

Welcome to 3.091

Lecture 10

September 30, 2009

Hybridized & Molecular Orbitals; Paramagnetism

3.091 Test #1

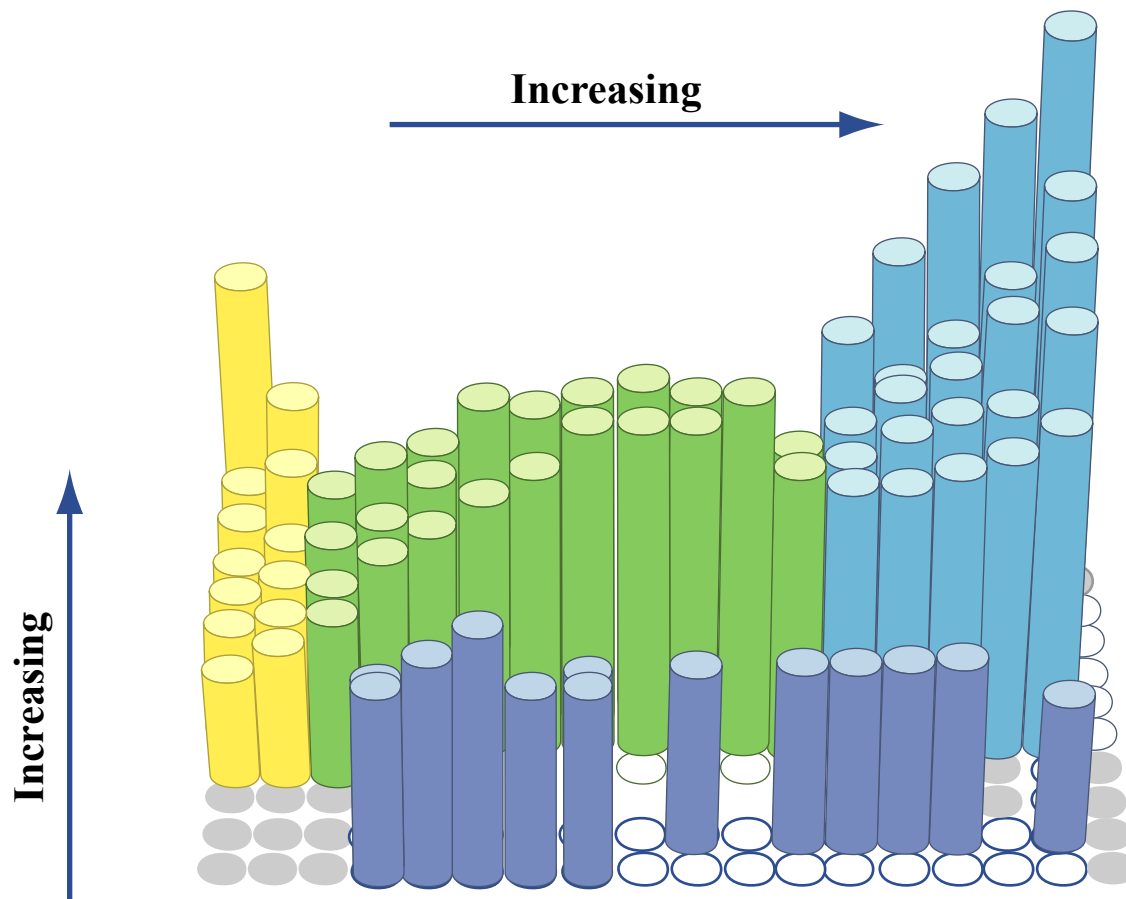
Wednesday, October 7, 2009

Room Assignments

A – Ha: 10-250

He - Sm: 26-100

So - ∞ : 4-270



Electronegativity, χ

● *s* Block

● *p* Block

● *d* Block

● *f* Block

$$\% \text{ ionic character} = \left\{ 1 - \exp \left(-\frac{1}{4} (\Delta X)^2 \right) \right\} \times 100$$

▼ % Ionic Character of a Single Chemical Bond

Difference in Electronegativity	%IC (by L. Pauling)	%IC (by Hannay & Smyth)
0.1	0.2	1.6
0.2	1.0	3.3
0.3	2.2	5.1
0.4	3.9	7.0
0.5	6.1	8.9
0.6	8.6	11
0.7	12	13
0.8	15	15
0.9	18	17
1.0	22	20
1.1	26	22
1.2	30	24
1.3	34	27
1.4	39	29
1.5	43	32
1.6	47	35
1.7	51	37
1.8	56	40
1.9	59	43
2.0	63	46
2.1	67	49
2.2	70	52
2.3	73	55
2.4	76	59
2.5	79	62
2.6	82	65
2.7	84	69
2.8	86	72
2.9	88	76
3.0	89	80
3.1	91	83
3.2	92	87

7
VIIA
VIIB

Group Classifications⁶

Atomic Number²

Oxidation States³

bold indicates
most stable state

Symbol⁴

Black = solid, red = gas,
blue = liquid,
outline = synthetically
prepared

Electronic⁵
Configuration

Name⁴

25

54.93805

2, 3, 4, 6, 7

1246

2061

7.47

1.55

7.435

Mn

[Ar]3d⁵4s²

Manganese

Atomic Weight¹

() Indicates most stable
or best known isotope

Melting Point⁷, °C

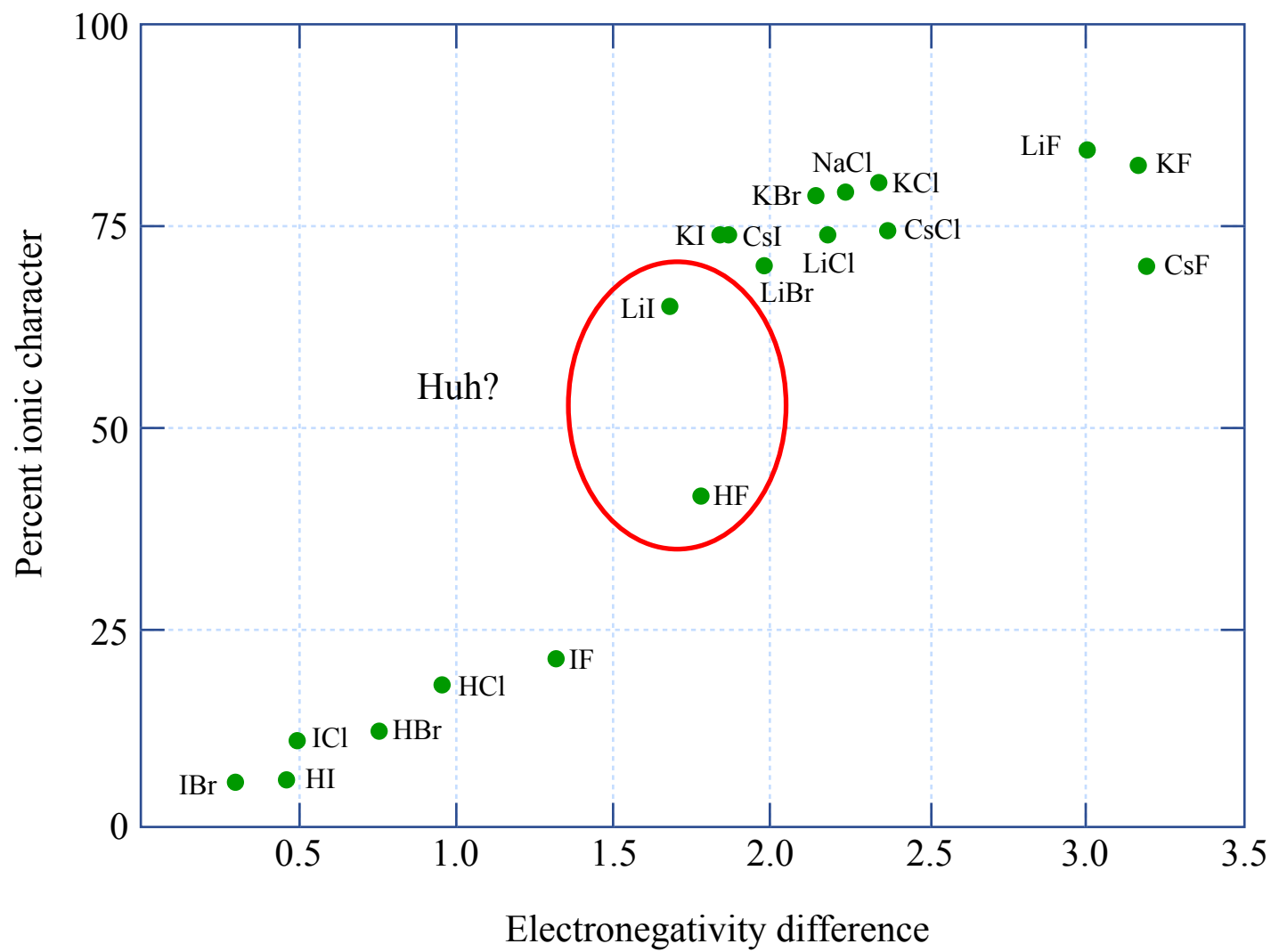
Boiling Point⁷, °C

Density⁸, g/cm³

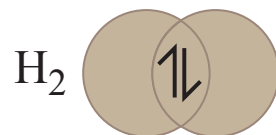
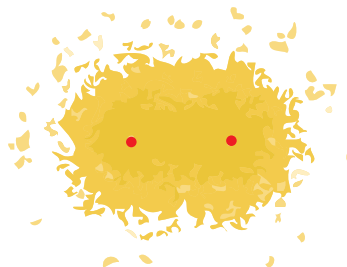
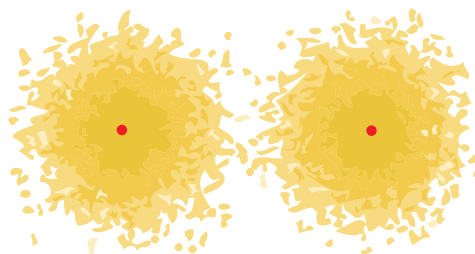
(gases: g/L at 0°C, 1atm)

