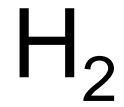
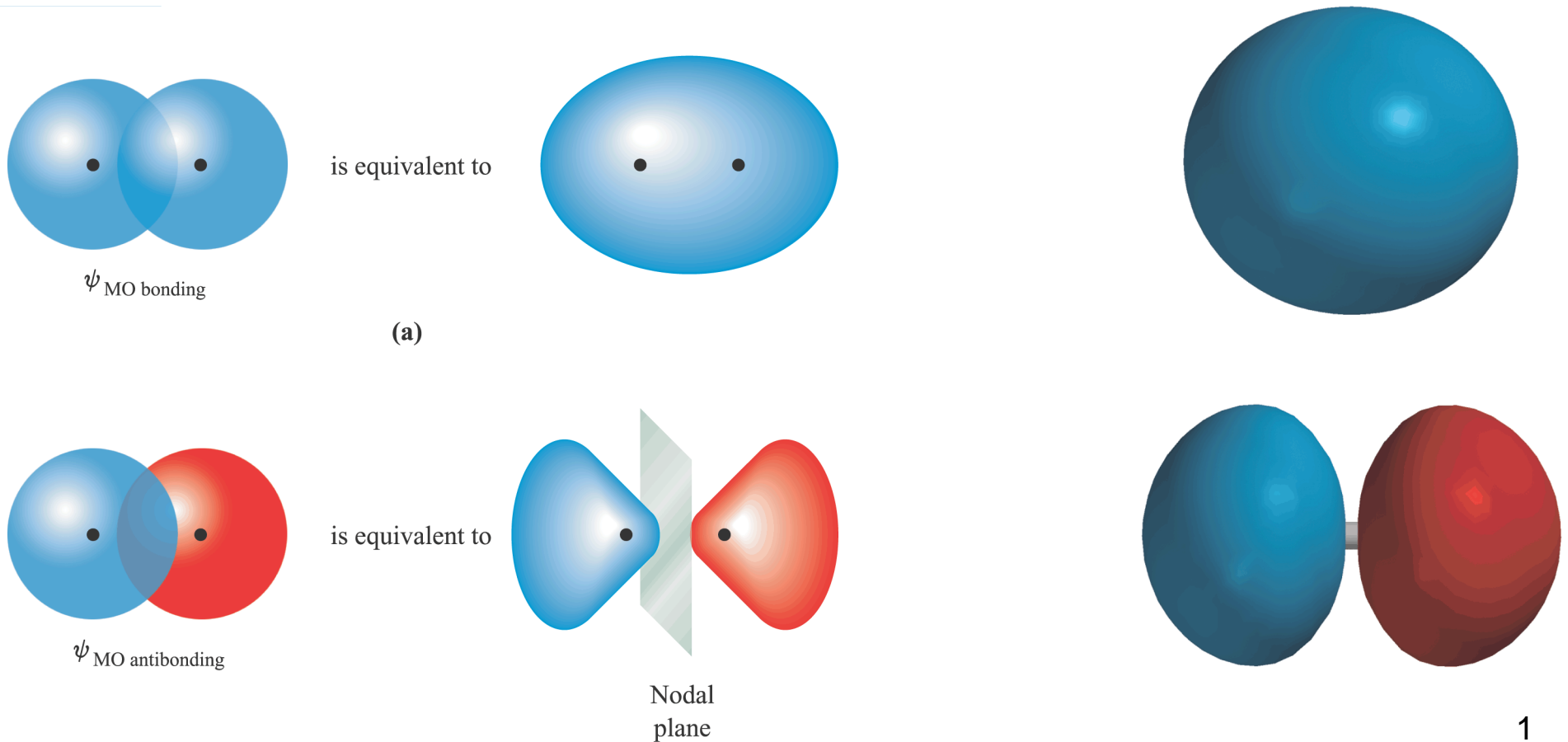


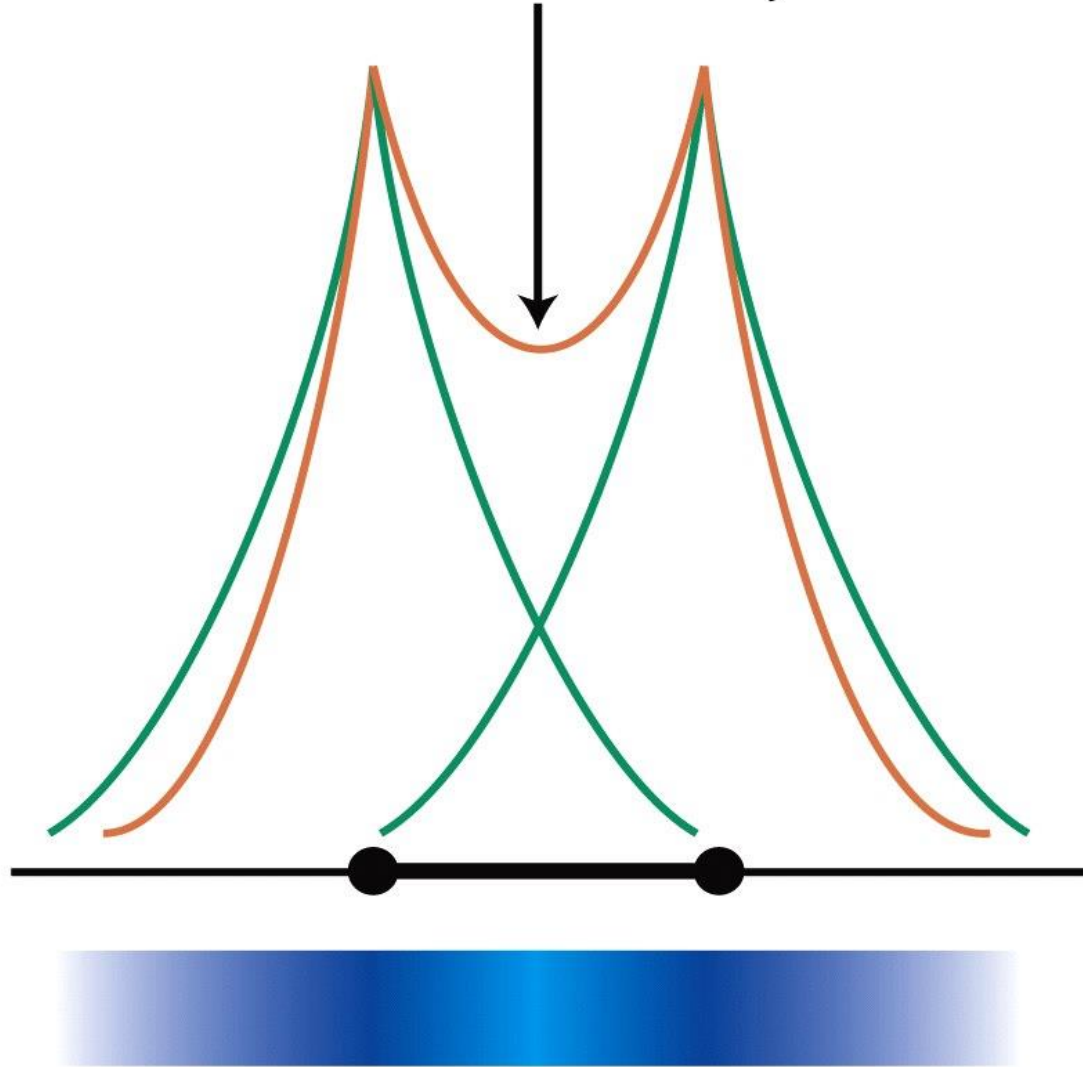
Teoria dell'Orbitale Molecolare

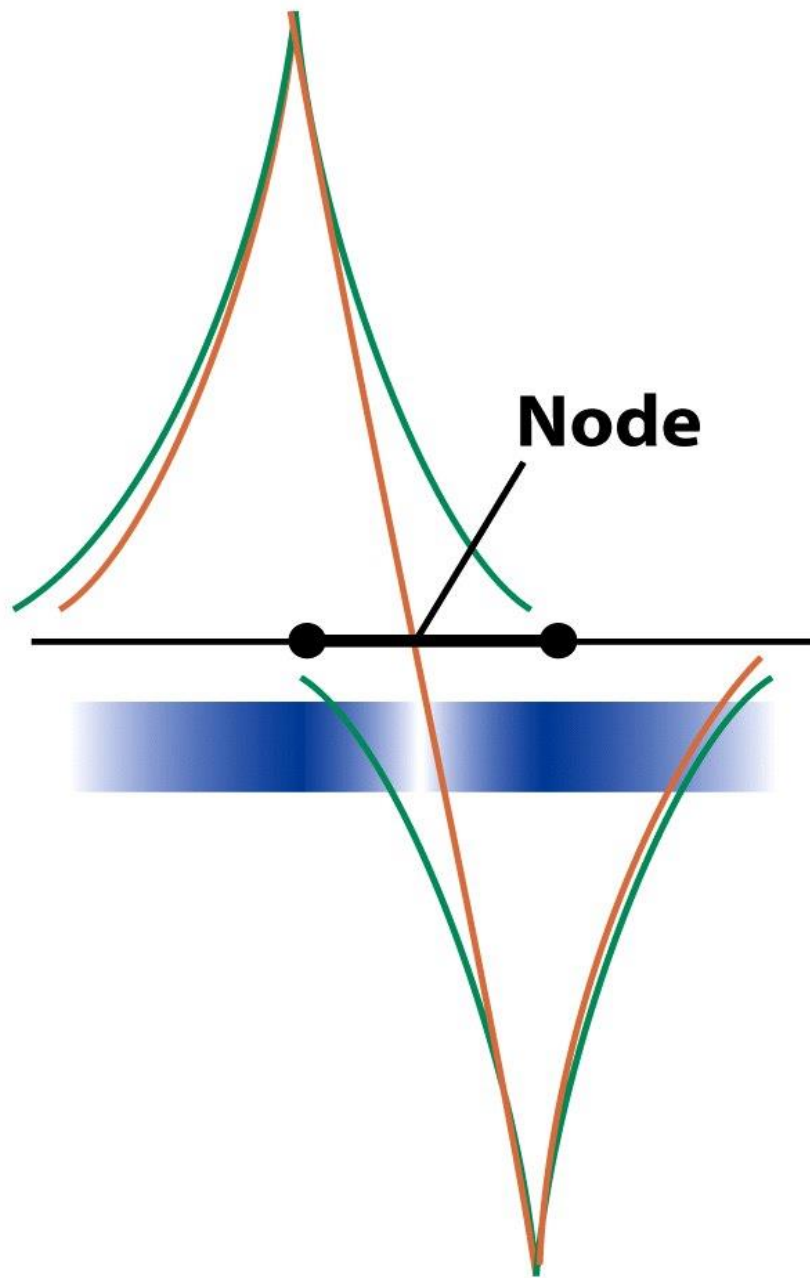


Linear Combination of Atomic Orbitals (LCAO)



