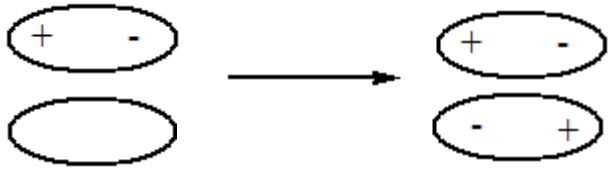
Punto di fusione
Punto di ebollizione

# FORZE DI VAN DER WAALS

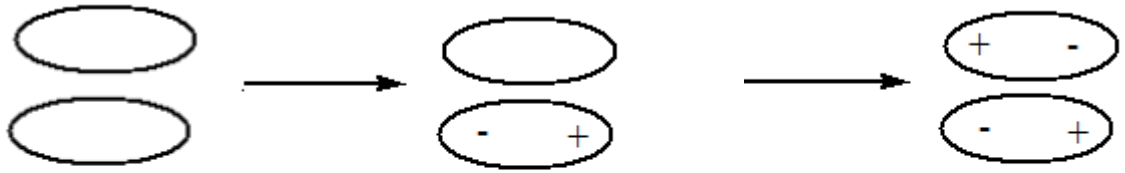
dipolo-dipolo



dipolo-dipolo indotto



dipolo istantaneo-dipolo indotto



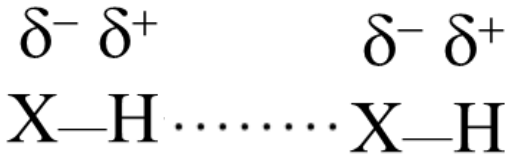
molecole apolari

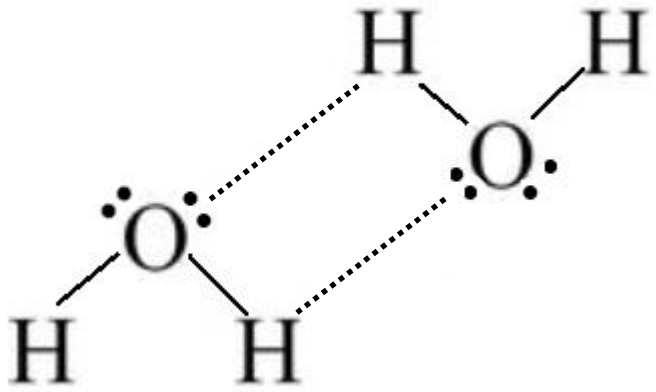