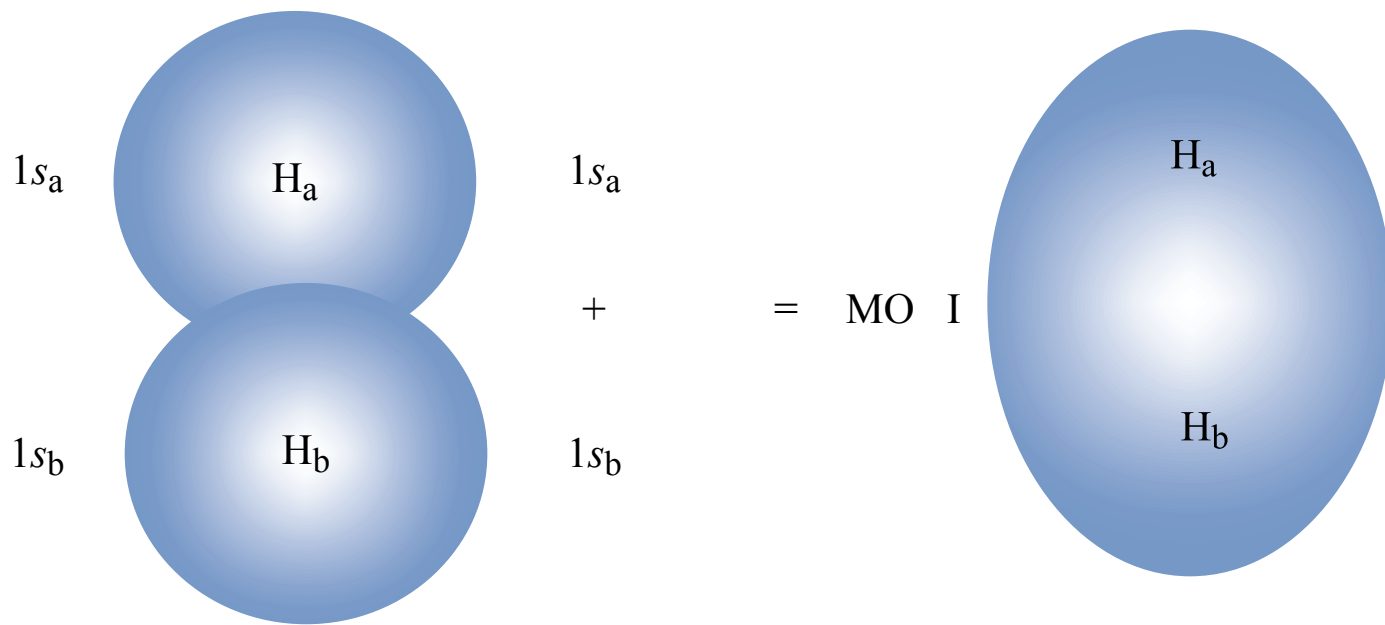
Electronegativity⁹

First Ionization
Potential¹⁰, eV

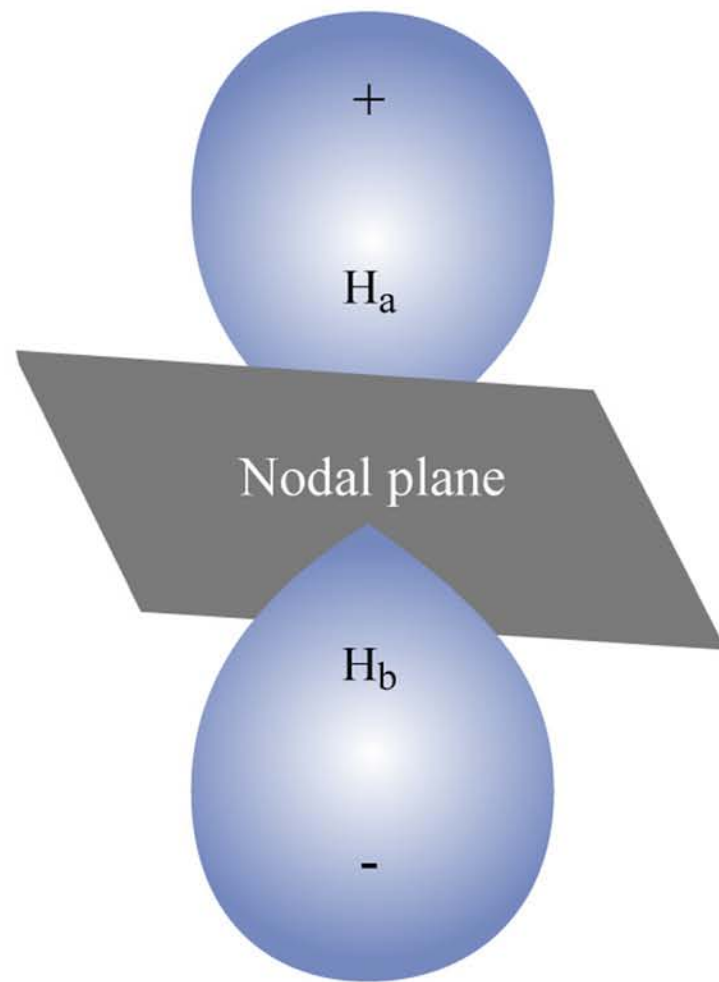
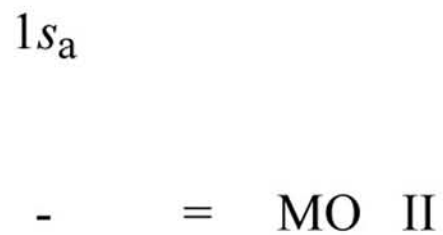
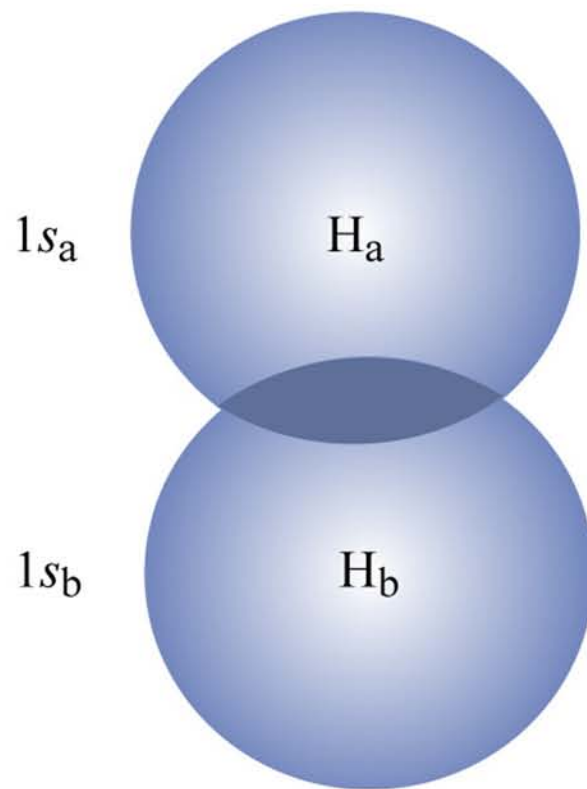


Electron-Pair Bond

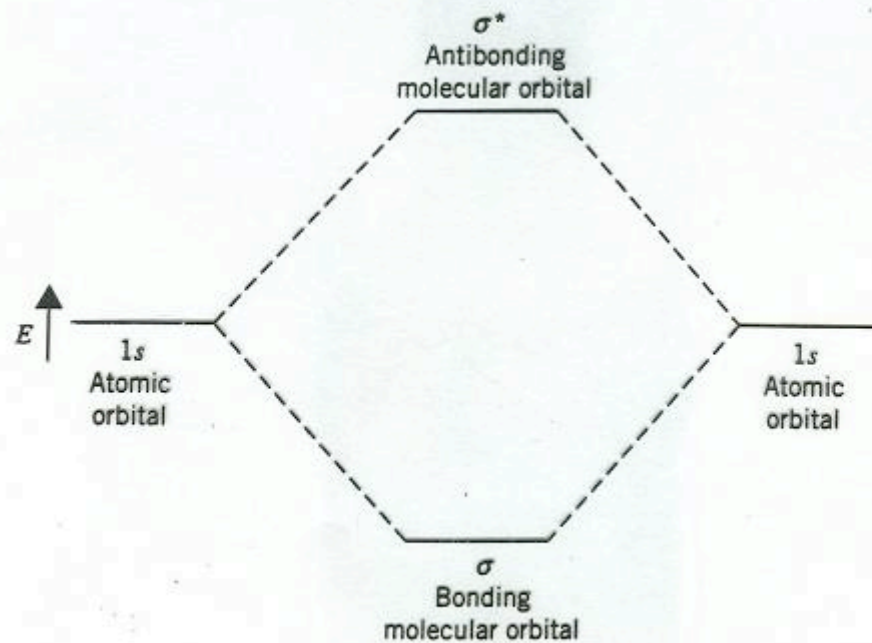
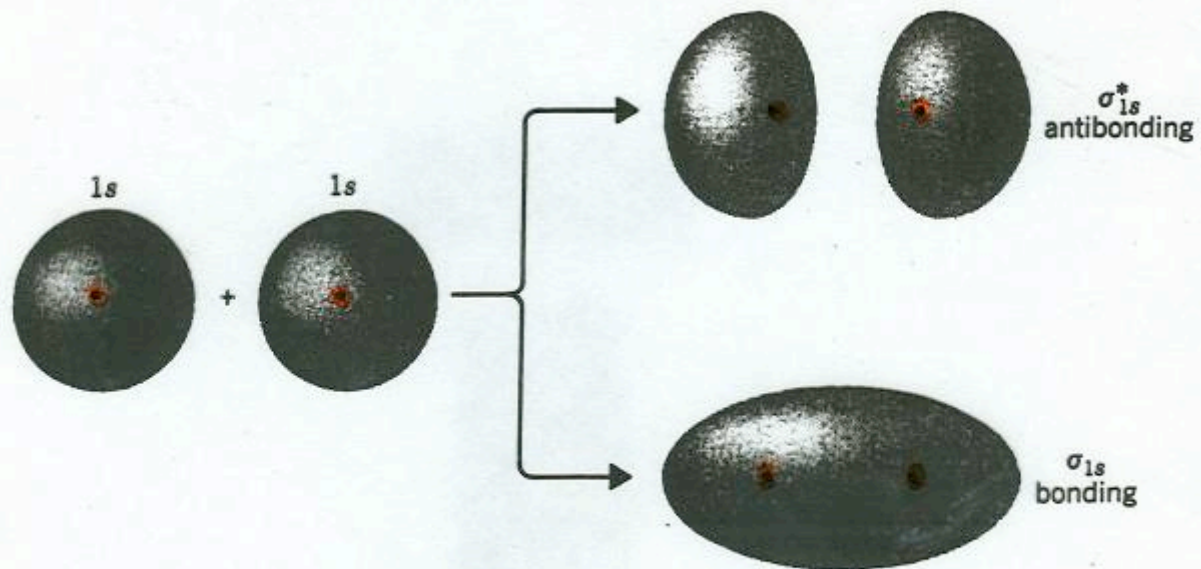




Molecular Orbital ——— Bonding



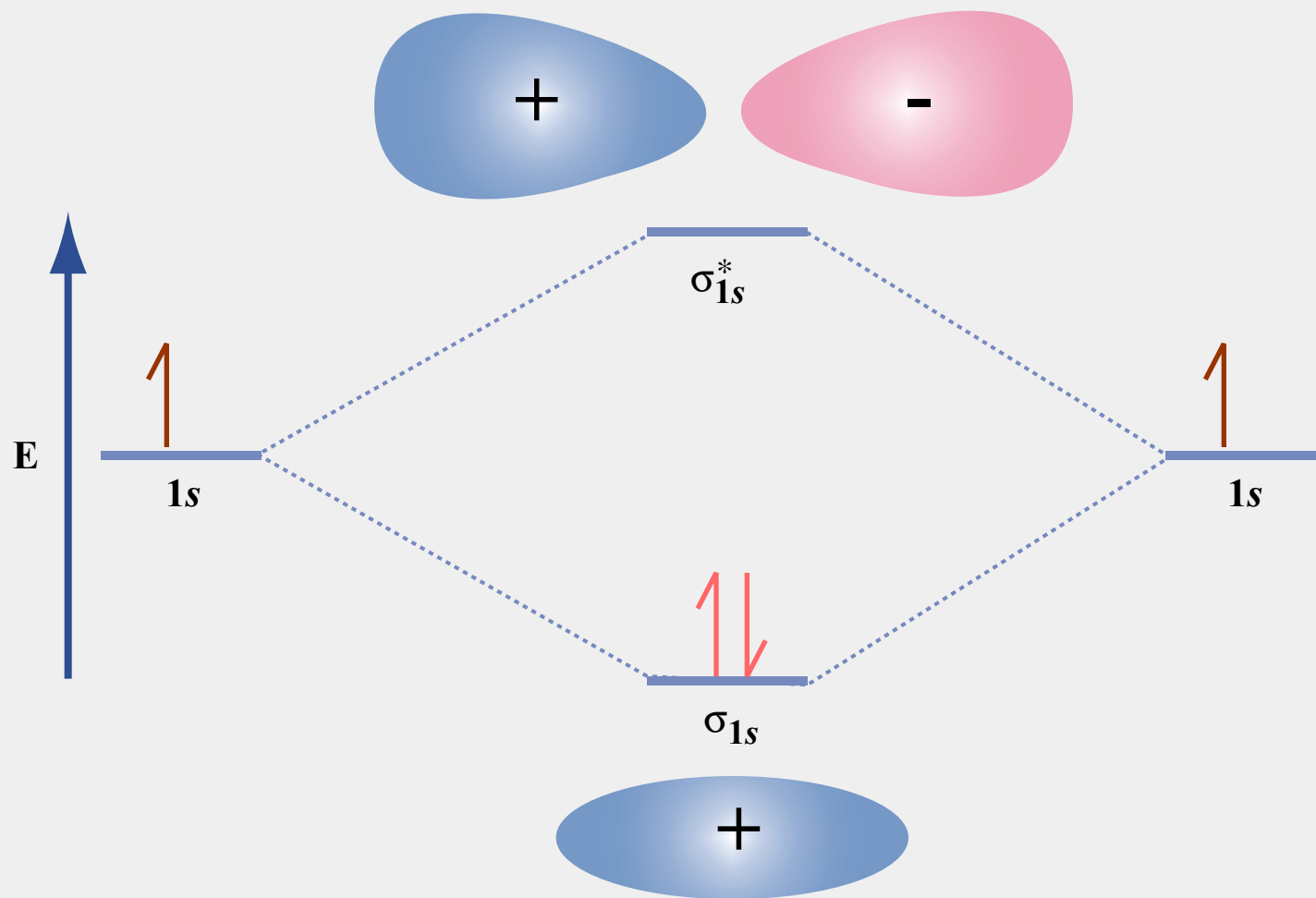
Molecular Orbital ——— Antibonding



H (AO)

H₂ (MOs)

H (AO)

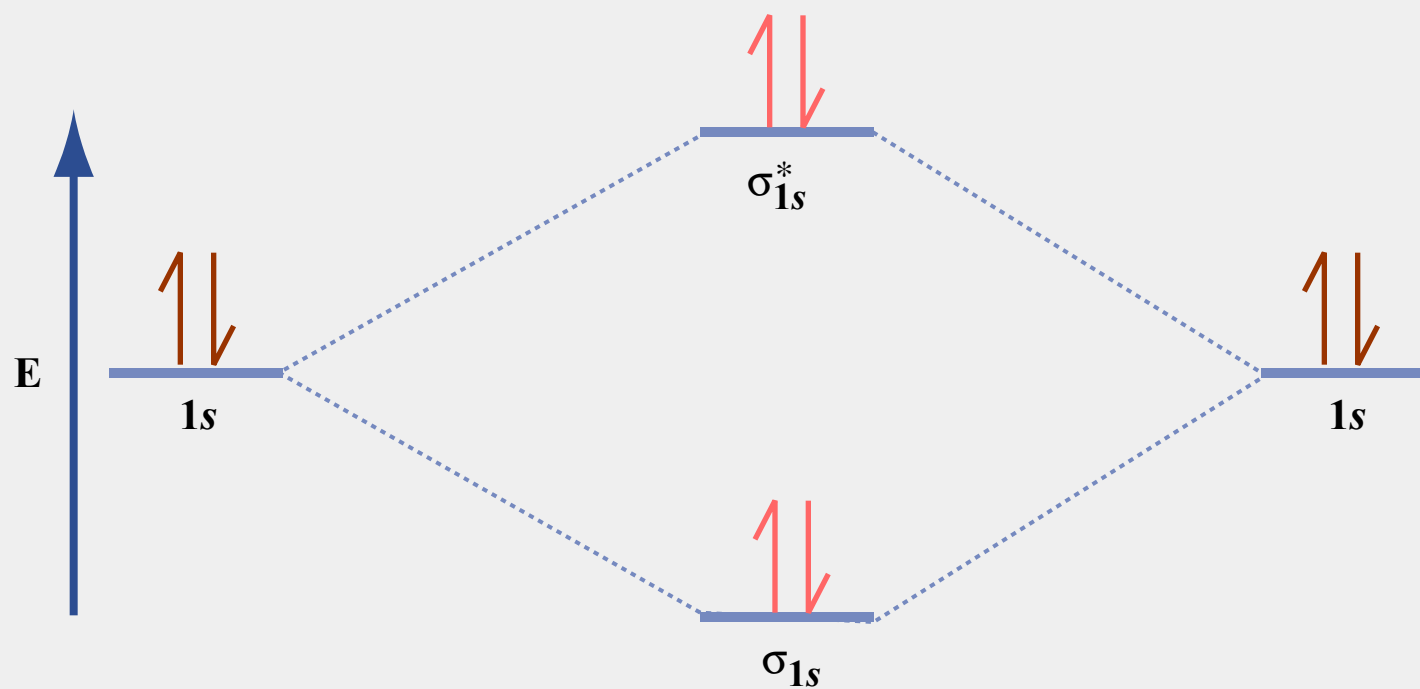


(c)