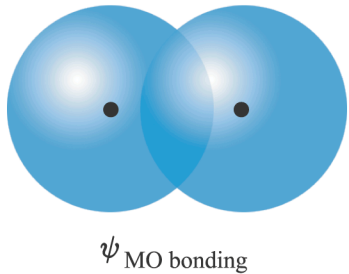
**Enhanced
density**



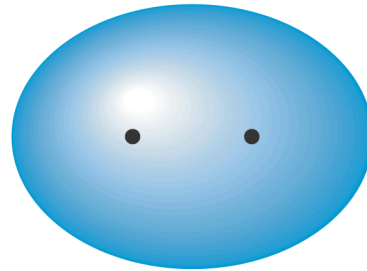


Teoria dell'Orbitale Molecolare

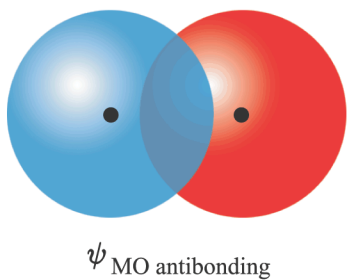
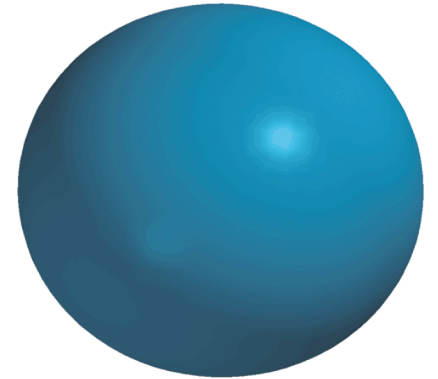
$$\Psi^2_{\text{legante}} = \Psi^2_A + \Psi^2_B + 2\Psi_A\Psi_B$$



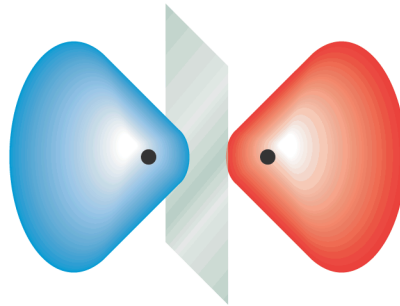
is equivalent to



(a)



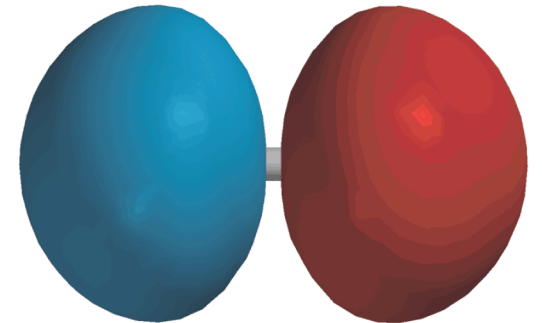
is equivalent to



(b)

$$\Psi^2_{\text{antilegante}} = \Psi^2_A + \Psi^2_B - 2\Psi_A\Psi_B$$

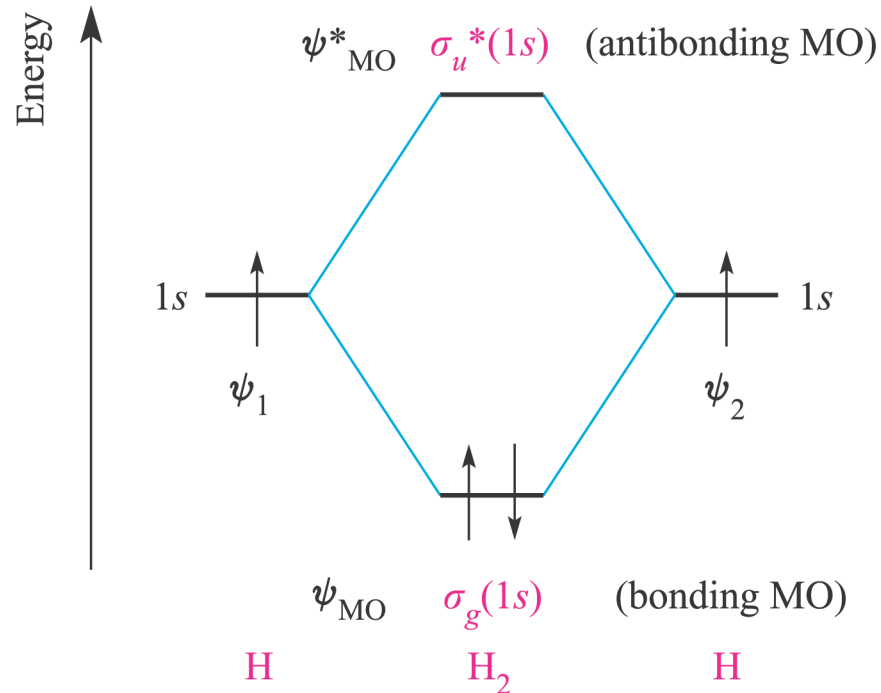
(c)



