Chem 111

Lecture 35

Announcement

- Final: Dec. ~~12~~ 17th; 1:30pm – 3:30pm in Totman Gym
  - No Makeups
  - No Pyramid
  - Bring pencils, calculator, ID card and a good erasers

- Review Schedule - ISB 135

Weds 4-6 PM C. Joseph
Weds 7-9 PM J. Tyson and M. Johnson
Thurs 4-6 PM B.Botch

- Office Hours only on Tuesday for Finals week

Homework

- Continue Reading Chapter 9
- Owl Homework

Recap

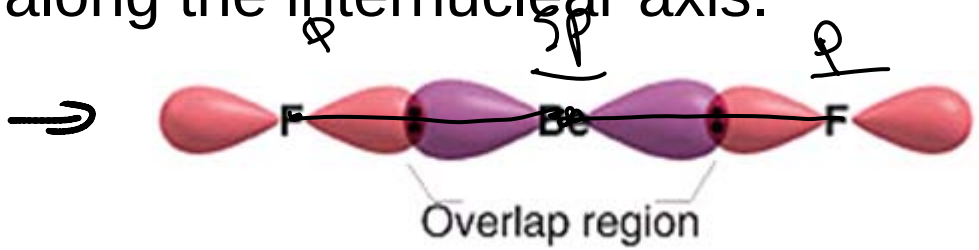
- Hybridization
- Multiple Bonds

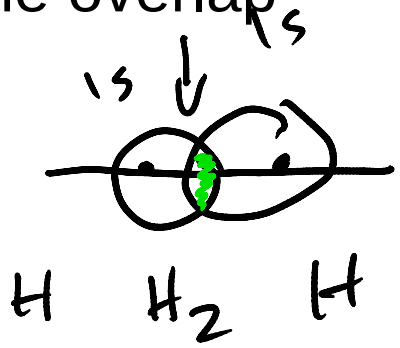
Multiple Bonds

Internuclear Axis - Line connecting the nuclei of two bonded atoms

⇒ single bonds

Sigma (σ) bond – is a covalent bond in which the overlap region lies along the internuclear axis.

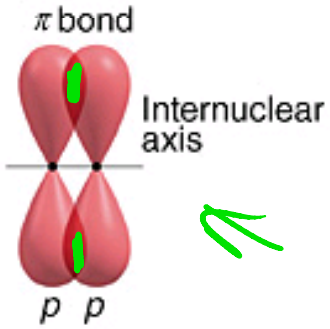




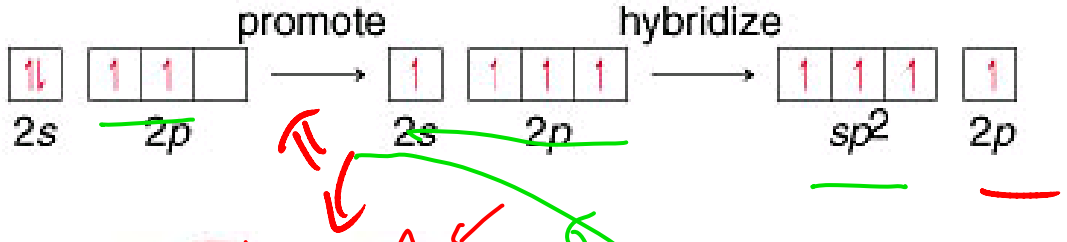
Pi (π) bonds – is a covalent bond in which the overlap regions lie above and below the internuclear axis.