He (AO)

He₂ (MOs)

He (AO)

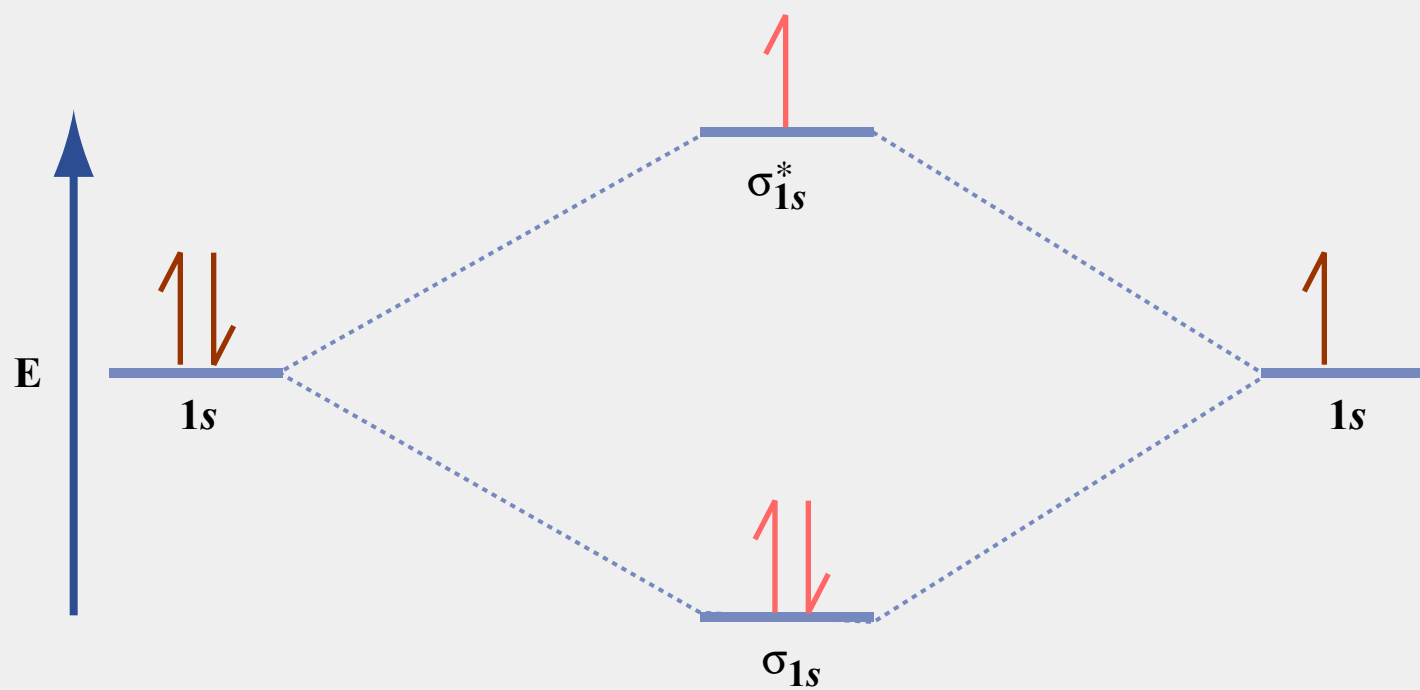


(b)

He (AO)

He₂⁺ (MOs)

He⁺ (AO)

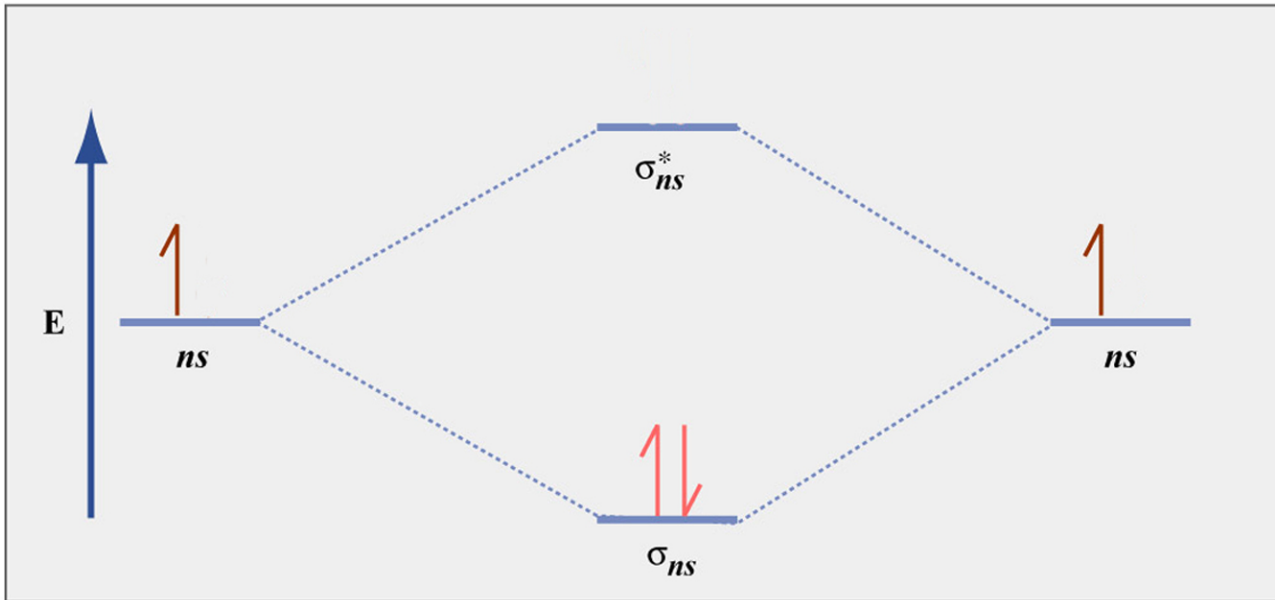


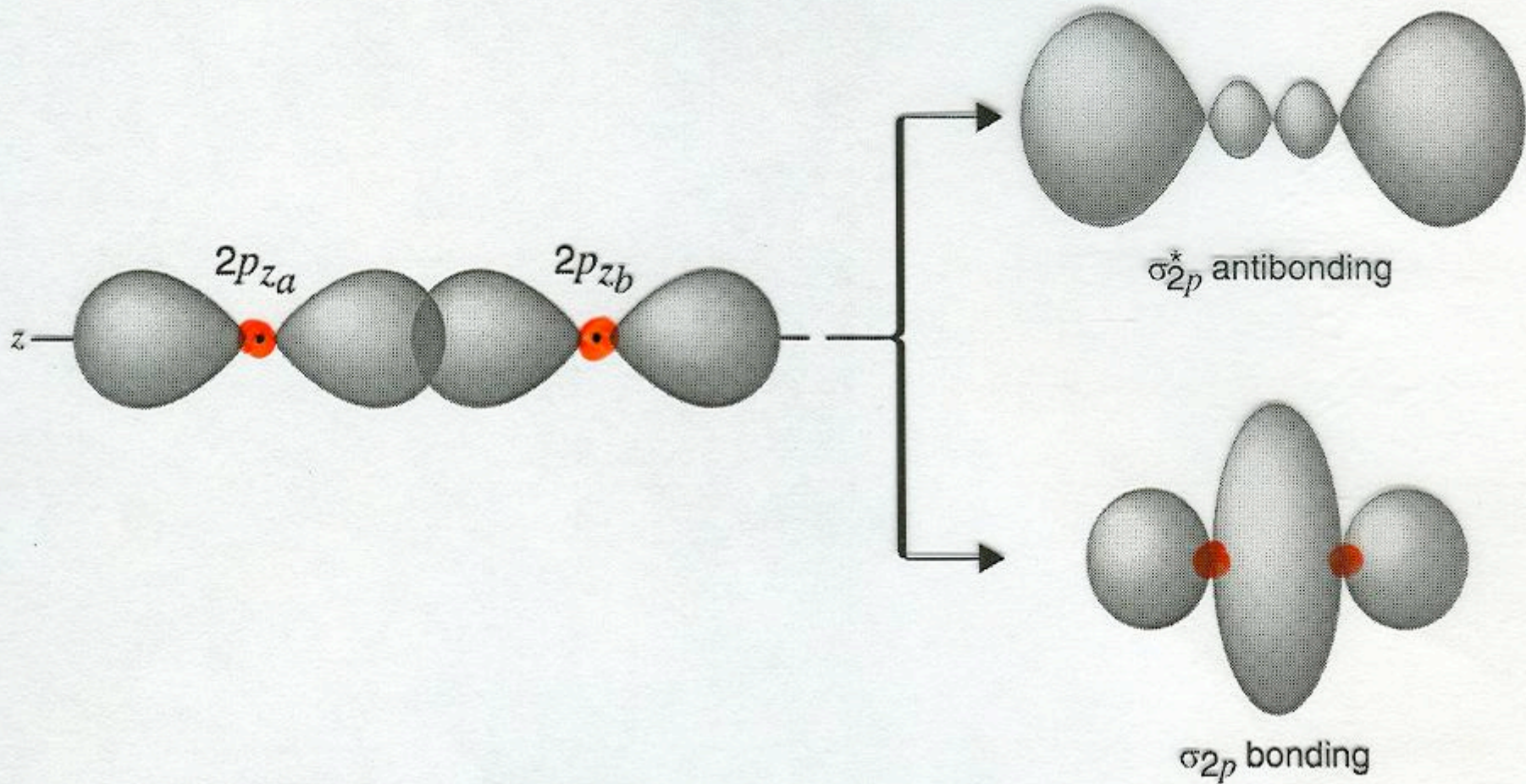
(a) Alkali metals

M (AO)

M₂ (MOs)

M (AO)





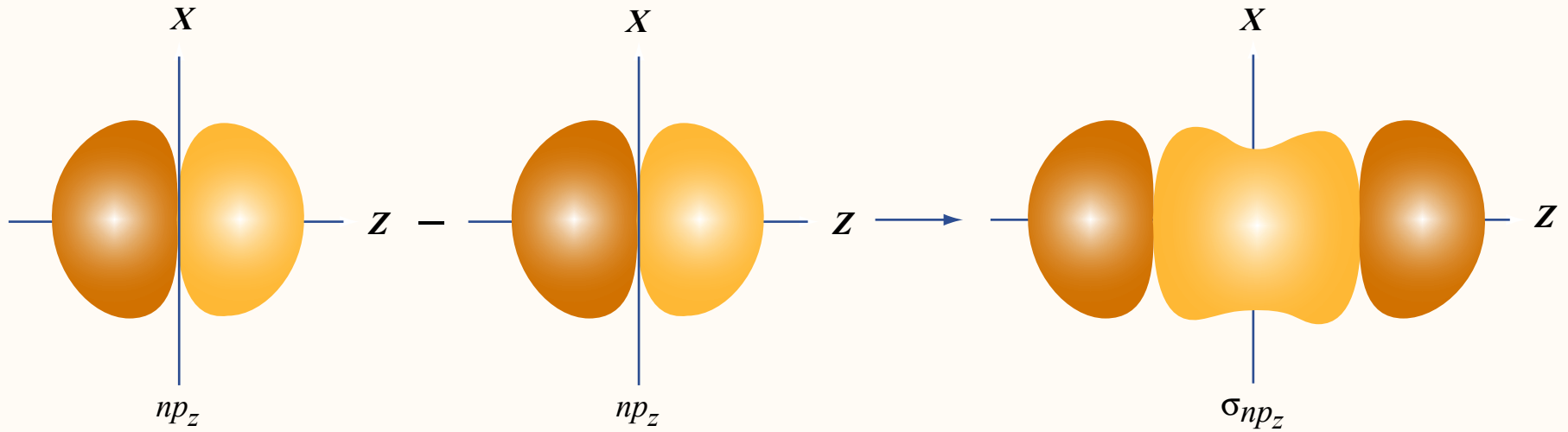
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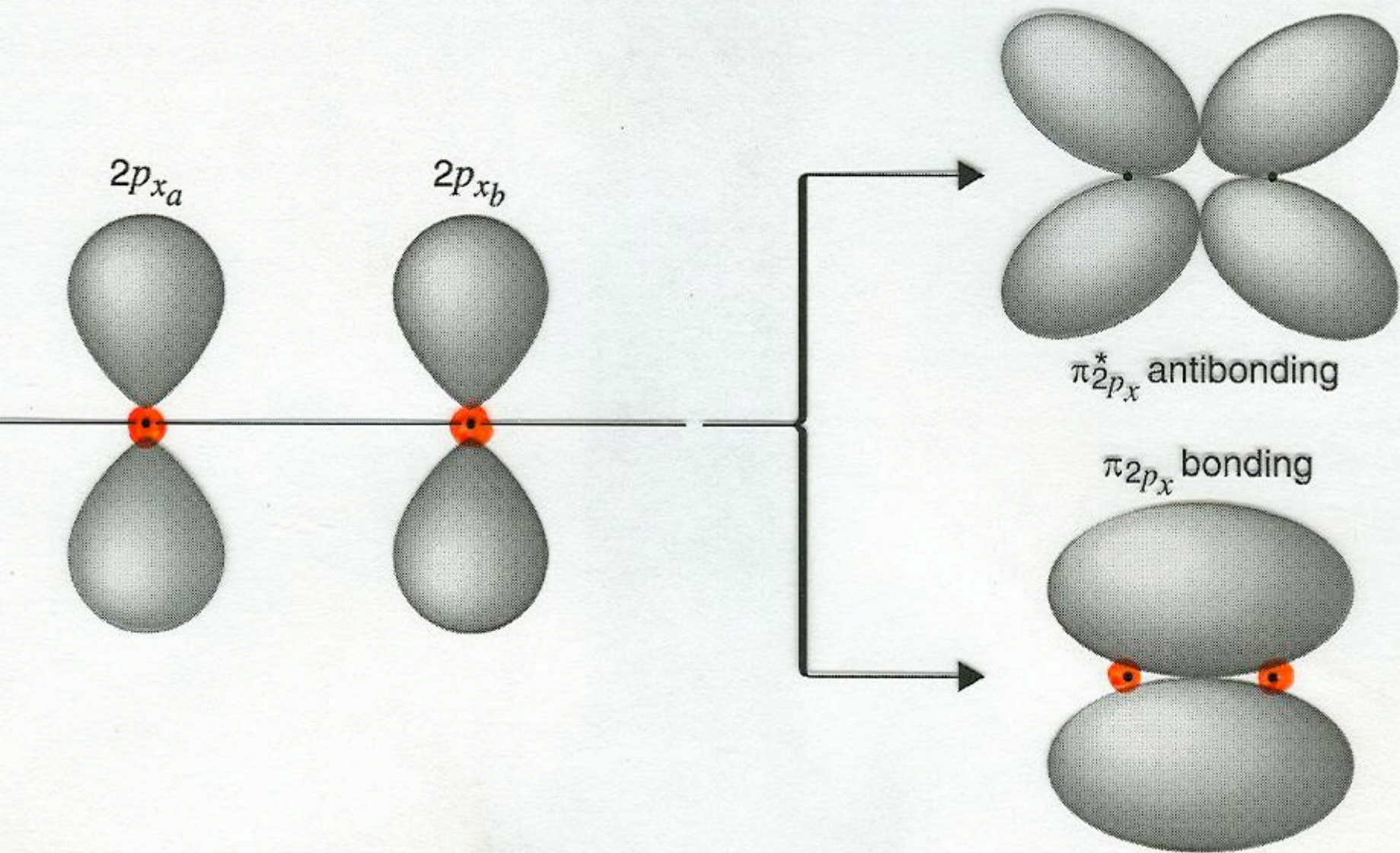
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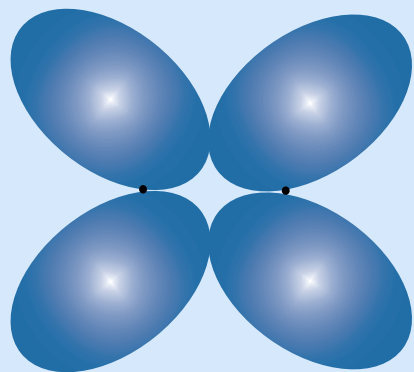
Bonding