$\int \Psi_A \Psi_B d\tau = \text{integrale di sovrapposizione } S$

$$N_b = \sqrt{1/(2 + 2S)}$$

$$N_a = \sqrt{1/(2 - 2S)}$$

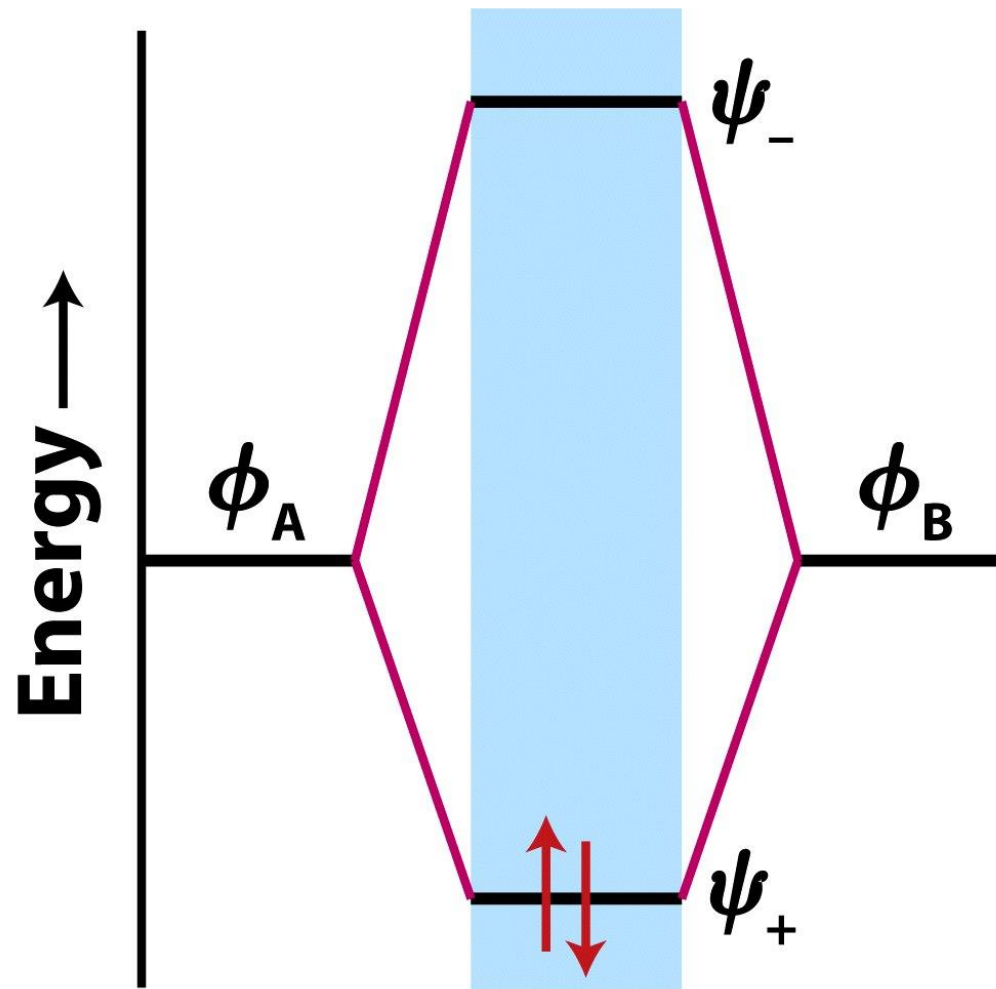


Trascurando l'integrale di sovrapposizione S

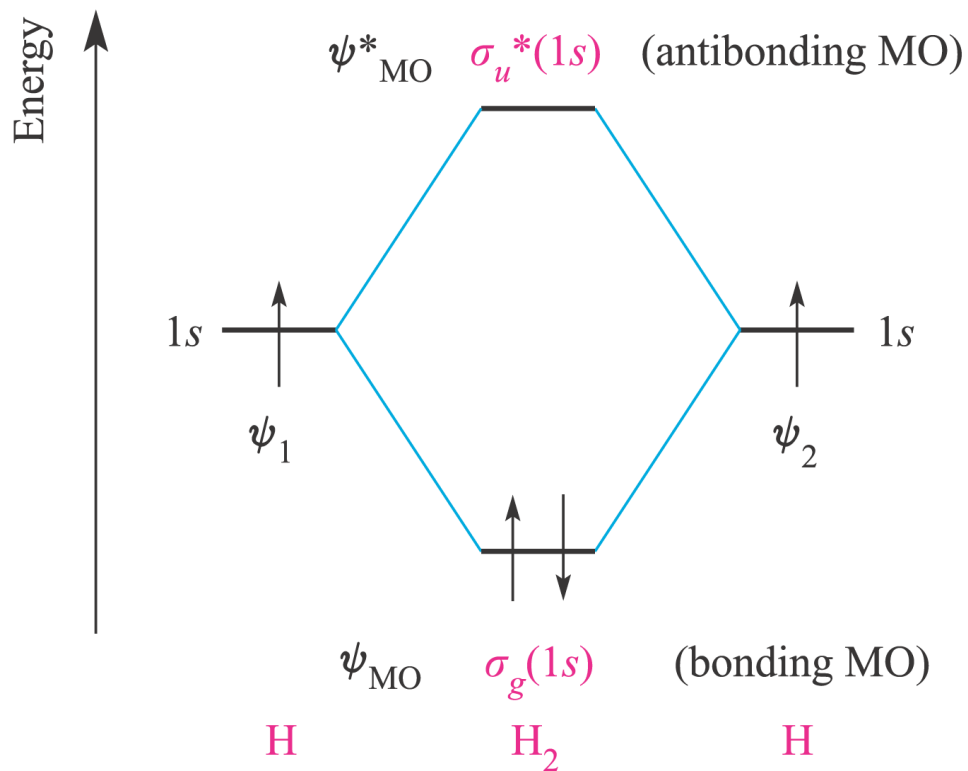
$$N_b = N_a = \sqrt{1/2} = 0.71$$

Considerando l'integrale di sovrapposizione S

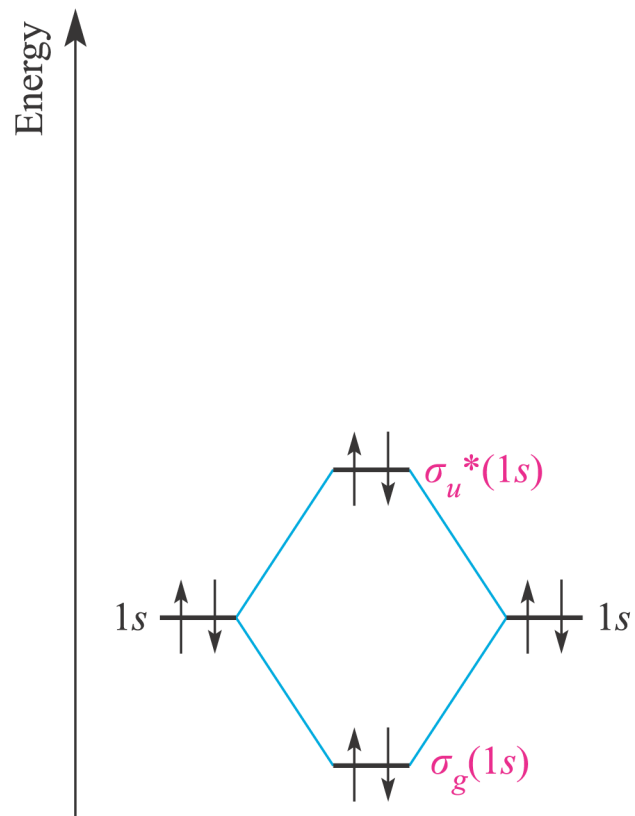
$$N_b < N_a$$



$$\text{ordine di legame} = \frac{1}{2}(n \cdot e_B - n \cdot e_{AB})$$

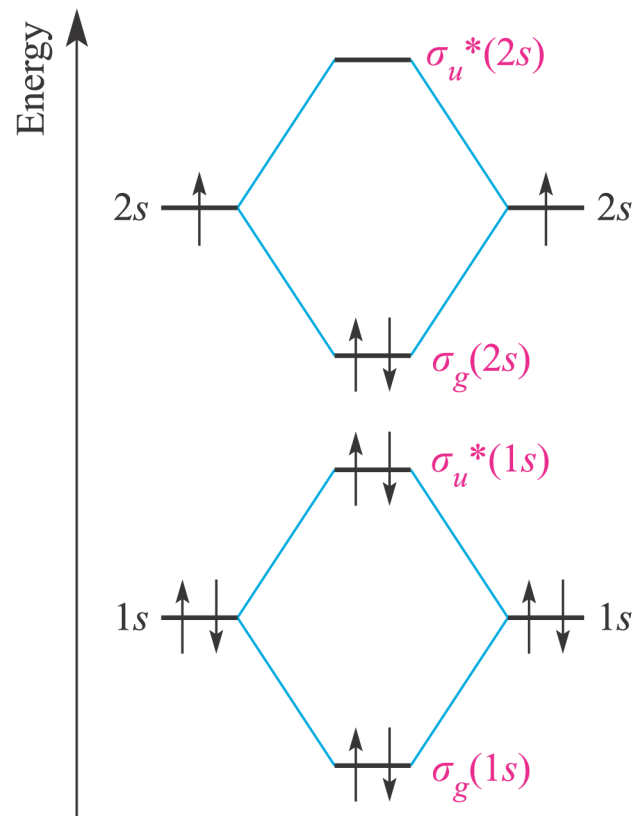


Molecola	Ordine di legame	Energia legame (kJ/mol)	Lunghezza legame (pm)
H_2	1	458	74
H_2^+	0.5	269	105



He He₂ He

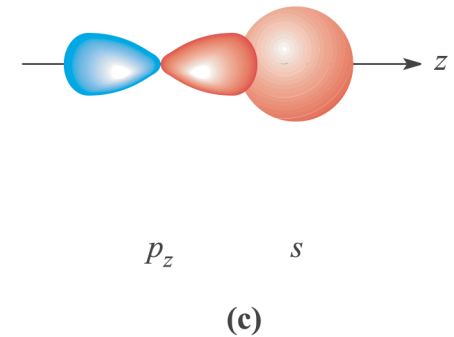
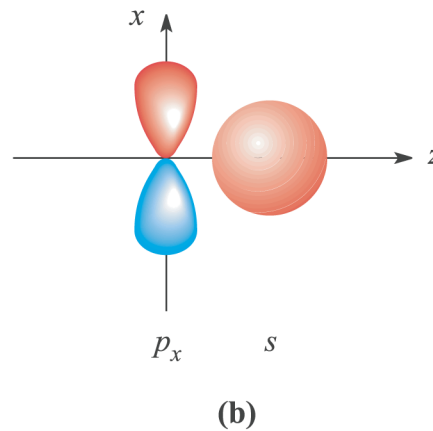
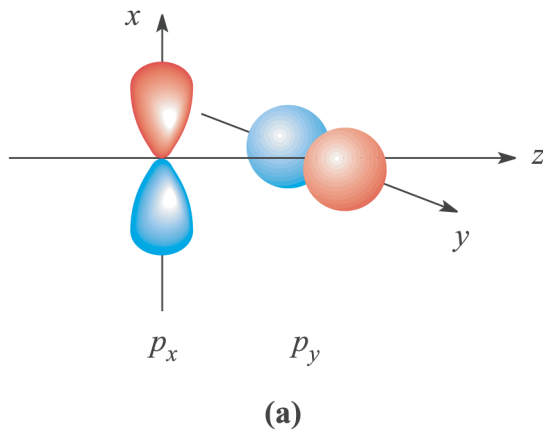
(a)