dipolo instantaneo

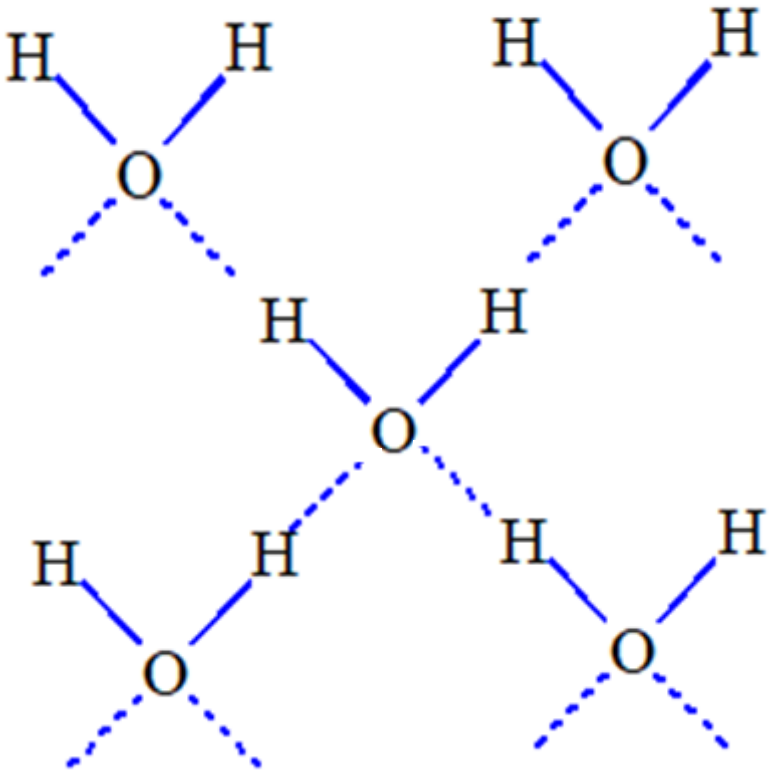
dipolo indotto

Es $F_2$, $Cl_2$, $Br_2$, $I_2$

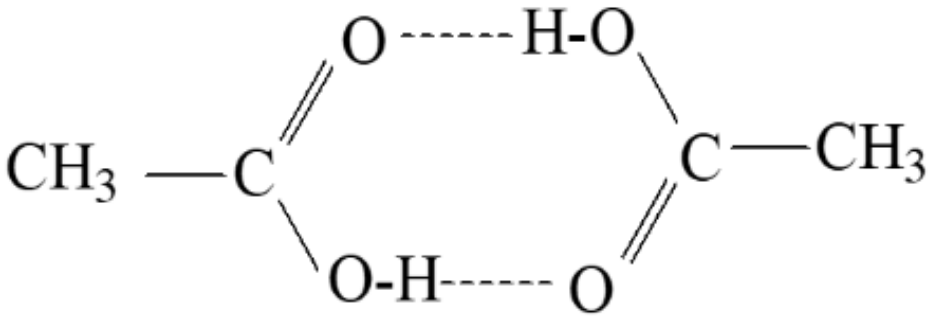
# LEGAME IDROGENO



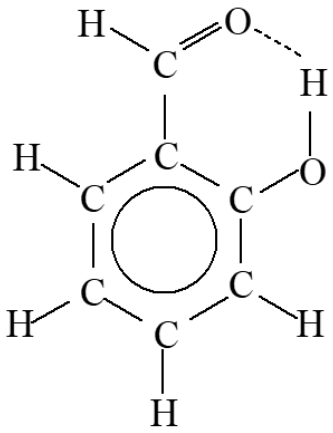



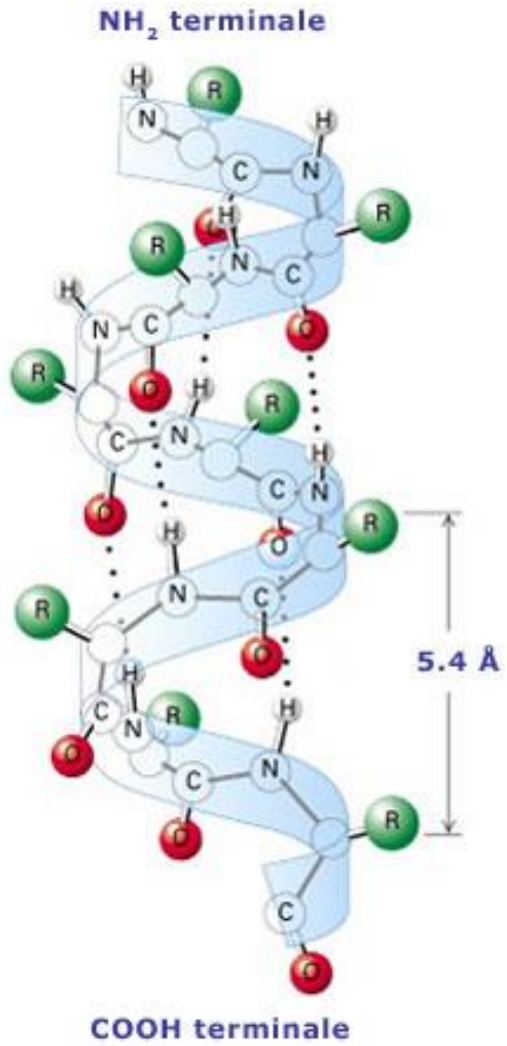



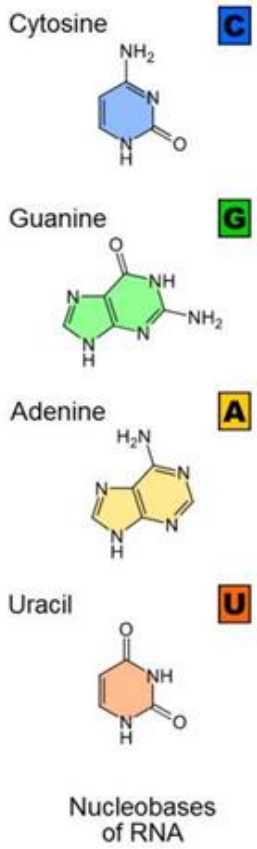

INTERMOLECOLARE

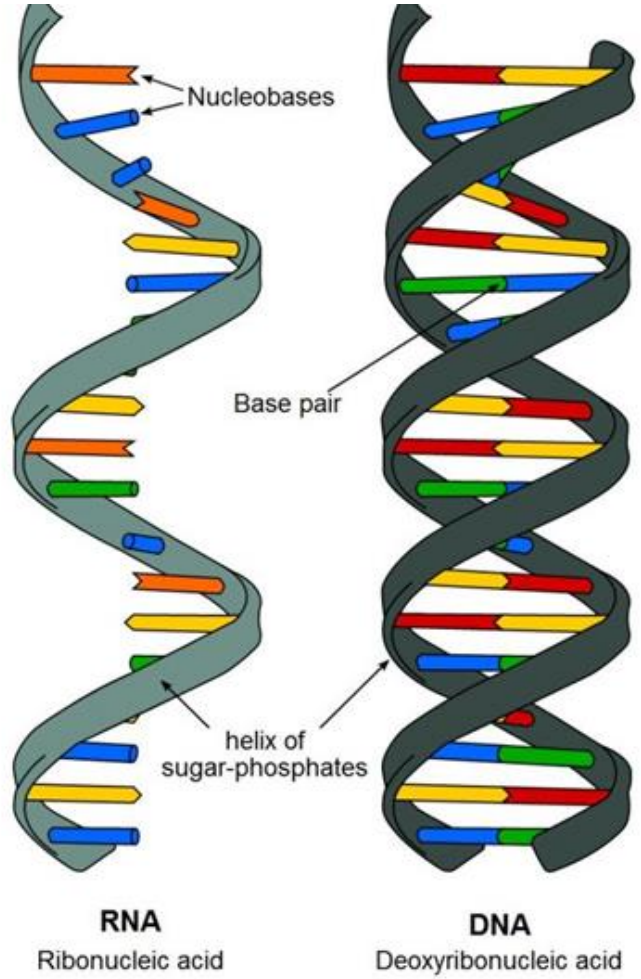


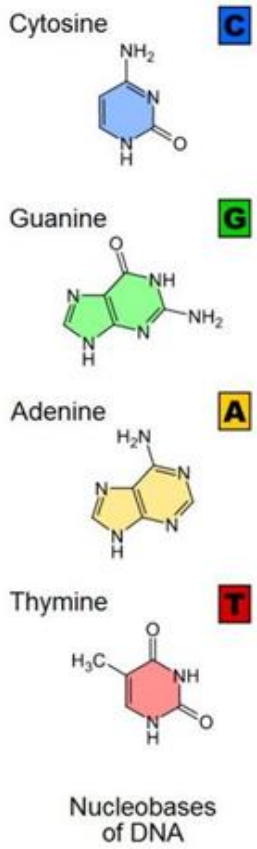

INTRAMOLECOLARE




NH2 terminale
5.4 Å
COOH terminale


Cytosine
C
Guanine
G
Adenine
A
Uracil
U
Nucleobases of RNA


Nucleobases
Base pair
helix of sugar-phosphates
RNA
Ribonucleic acid
DNA
Deoxyribonucleic acid


Cytosine
C
Guanine
G
Adenine
A
Thymine
T
Nucleobases of DNA