Atomic orbitals

Molecular orbital

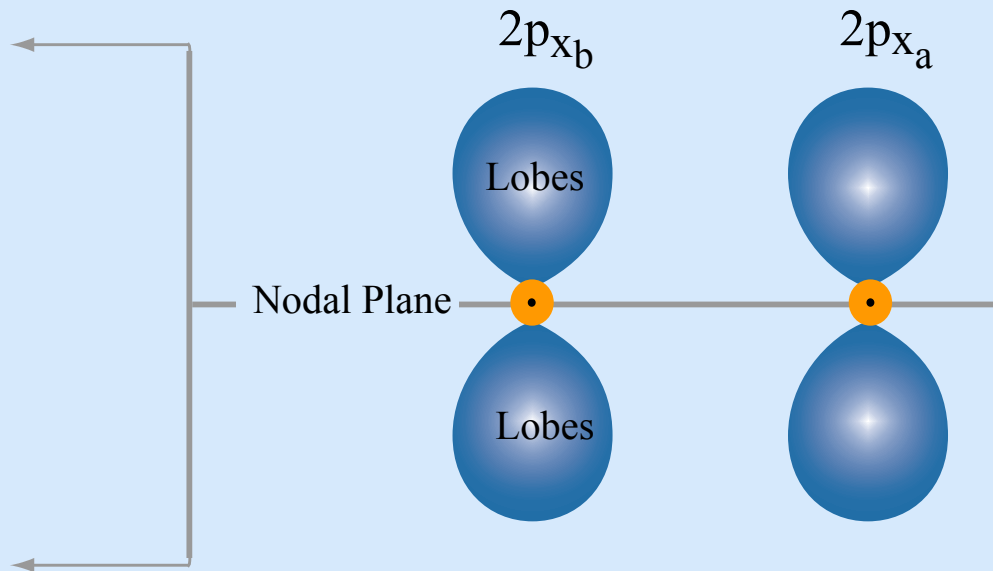
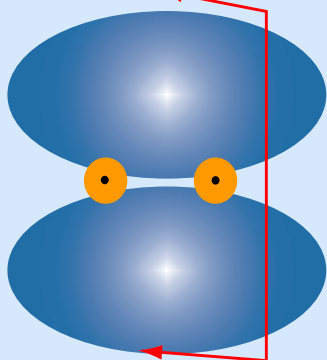