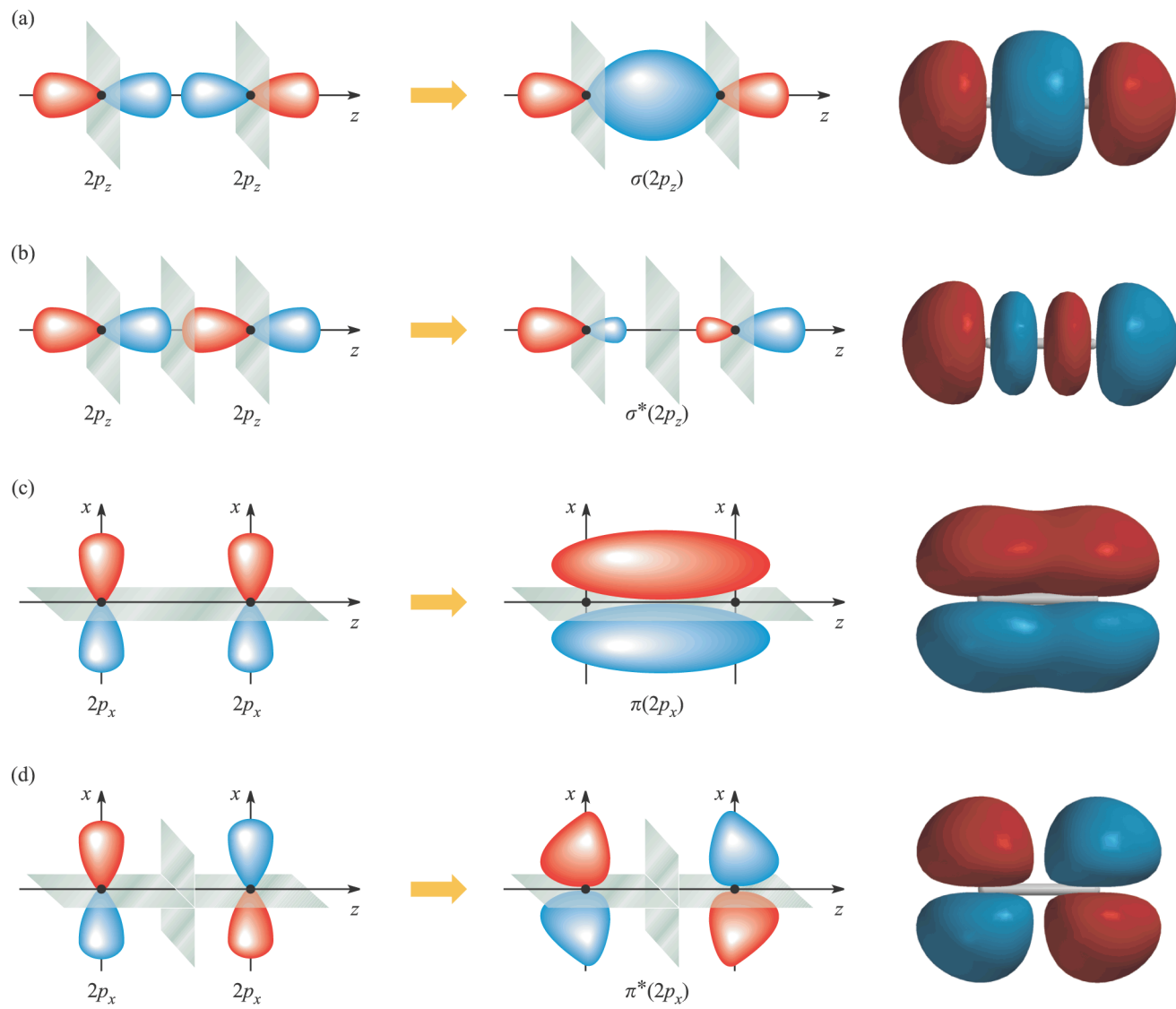
Li Li₂ Li

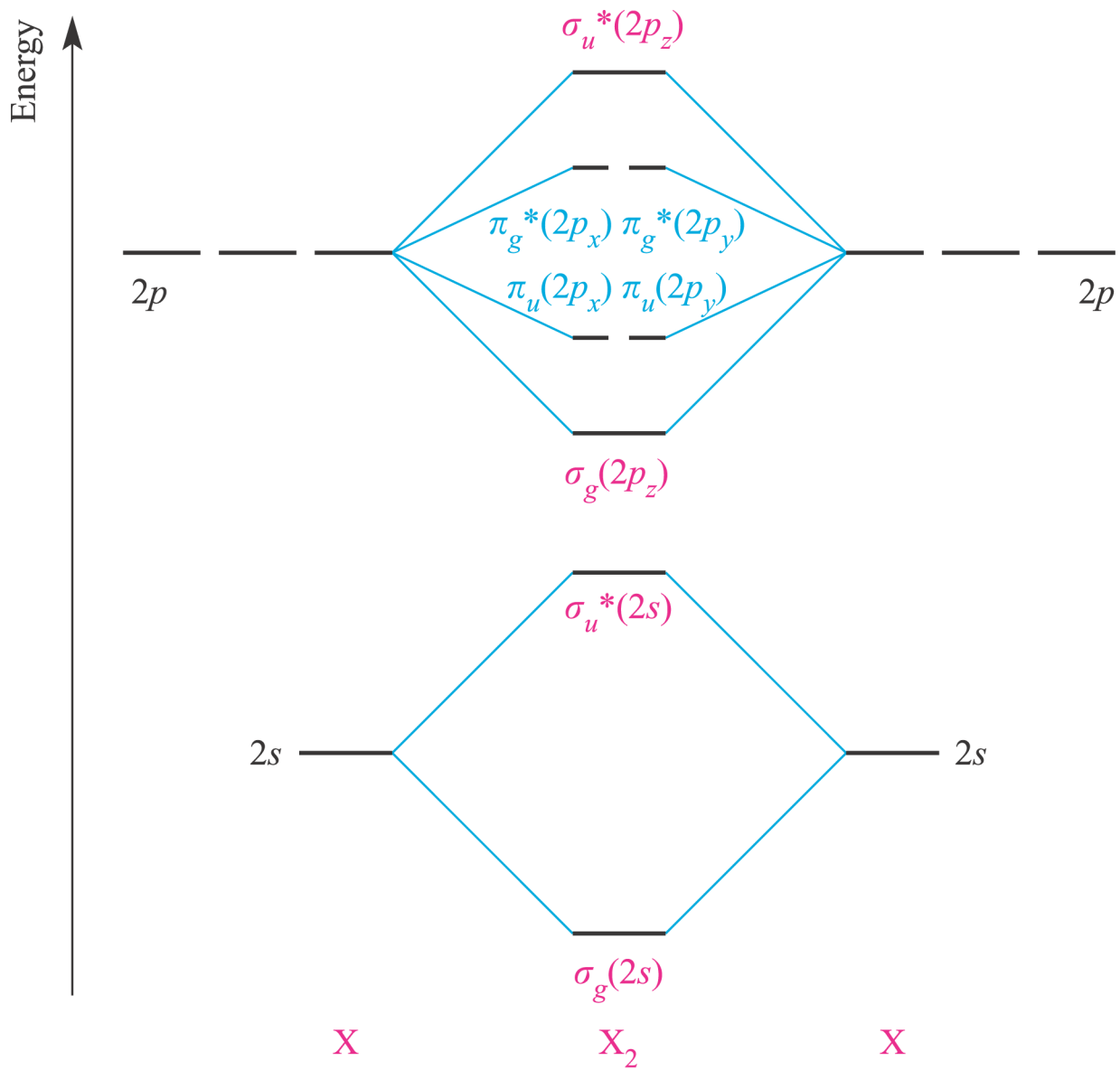
(b)

Interazioni di non-legame



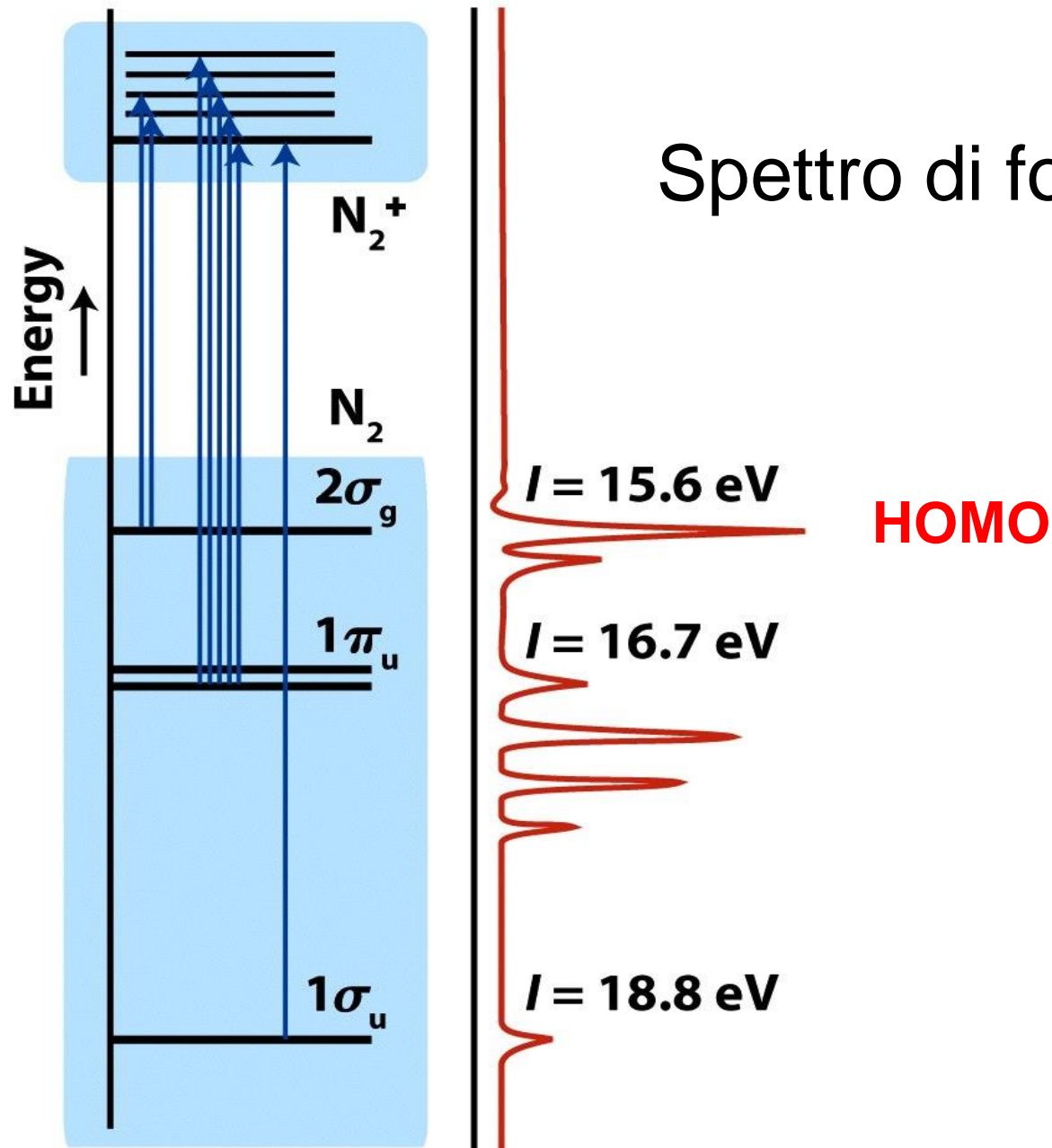
- Simmetria
- Entità sovrapposizione
- Energia relativa