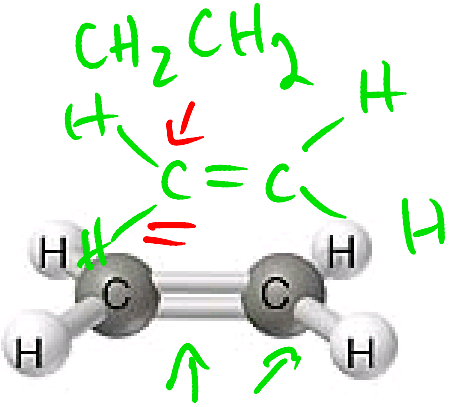
= double bonds

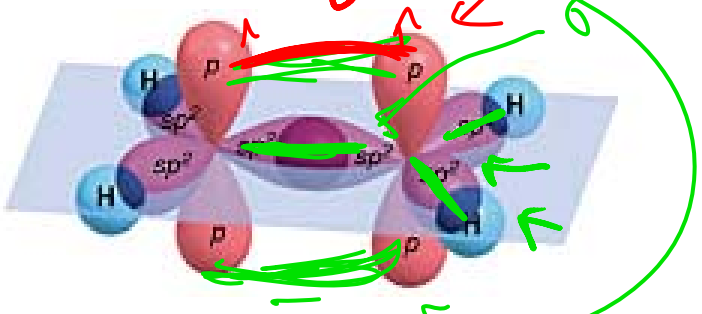
≡ triple

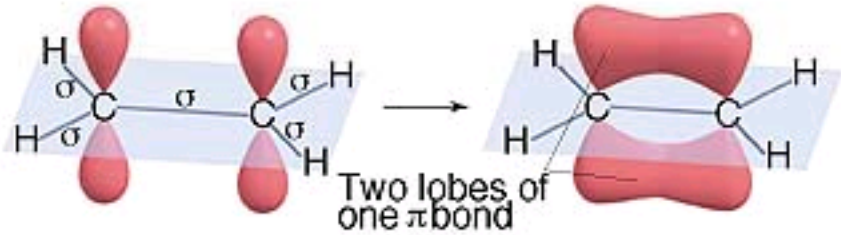


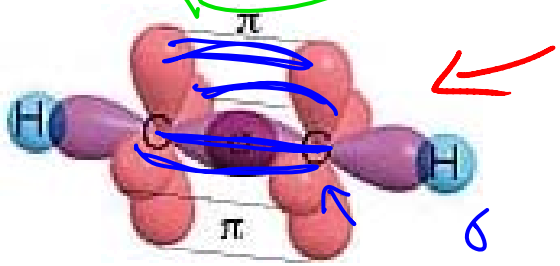
Multiple Bonds











$sp \Rightarrow p, p$

$sp^2 \Rightarrow p$

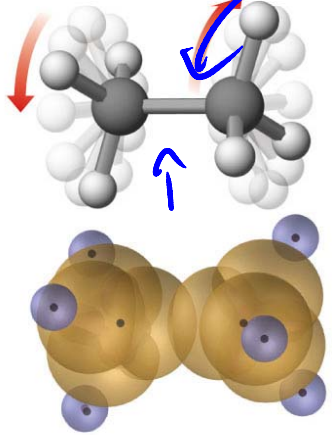
$sp^3 \Rightarrow \not{p}$

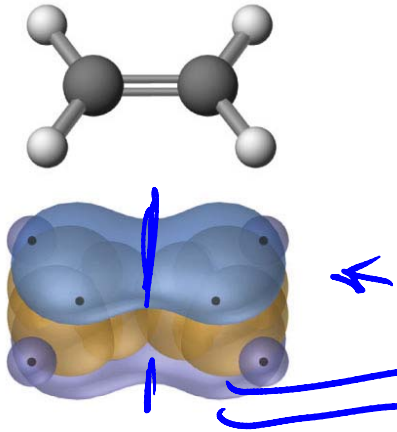
Double bond = 1 σ bond and 1 π bond
Triple bond = 1 σ bond and 2 π bond

πbond usually happen with unhybridized p orbitals, therefore sp and sp^2 hybridization.