$\pi_{2p_x}^*$ Antibonding

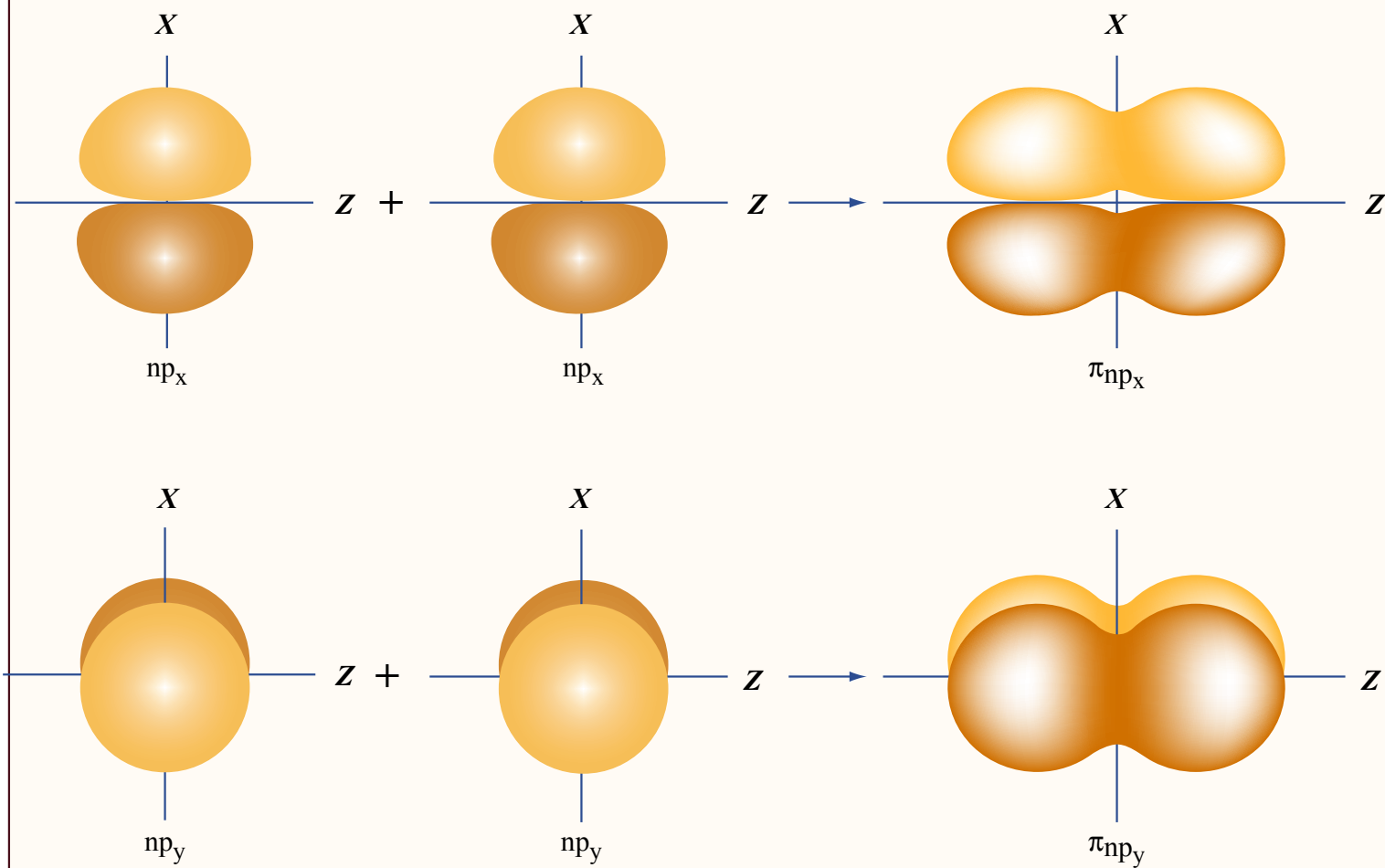
π_{2p_x} Bonding

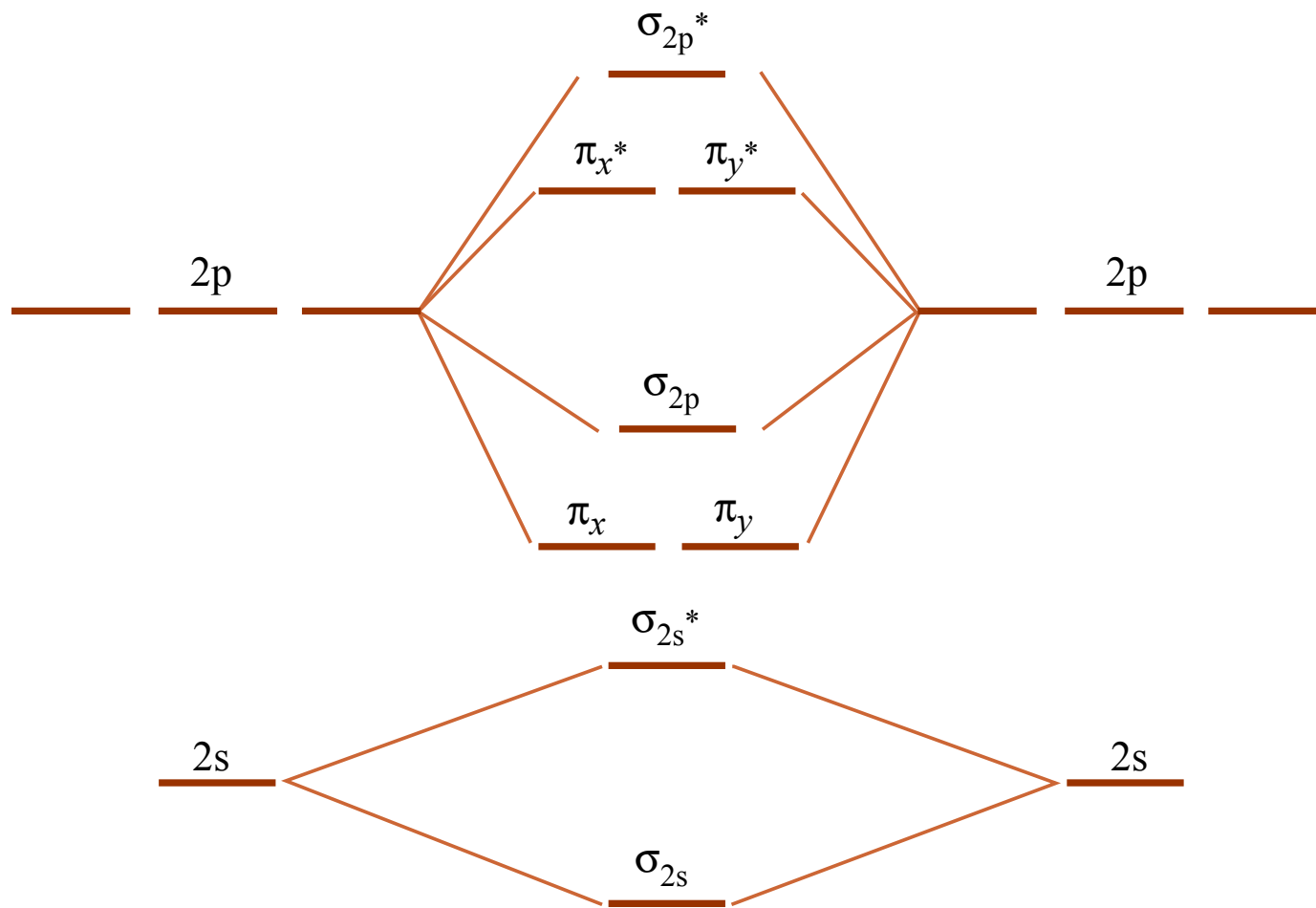


Bonding

Atomic orbitals

Molecular orbitals





e.g. N_2 , B_2 , C_2

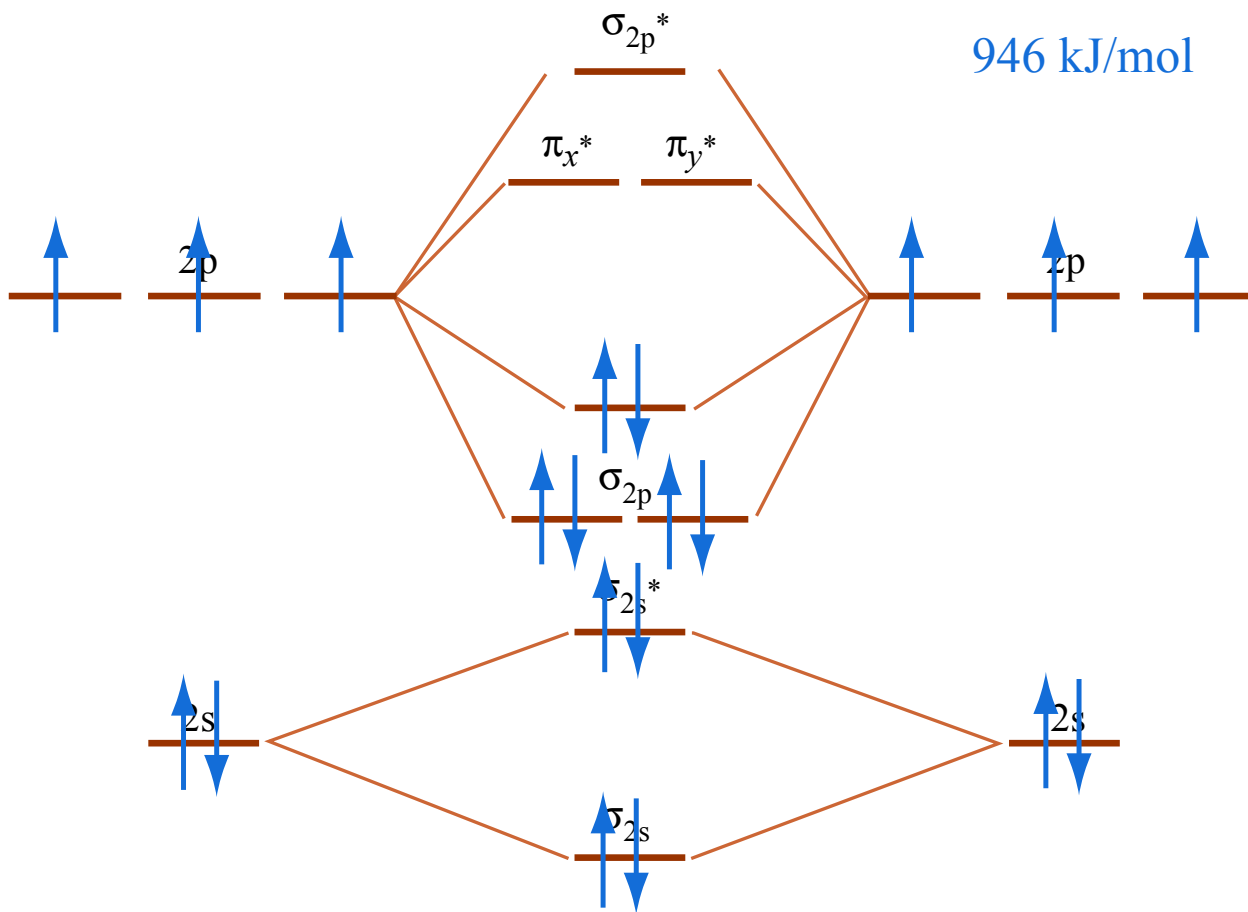


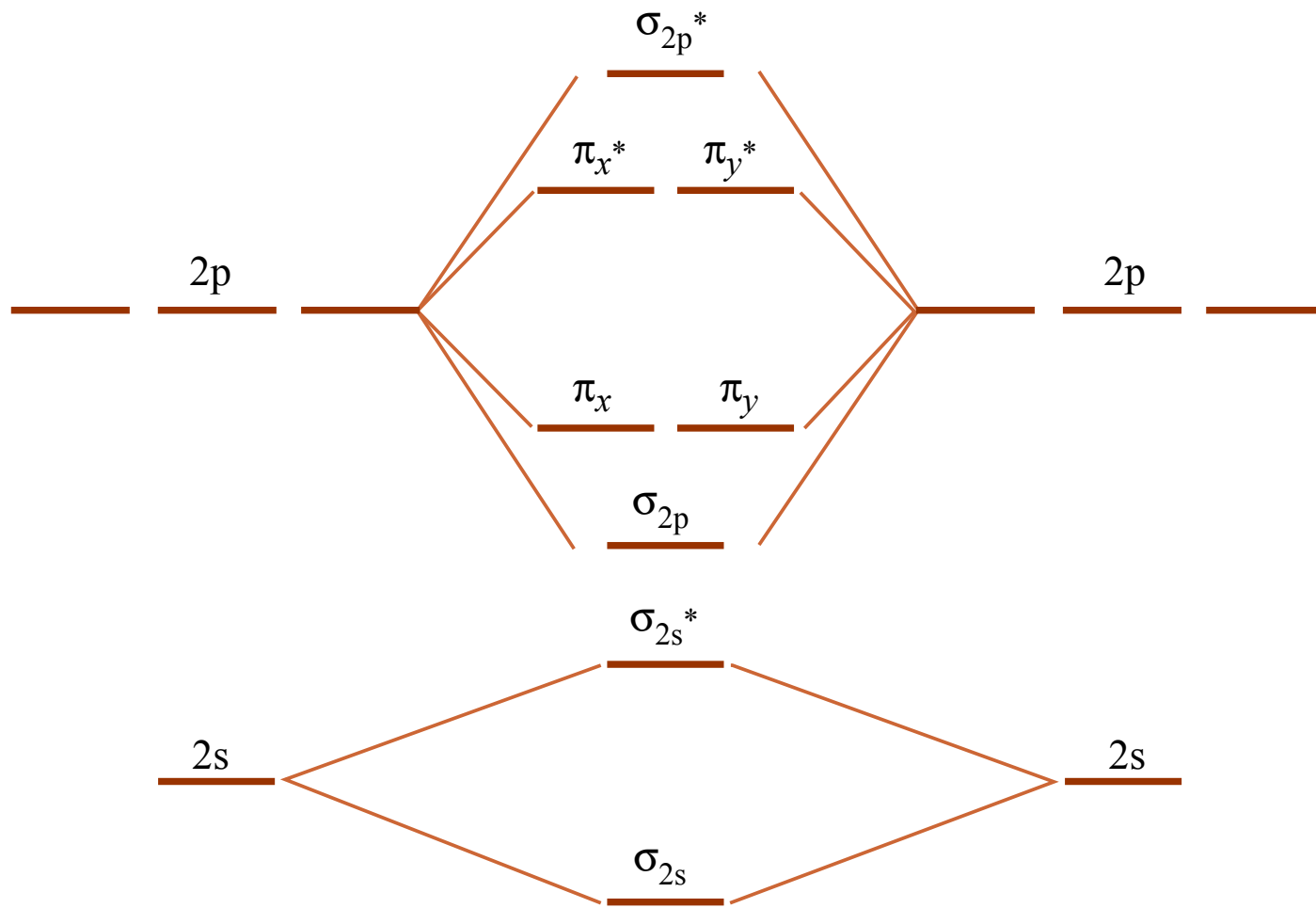
6 bonding electrons

⇒ triple bond

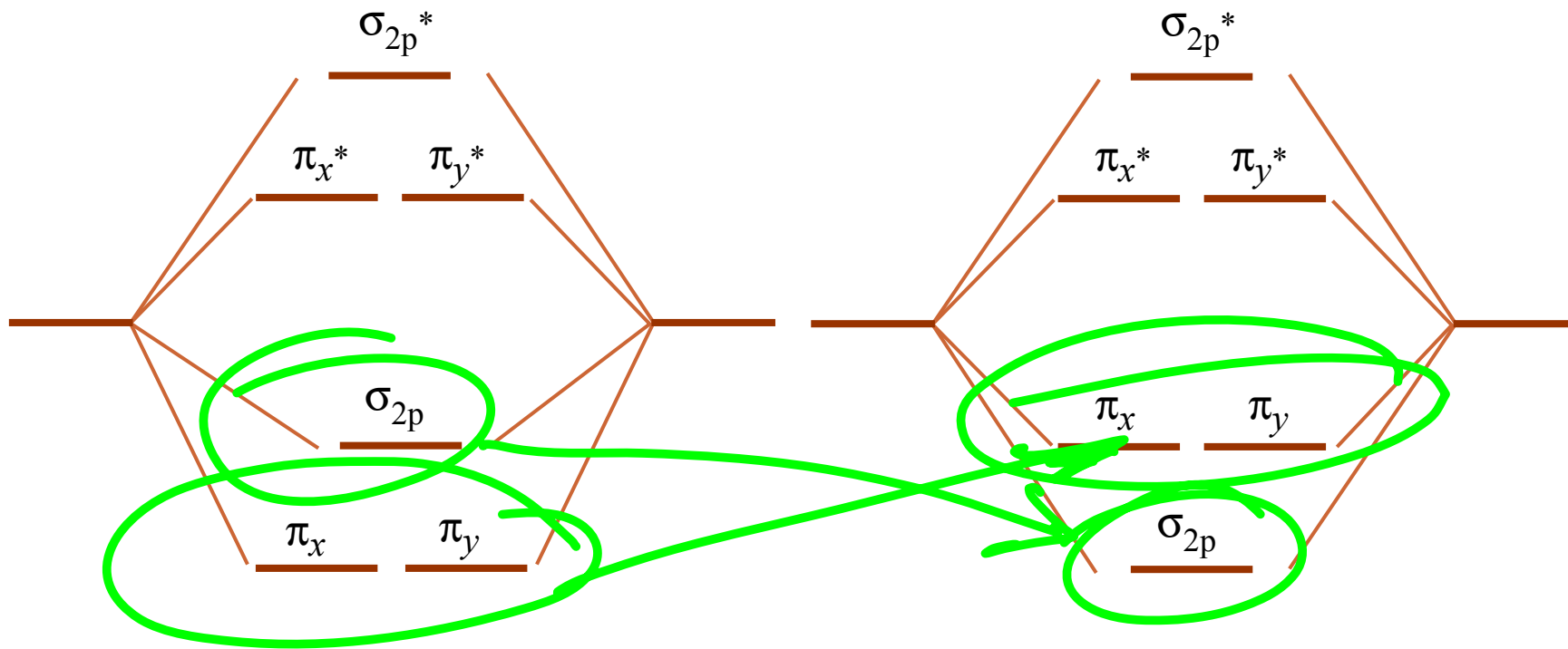


946 kJ/mol

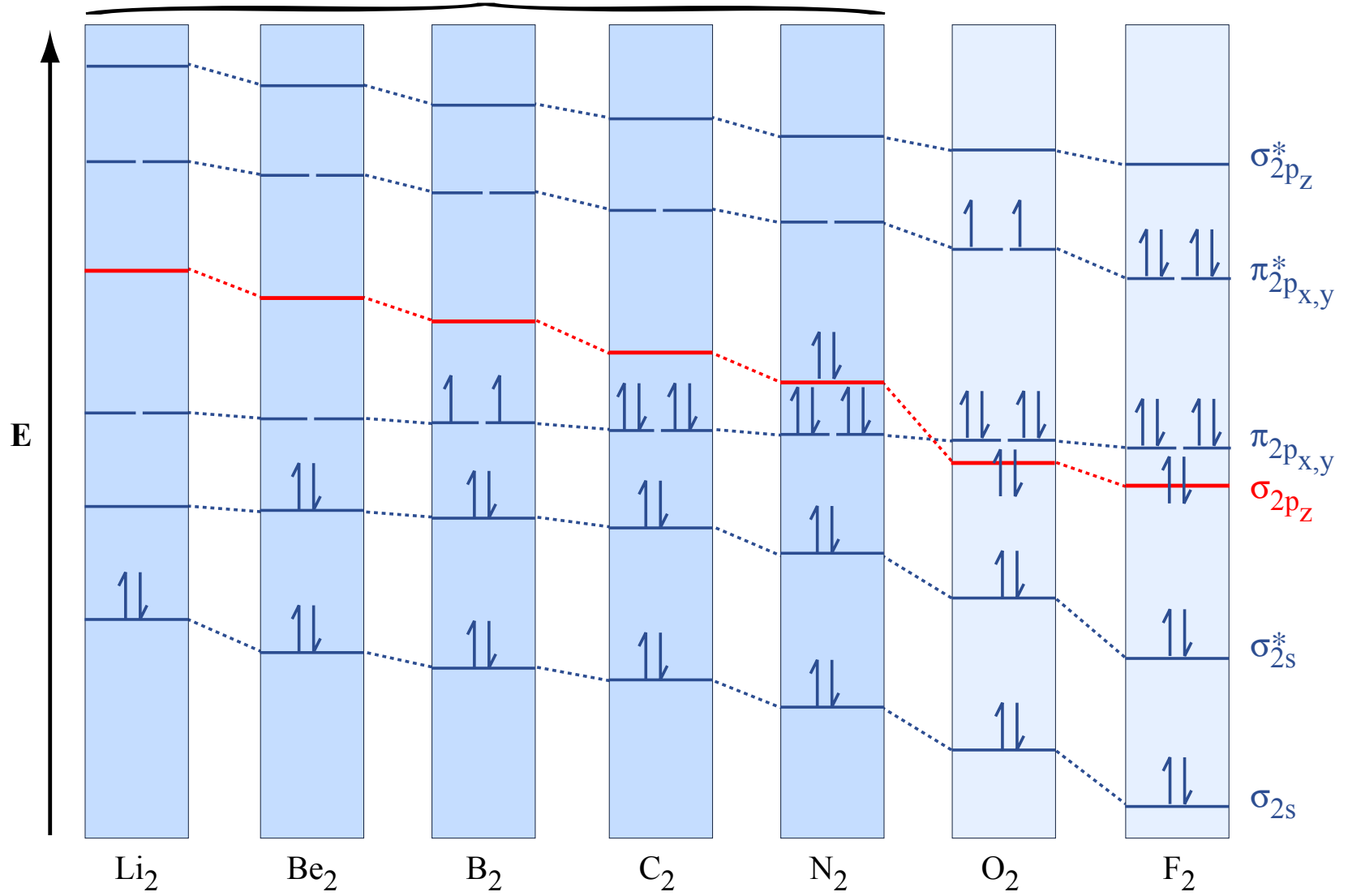




e.g. O_2 & F_2



2s-2p_z interaction

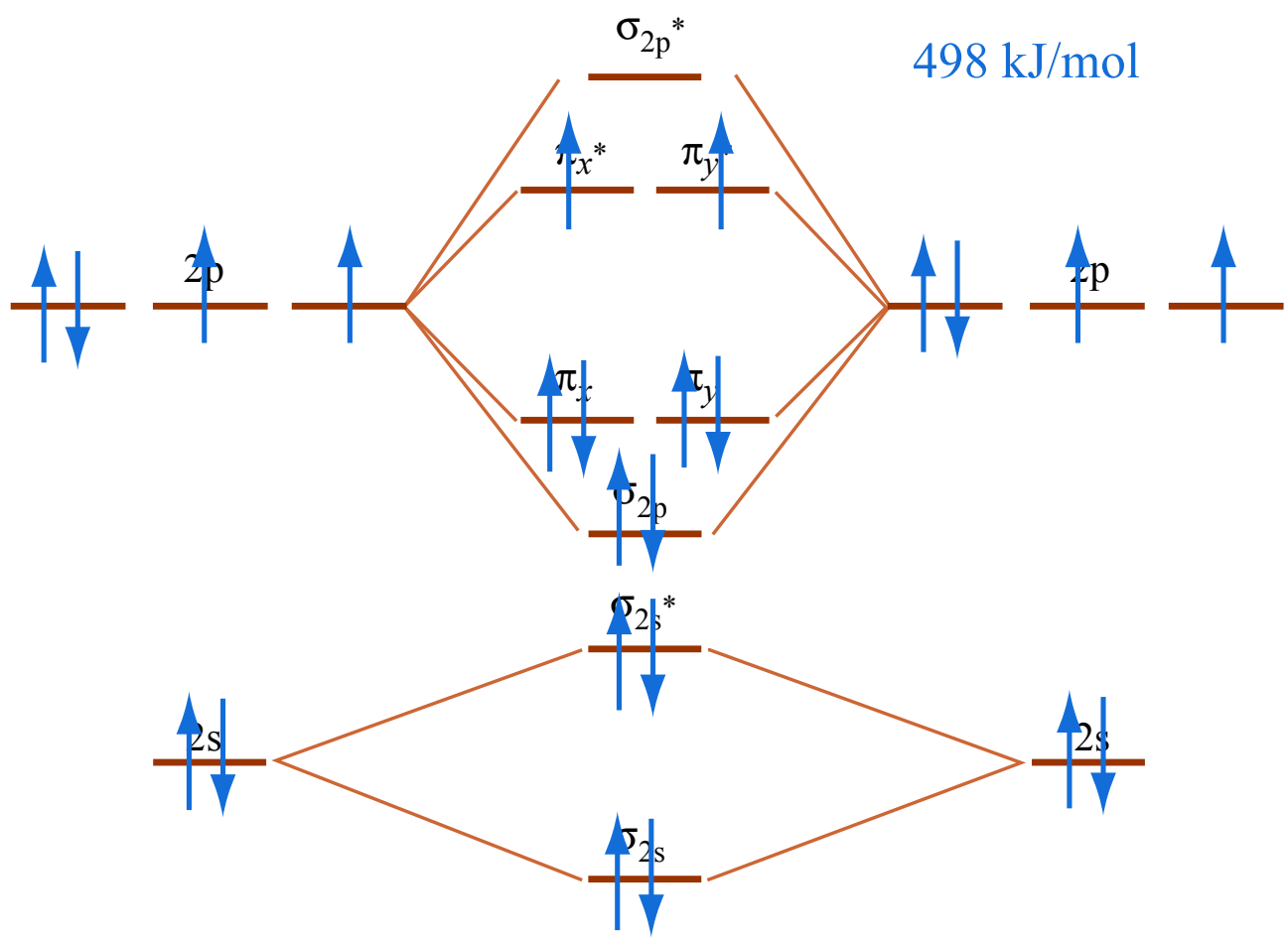