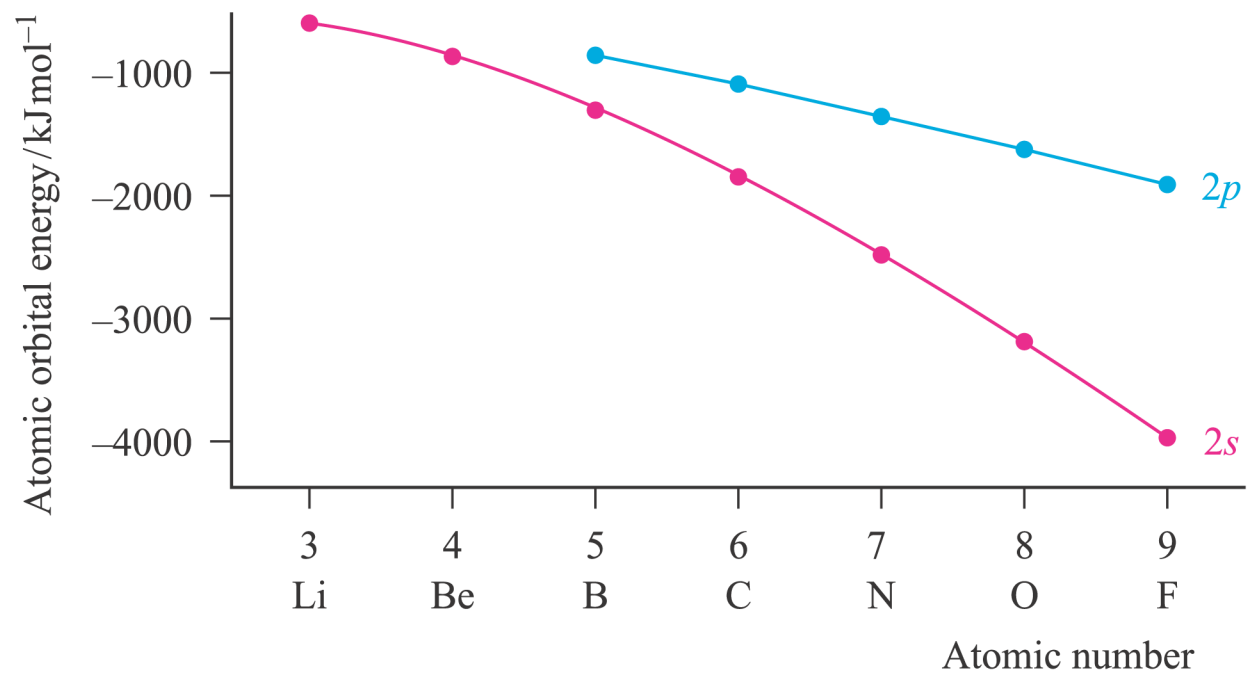


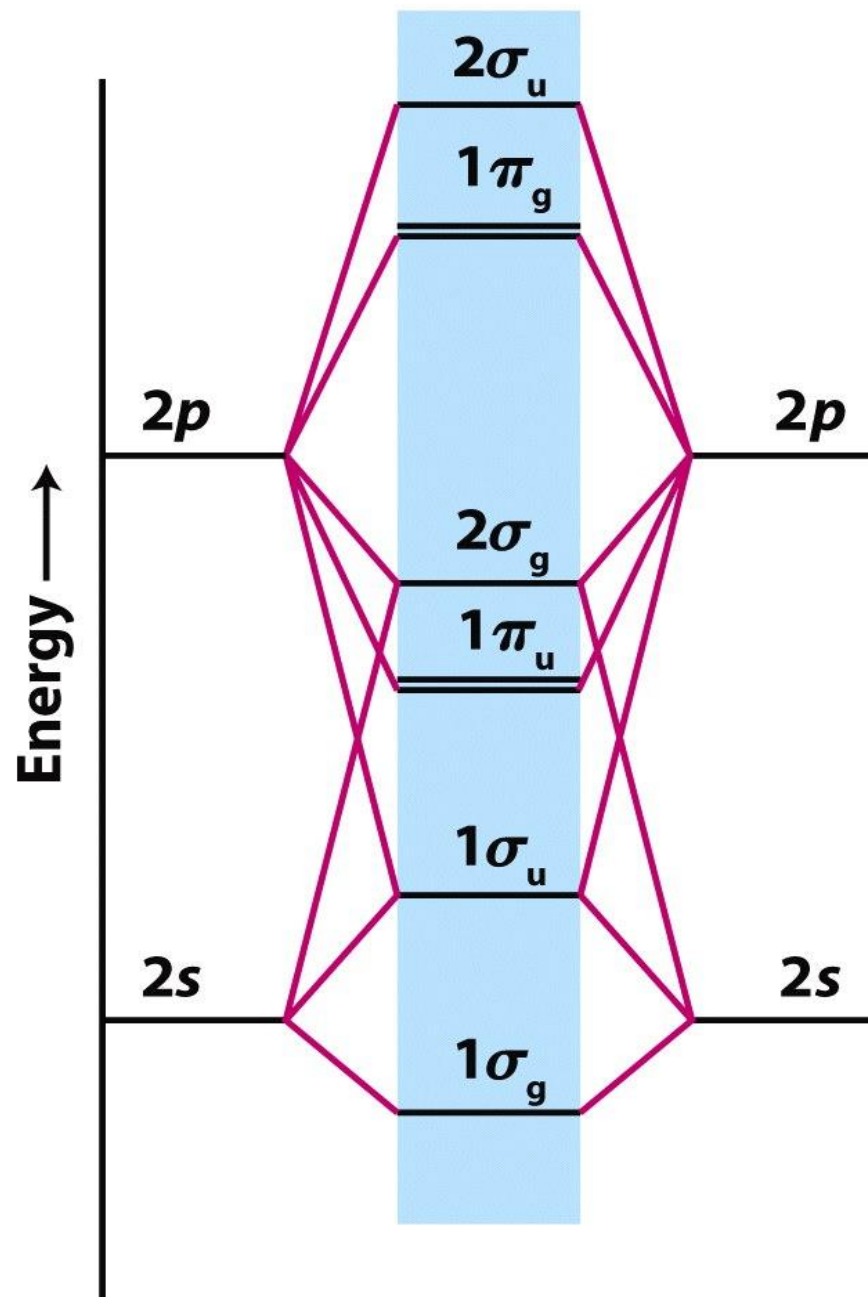


X = O, F

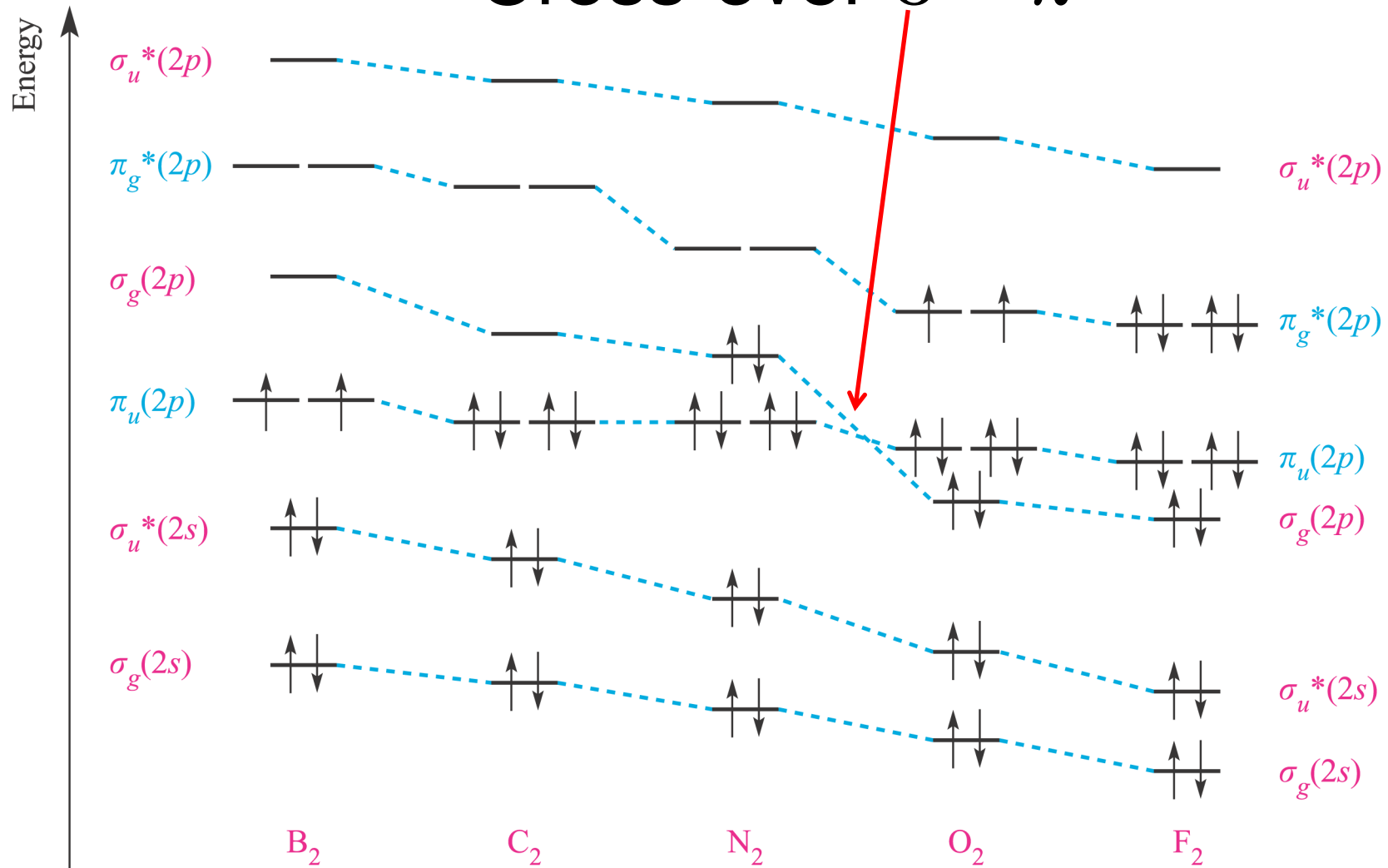
Spettro di fotoelettroni di N_2







Cross-over $\sigma - \pi$



Diatomic	Bond distance / pm	Bond dissociation enthalpy / kJ mol^{-1}	Bond order	Magnetic properties
Li_2	267	110	1	Diamagnetic
Be_2^\dagger	—	—	0	—
B_2	159	297	1	Paramagnetic
C_2	124	607	2	Diamagnetic
N_2	110	945	3	Diamagnetic
O_2	121	498	2	Paramagnetic
F_2	141	159	1	Diamagnetic