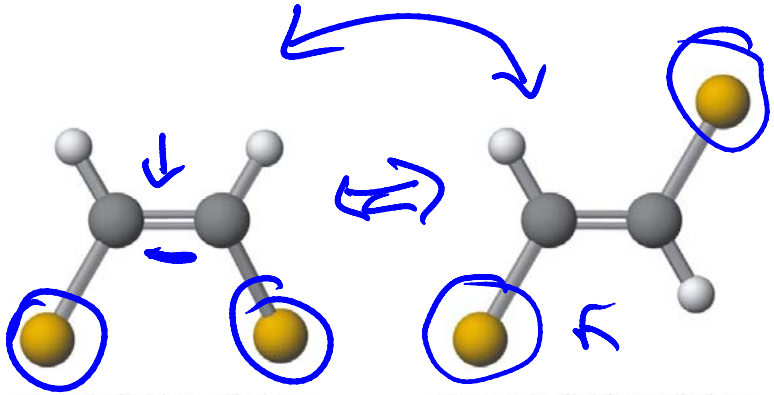
πUsually C, O, N, and S

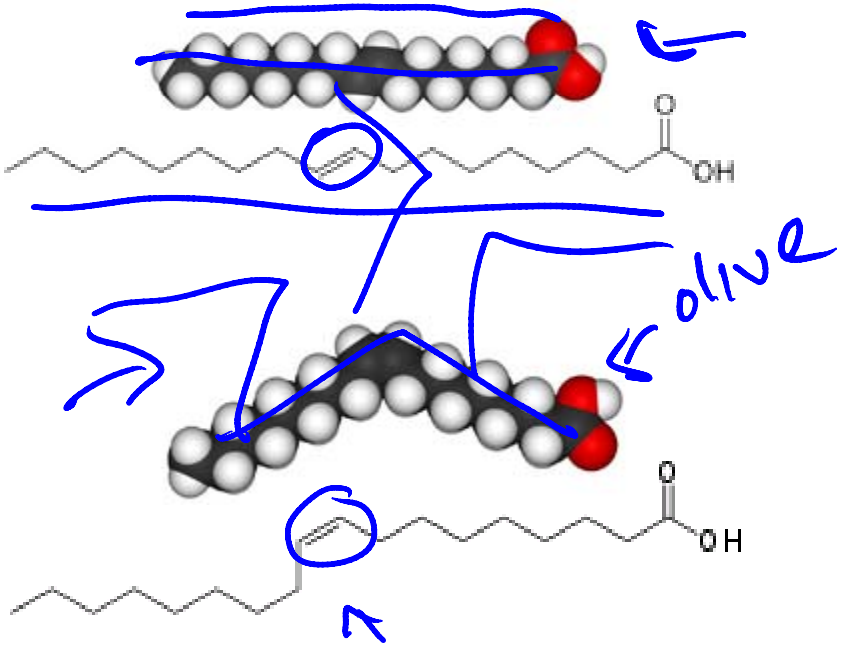
Cis-Trans Isomers





Isomers – are compounds that have the same formula but different structures.