6 bonding electrons
2 anti bonding electrons
⇒ double bond

$0 = 0$

498 kJ/mol

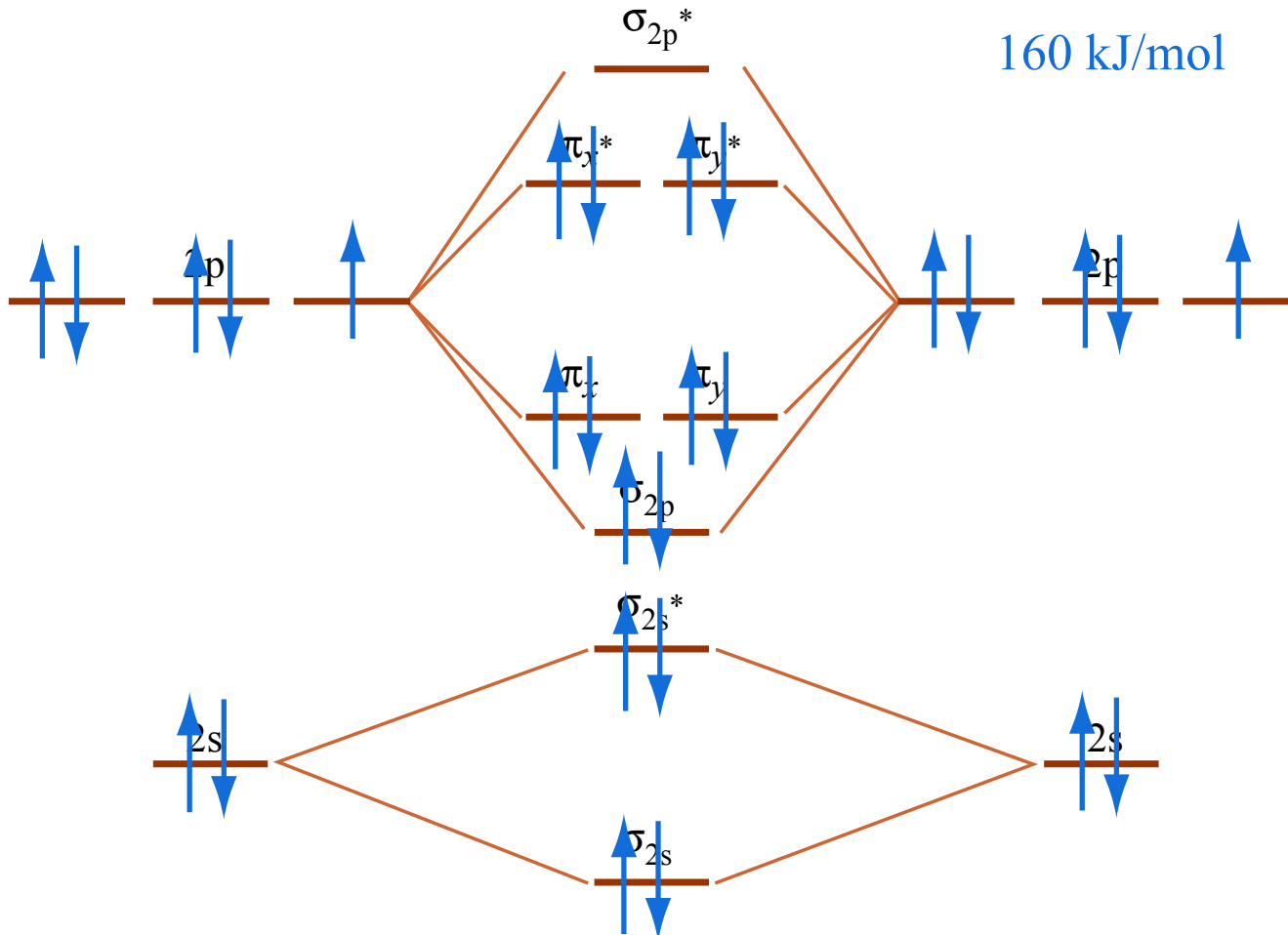


F_2

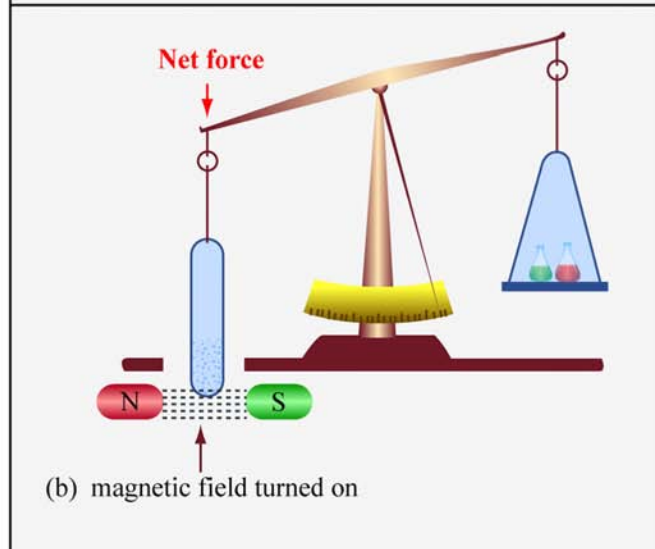
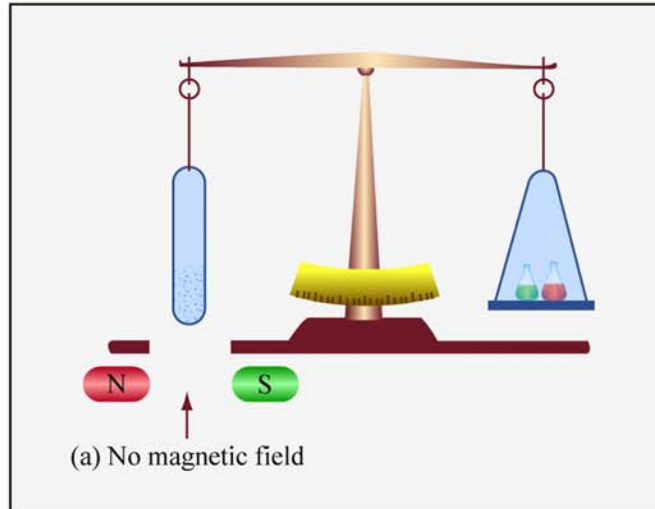
6 bonding electrons
4 anti bonding electrons
 \Rightarrow single bond

F-F

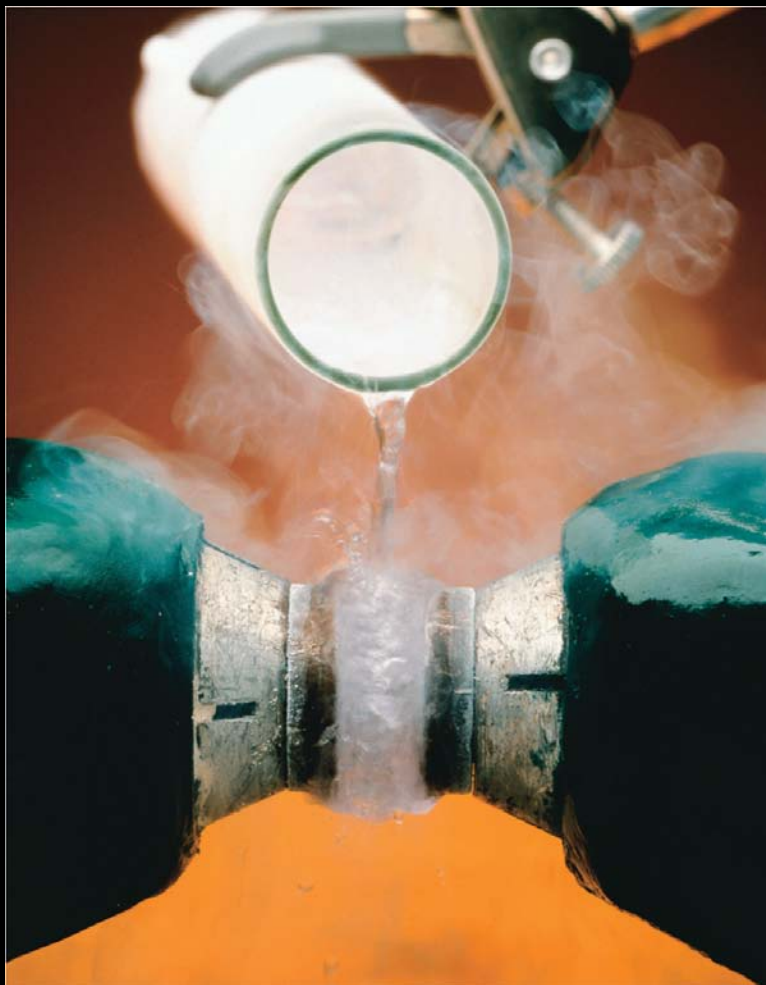
160 kJ/mol



Paramagnetism



unpaired electrons



Averill, B., and P. Eldredge. *Chemistry: Principles, Patterns, and Applications*. Flat WorldKnowledge, 2011. ISBN: 9781453331224.