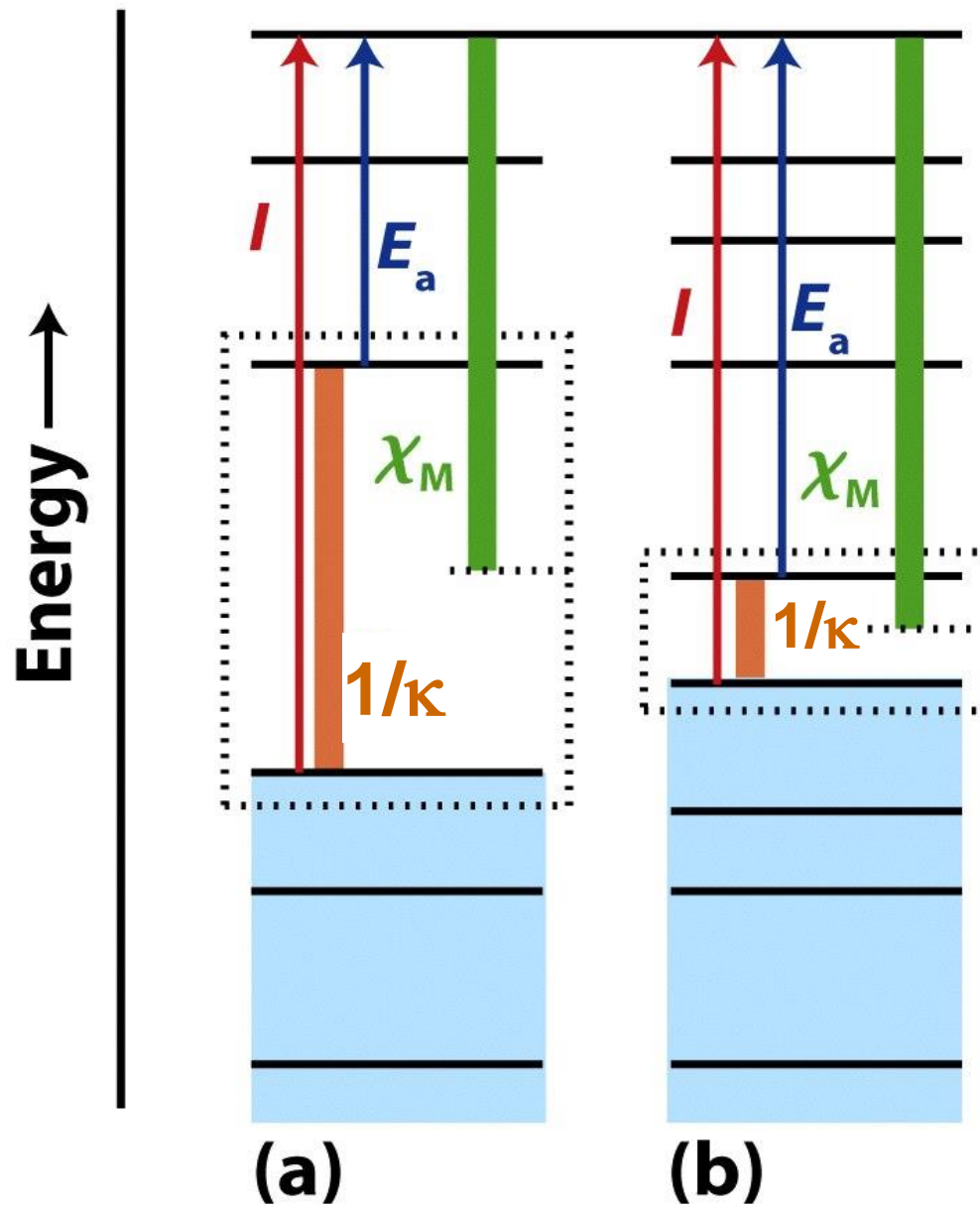
Molecola	Ordine di legame	Lunghezza di legame (pm)
O ₂	2	121
O ₂ ⁻	1.5	126
O ₂ ²⁻	1	149
O ₂ ⁺	2.5	112

Au₂(g) (221 kJ/mol)

Elettronegatività di Pauling, χ^P

Group 1	Group 2		Group 13	Group 14	Group 15	Group 16	Group 17
H 2.2							
Li 1.0	Be 1.6		B 2.0	C 2.6	N 3.0	O 3.4	F 4.0
Na 0.9	Mg 1.3		Al(III) 1.6	Si 1.9	P 2.2	S 2.6	Cl 3.2
K 0.8	Ca 1.0	<i>(d-block elements)</i>	Ga(III) 1.8	Ge(IV) 2.0	As(III) 2.2	Se 2.6	Br 3.0
Rb 0.8	Sr 0.9		In(III) 1.8	Sn(II) 1.8 Sn(IV) 2.0	Sb 2.1	Te 2.1	I 2.7
Cs 0.8	Ba 0.9		Tl(I) 1.6 Tl(III) 2.0	Pb(II) 1.9 Pb(IV) 2.3	Bi 2.0	Po 2.0	At 2.2

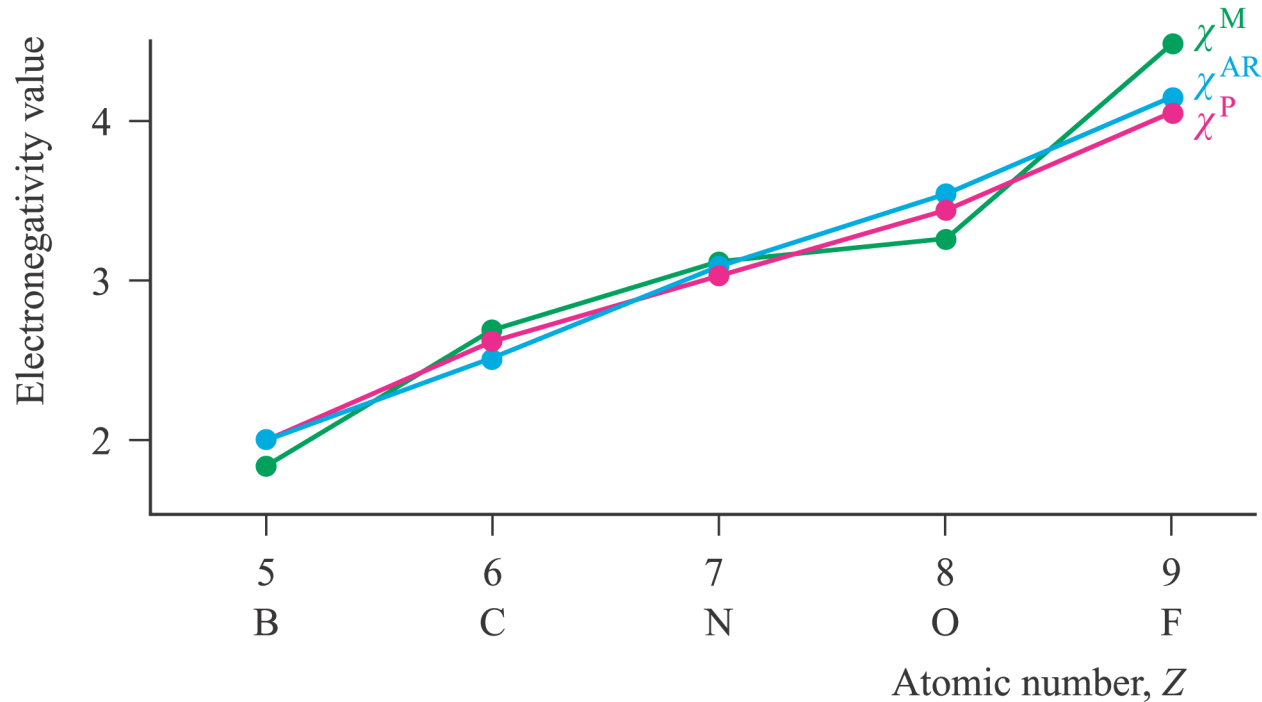
Ionization limit



Elettronegatività di Mulliken, χ^M

$$\chi^M = \frac{1}{2}(I_v + Ea_v)$$

$$\chi^{AR} = (3590 \times Z_{\text{eff}}/r_{\text{cov}}^2) + 0.744$$



χ^M = Mulliken

χ^{AR} = Allred e Rochow (elettronegatività = forza elettrostatica esercitata dal nucleo sugli elettroni di valenza)

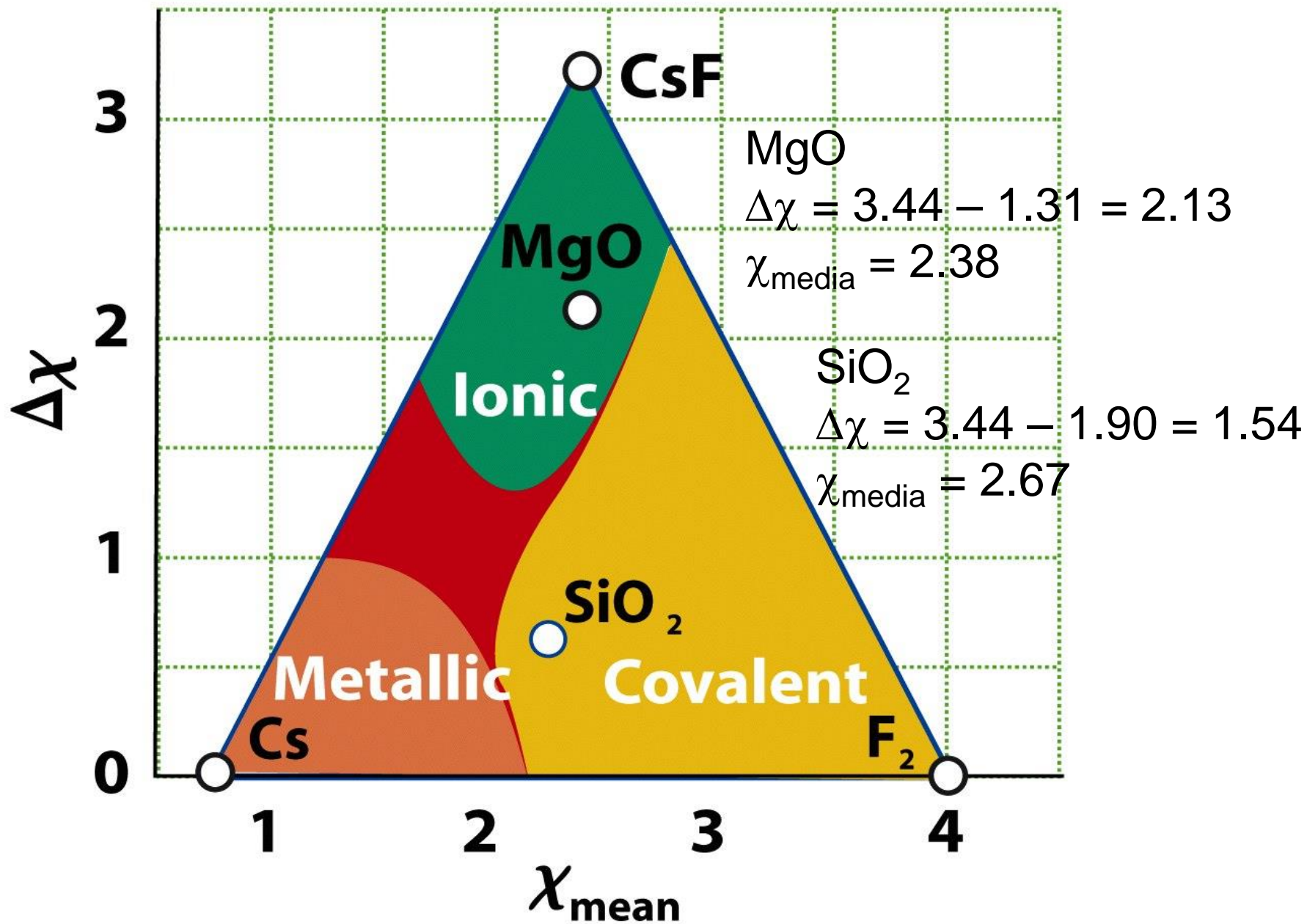
Dipendenza di χ^M da carica parziale δ e ibridizzazione

$\chi = a + b\delta$ **equazione di Mulliken-Jaffè** (b = coefficiente di carica)
 $b = 1/\kappa$ (κ = capacità di carica o **polarizzabilità**)

orbitali ibridi aventi maggiore carattere s sono più elettronegativi

	Ibridizzazione C	χ^M
HC≡CH	sp (50% s)	2.99
CH ₄	sp ³ (25% s)	2.48

	Ibridizzazione N	χ^M	pK _b
Me ₃ N	sp ³ (25% s)	3.04	4.2
C ₅ H ₅ N	sp ² (33% s)	3.26	8.8

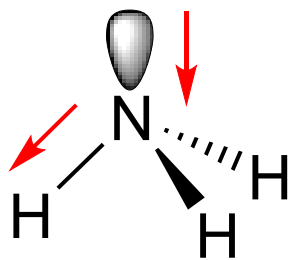


Triangolo di Ketelaar

momento di dipolo elettrico μ

$$\mu = q \times e \times d$$

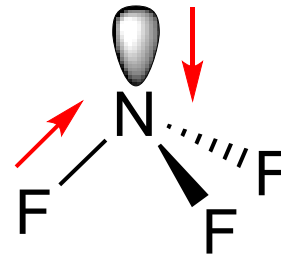
$$1\text{D} = 3.336 \times 10^{-30} \text{ C}\times\text{m}$$