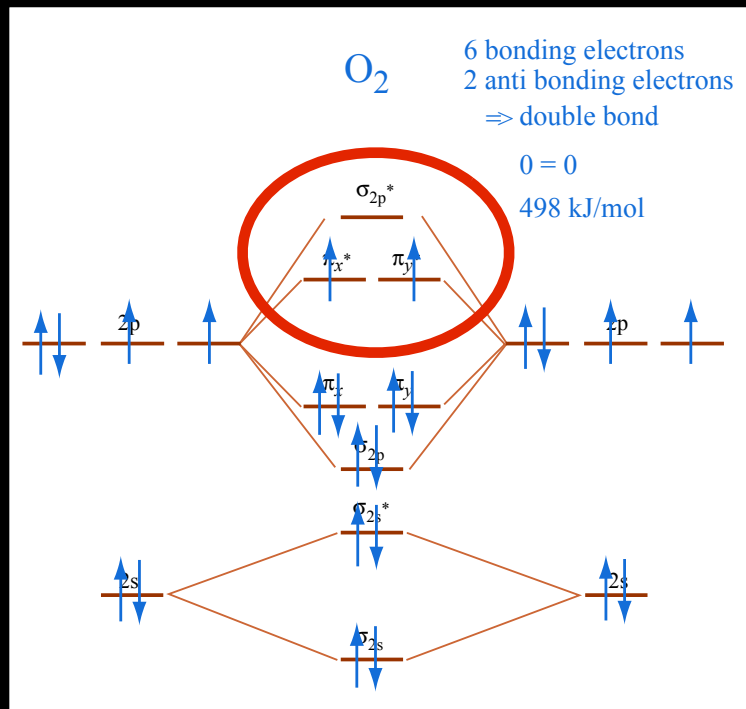
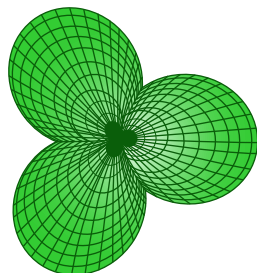


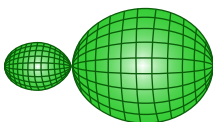
Image by MIT OpenCourseWare.

paramagnetism
in liquid oxygen

Three sp^2
Hybrid Orbitals



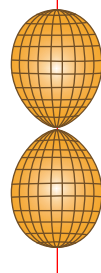
An sp^2
Hybrid Orbital



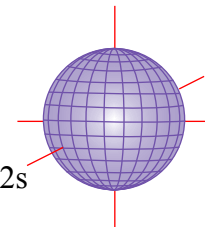
Hybridization



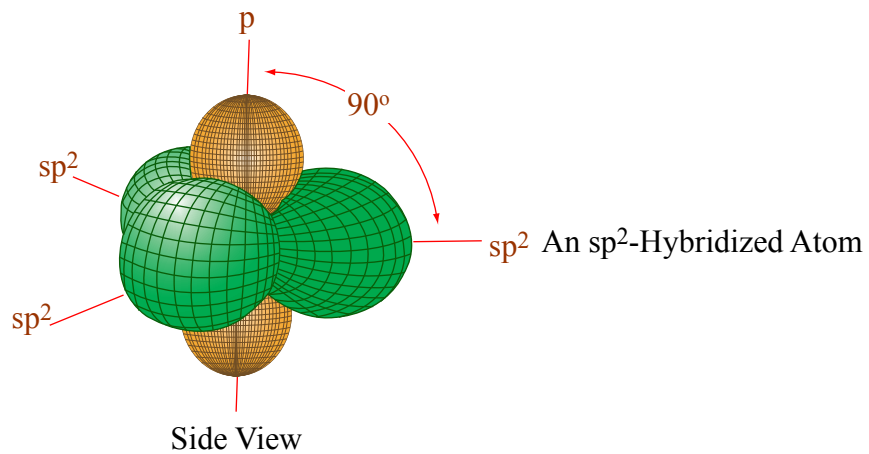
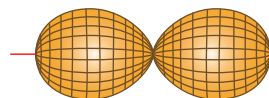
$2p_y$

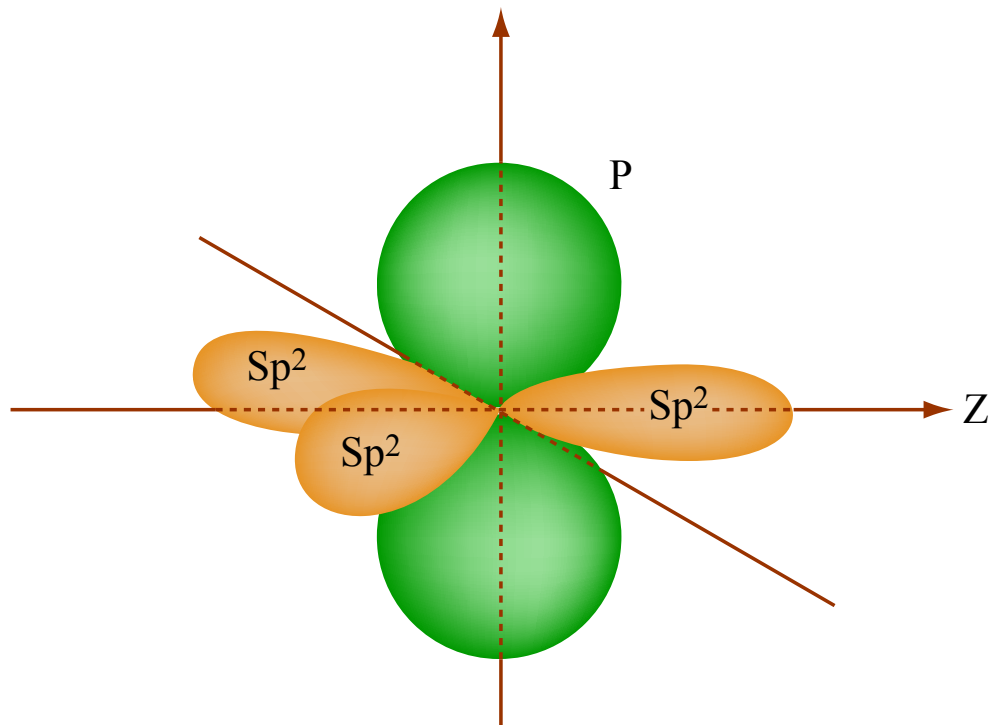


$2s$

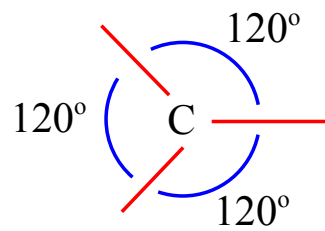


$2p_x$





Top View



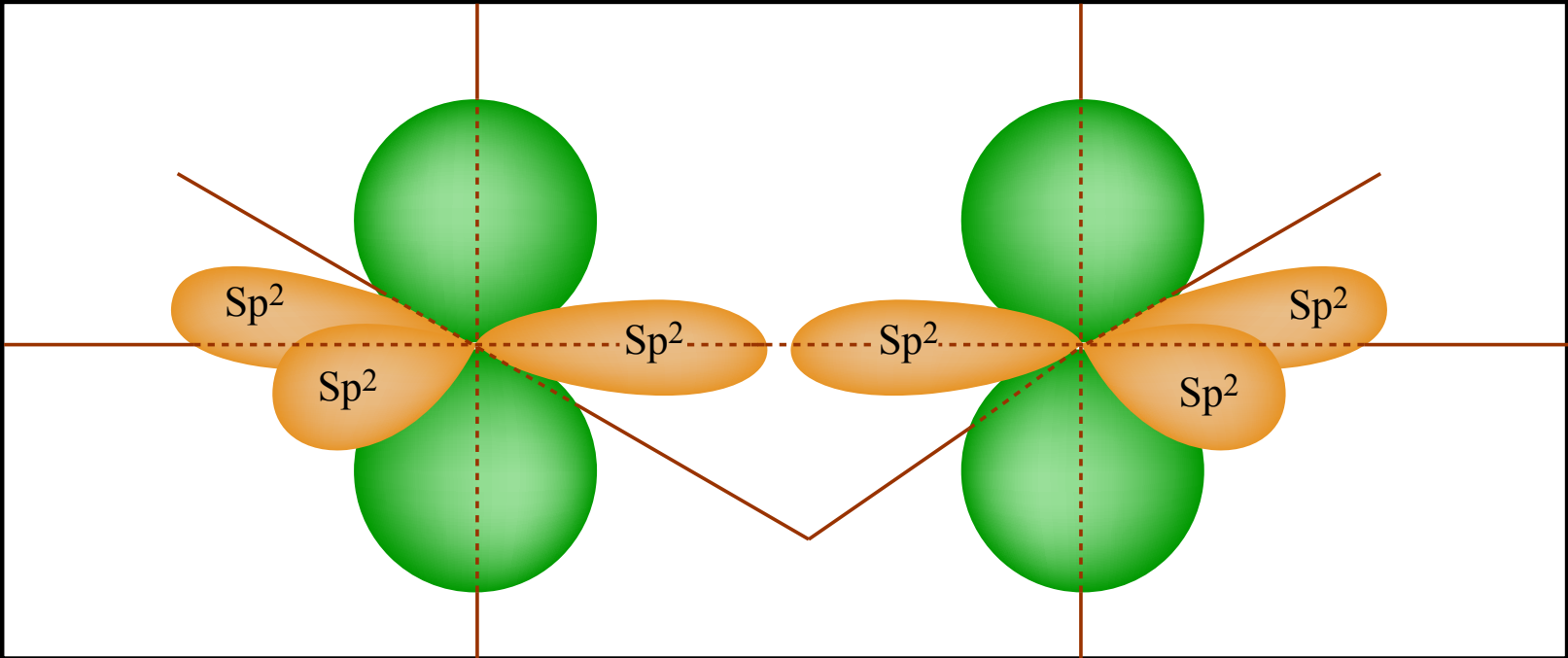


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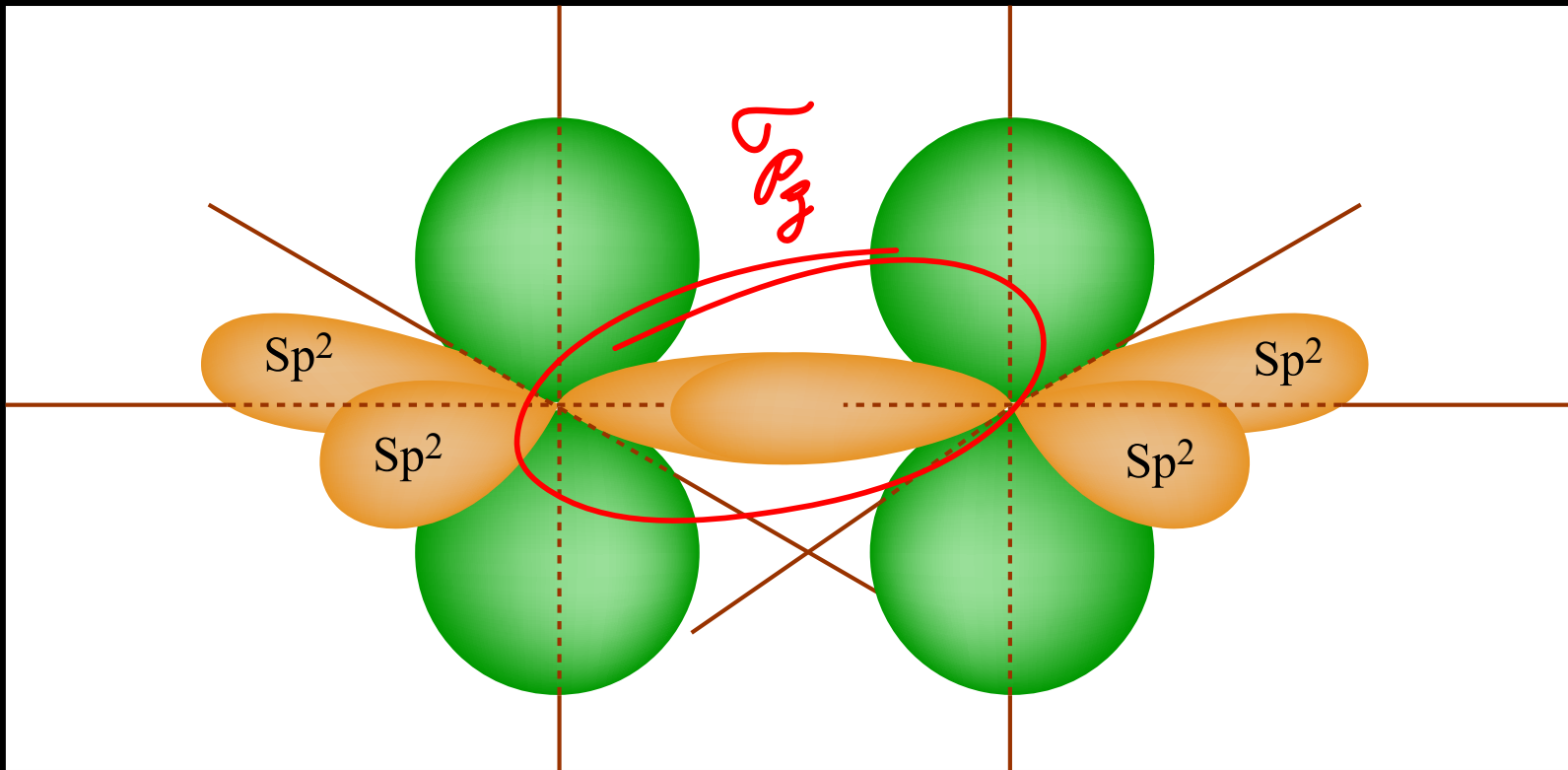


Image by MIT OpenCourseWare.