$$\chi_{\text{N}} = 3.0$$

$$\chi_{\text{H}} = 2.2$$

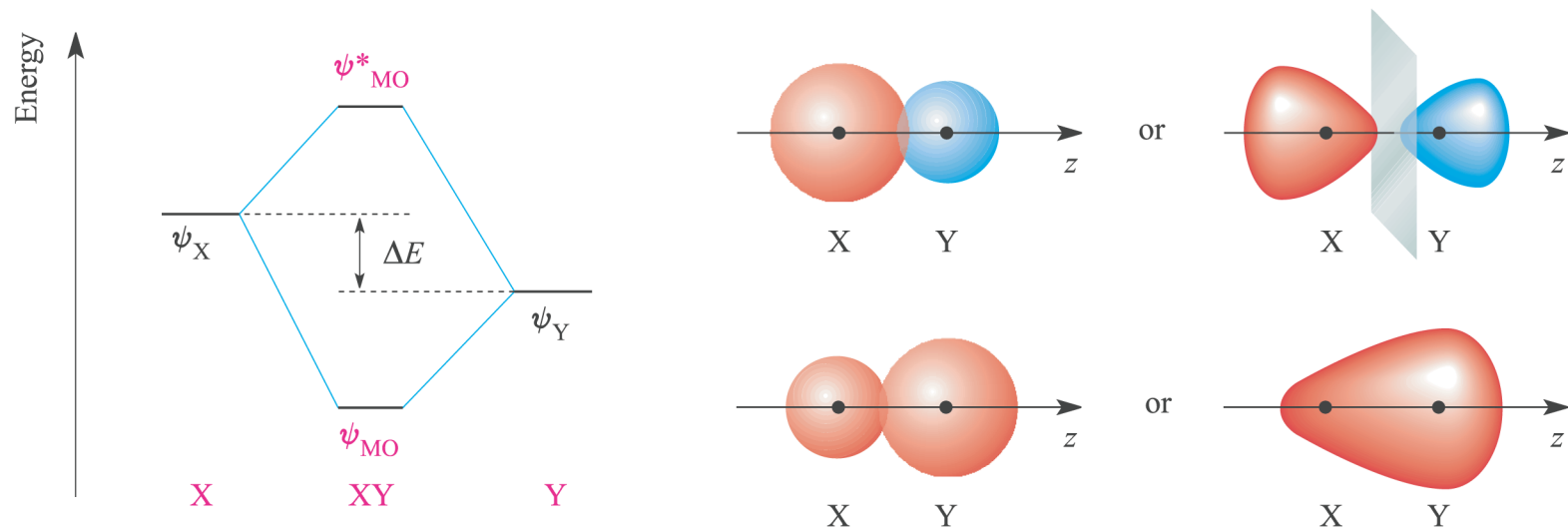
1.47 D



$$\chi_{\text{N}} = 3.0$$

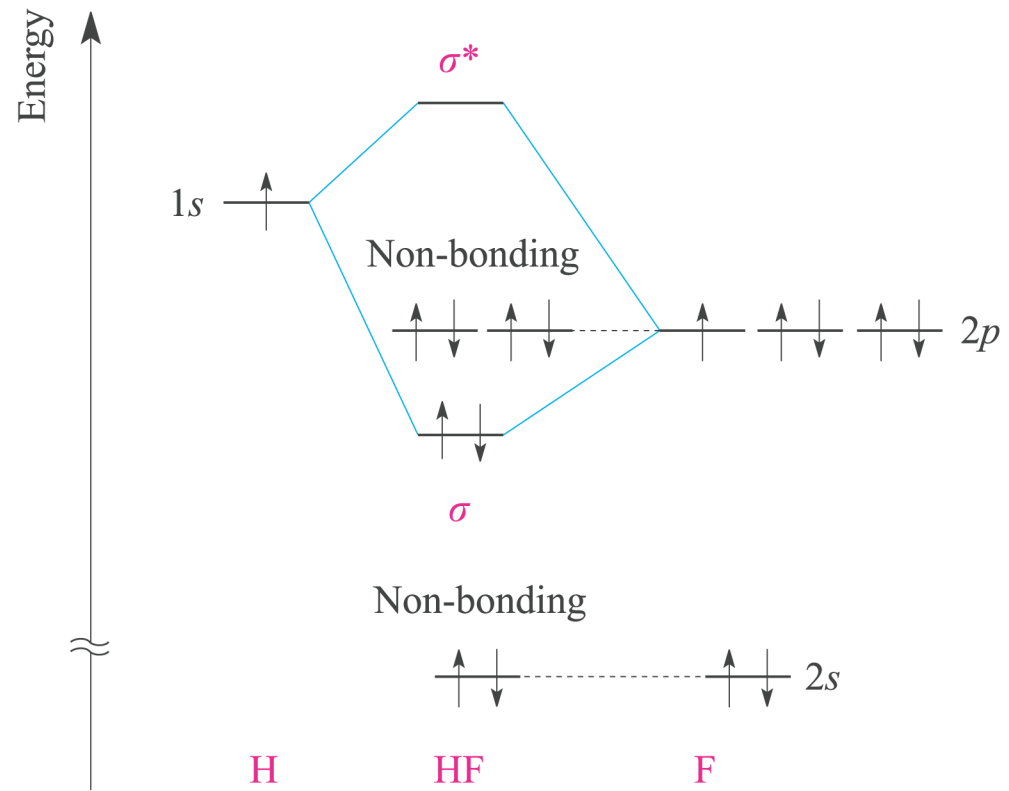
$$\chi_{\text{F}} = 4.0$$

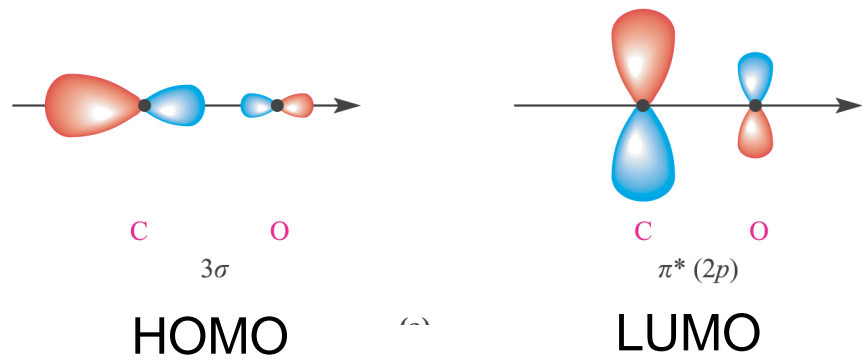
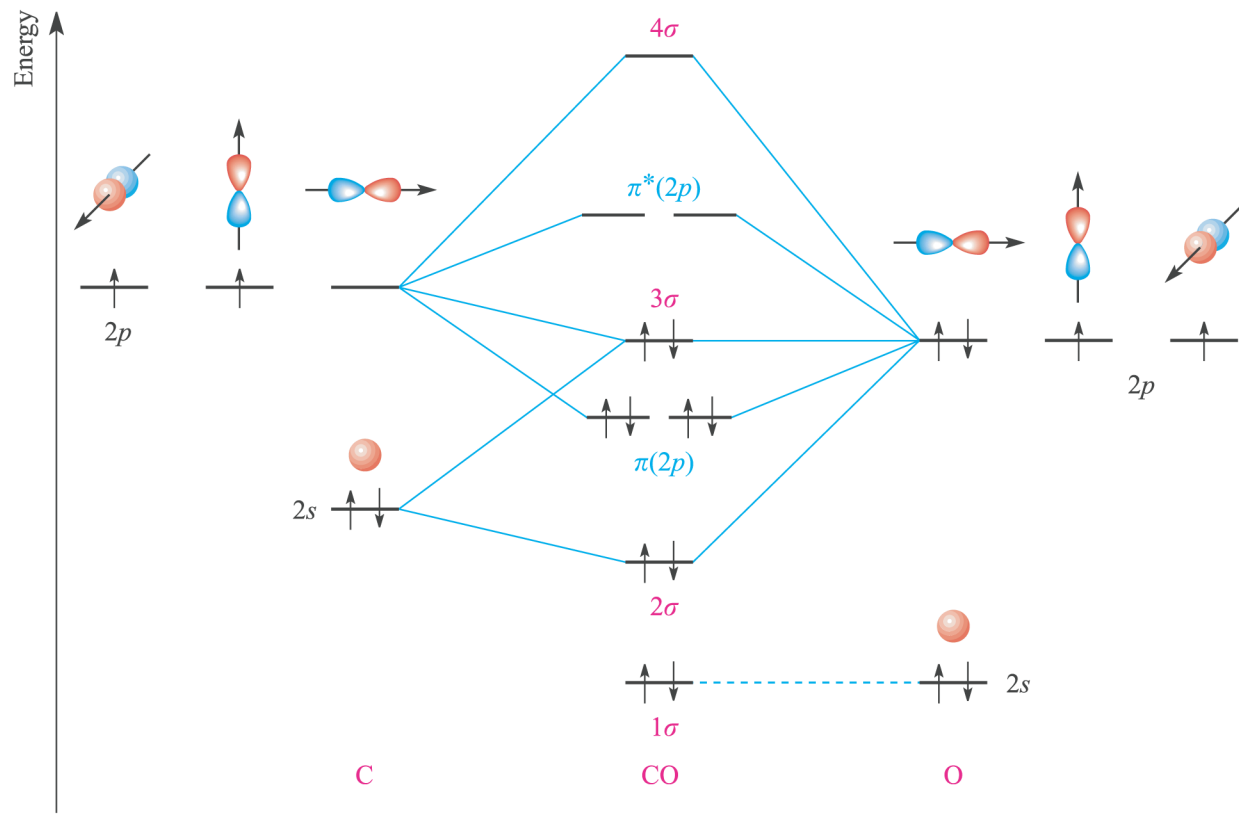
0.24 D

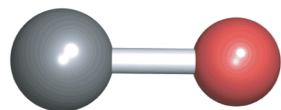
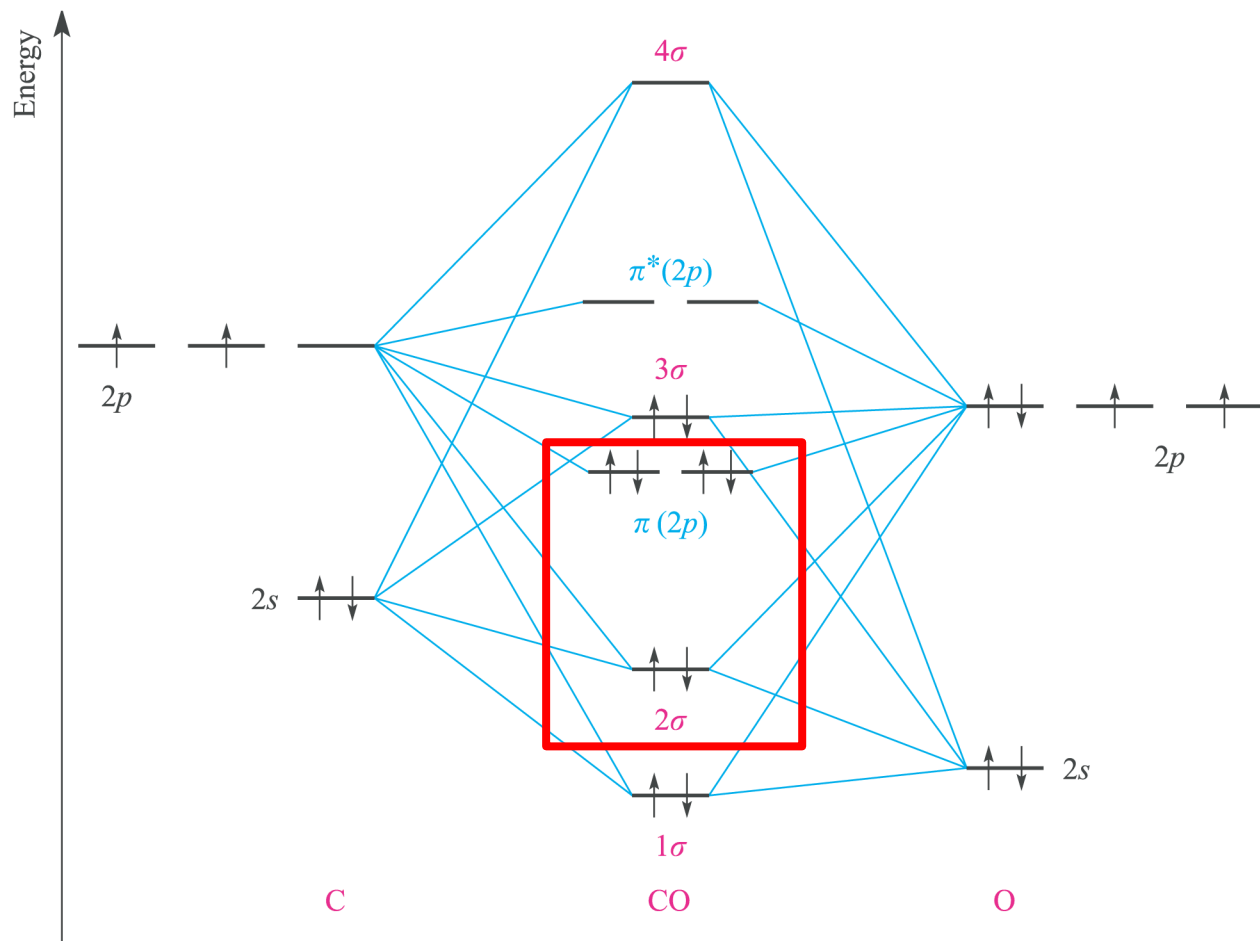


$$\Psi_{MO} = N[(c_1 \times \Psi_X) + (c_2 \times \Psi_Y)] \text{ con } c_2 > c_1$$

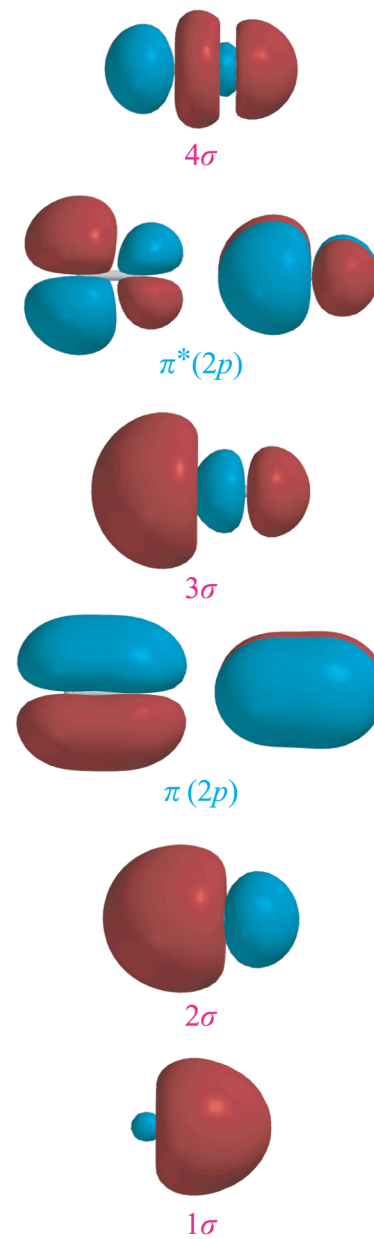
$$\Psi_{MO}^* = N[(c_2 \times \Psi_X) + (c_1 \times \Psi_Y)]$$







(b)



Dov'è l'errore?