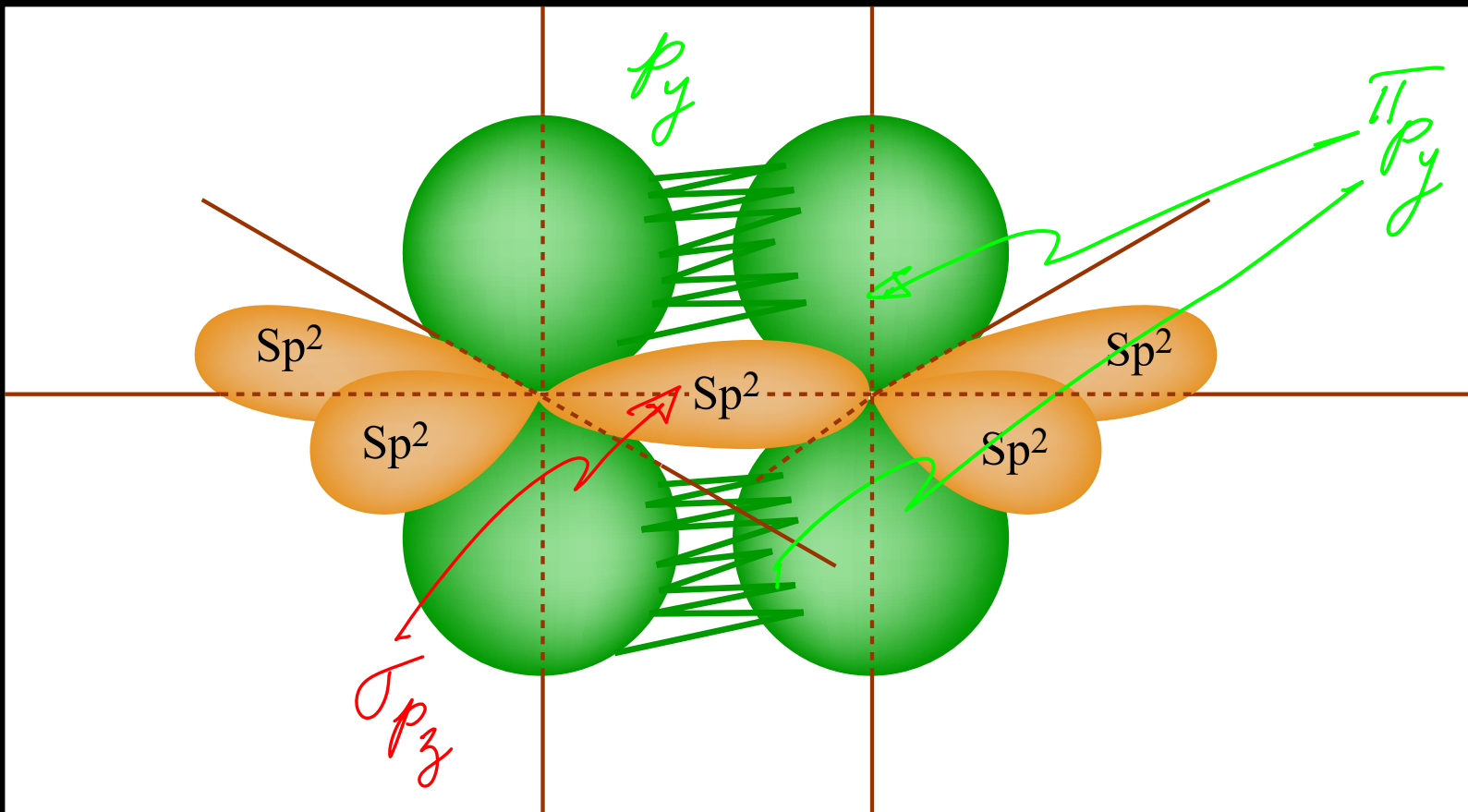
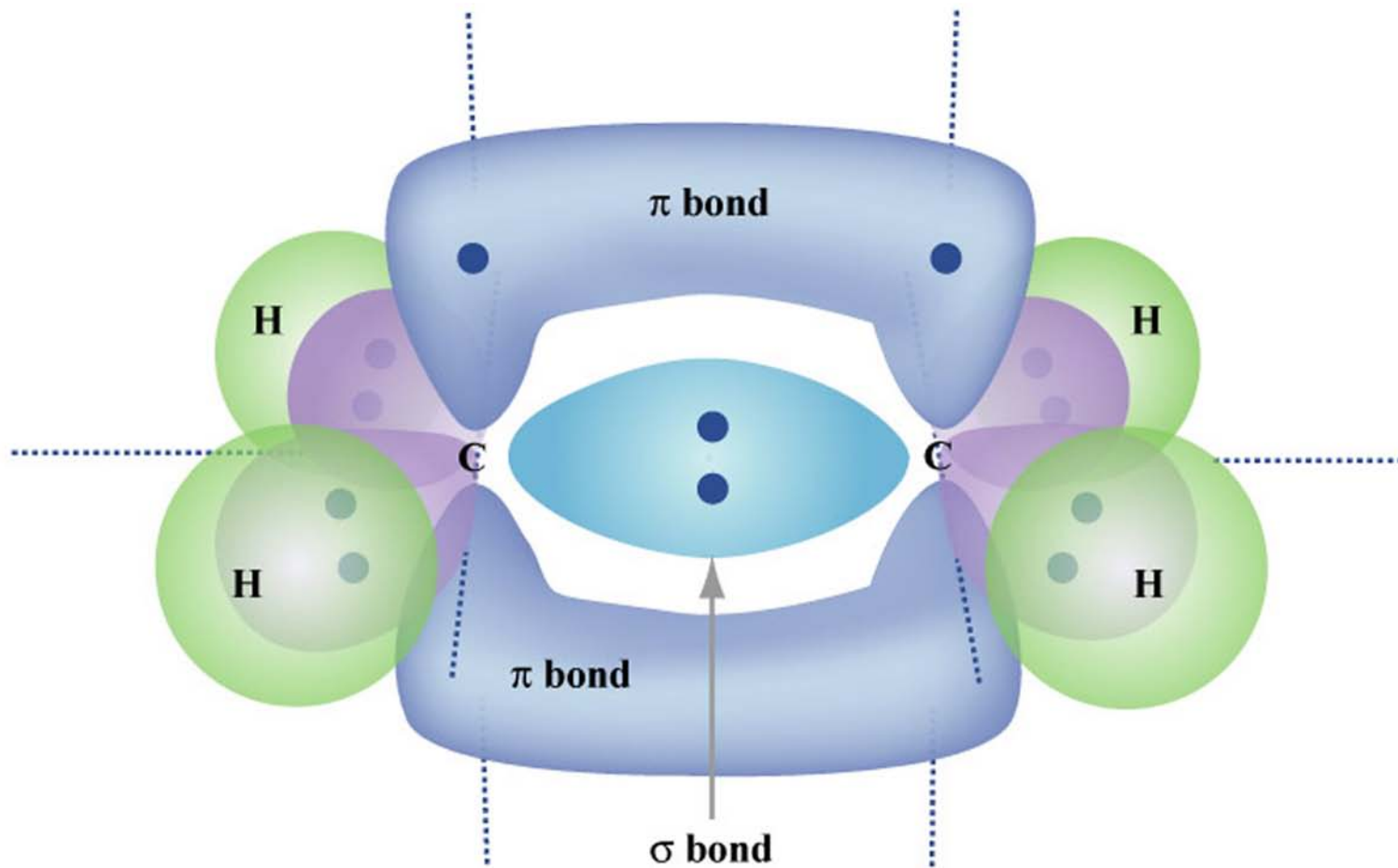
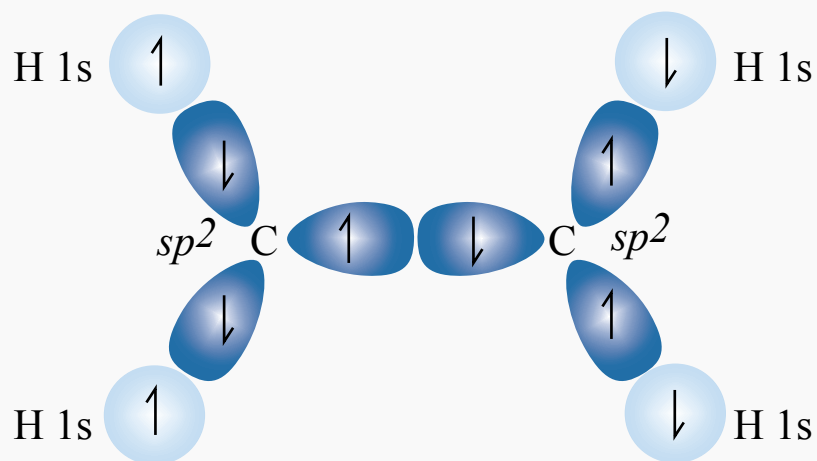


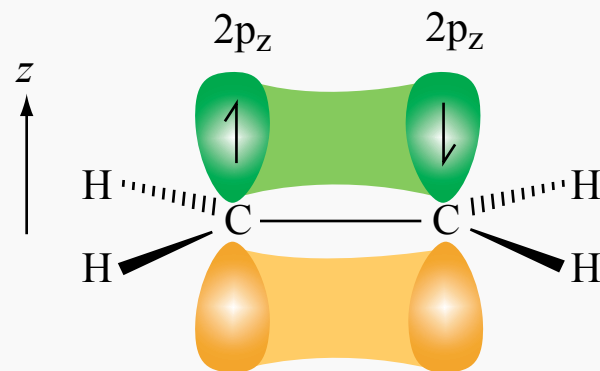
Image by MIT OpenCourseWare.



(a) C_2H_4 sigma-bonded framework



(b) C_2H_4 pi bonding



Extremes in electronegativity

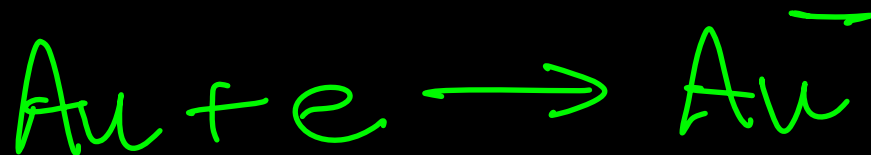
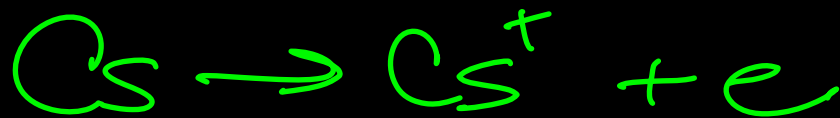
NaI: $\Delta\chi = 1.73$

CsAu: $\Delta\chi = 1.75$

Cs and Au, both metals, melt to form metallic liquids, *but...*
when the concentration nears 50%

(equal numbers of donors & acceptors)

💣* electron transfer occurs 💣* !



Extremes in electronegativity

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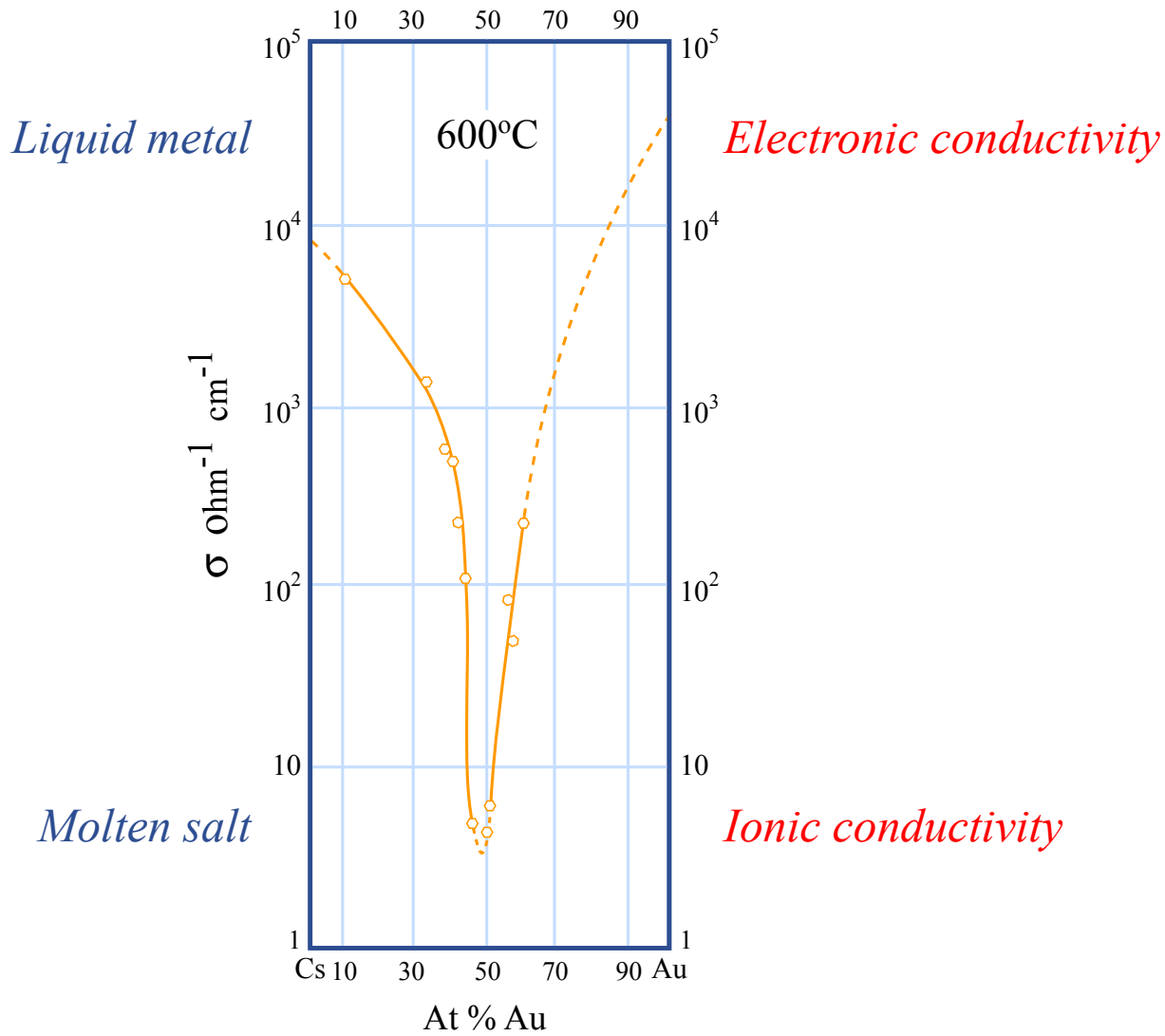
metallic melt turns into molten salt!!

☞ clear, colorless liquid

☞ big drop in electrical conductivity

☞ shift from electronic to ionic conduction

Specific electrical conductivity of liquid Cs – Au alloys as a function of concentration
(Hoshino *et al.* 1975)



Extremes in electronegativity

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- 👉 **cesium auride**

Amazing!

Extremes in electronegativity

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3.091SC Introduction to Solid State Chemistry
Fall 2009

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