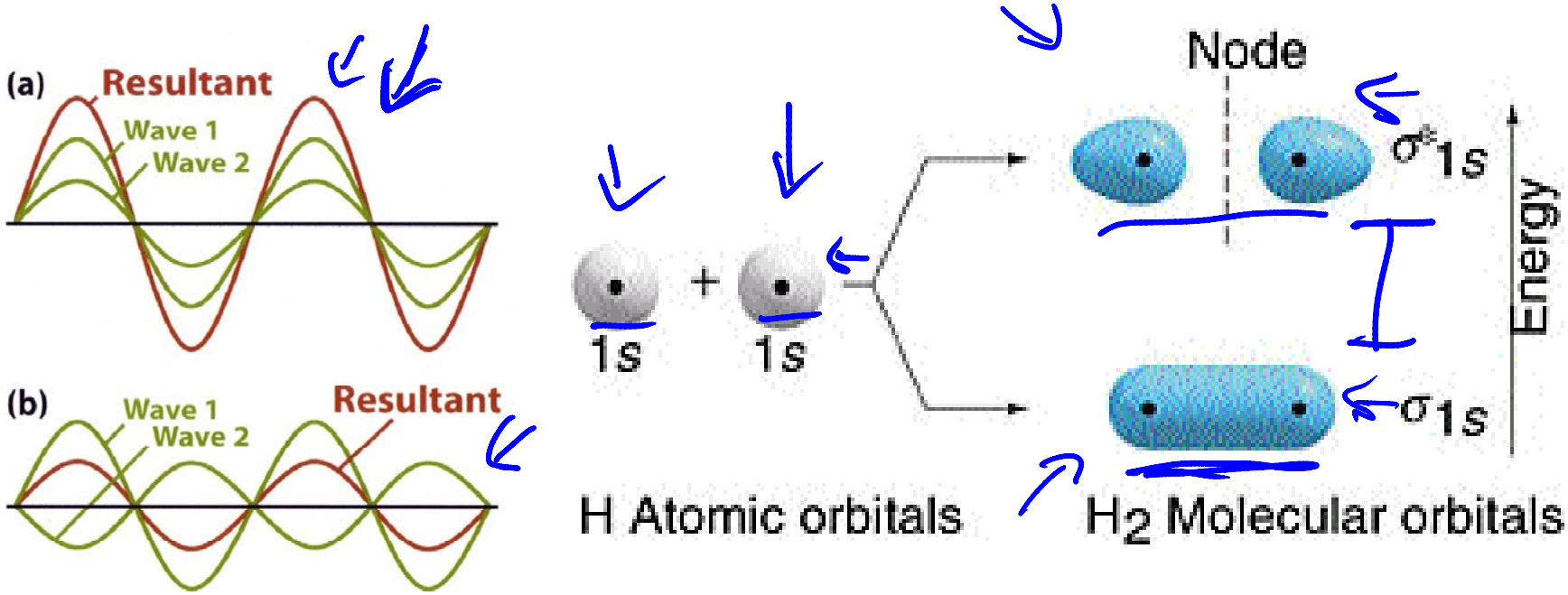




Molecular Orbital Theory

Molecular orbitals have many characteristics similar to atomic orbitals: hold two electrons, have discreet energies.

Consider H_2



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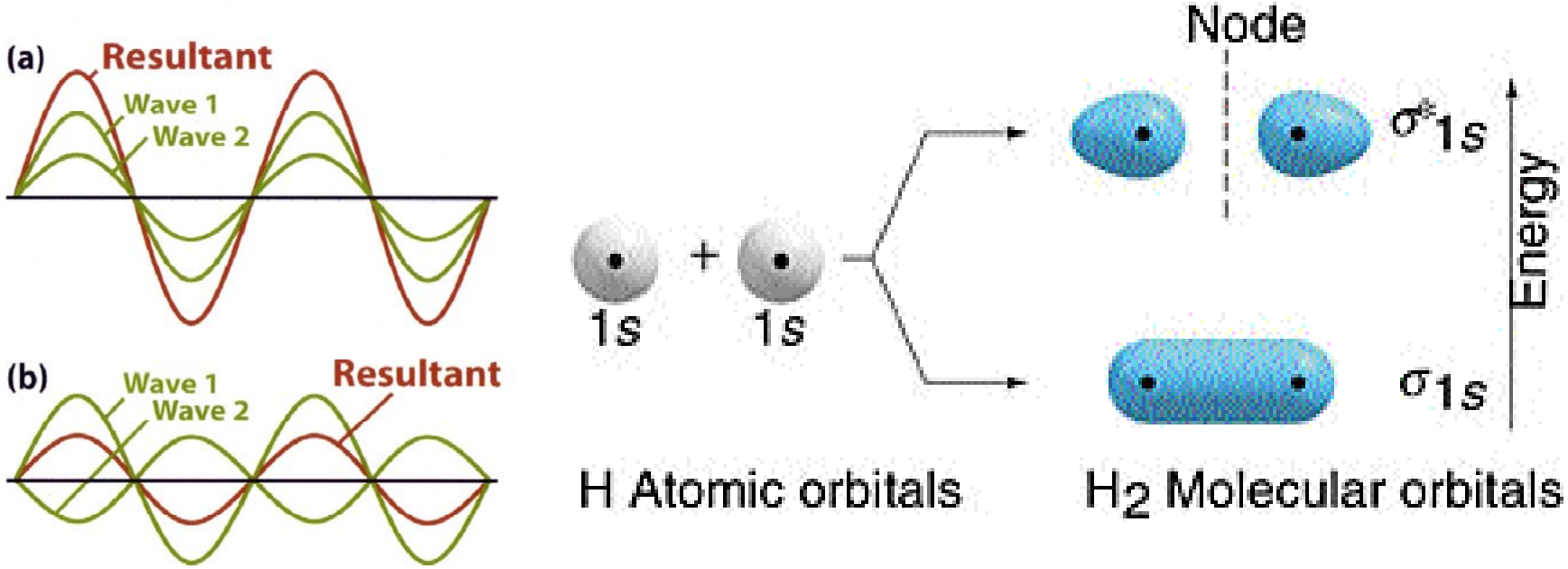
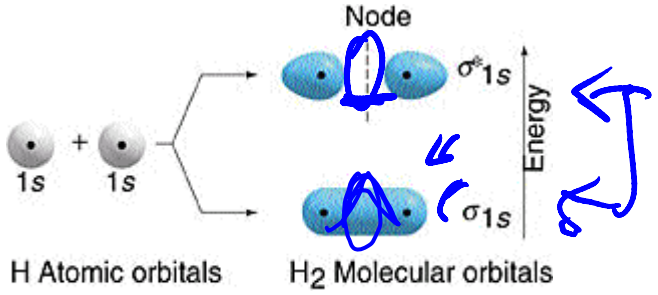


Molecular Orbital Theory

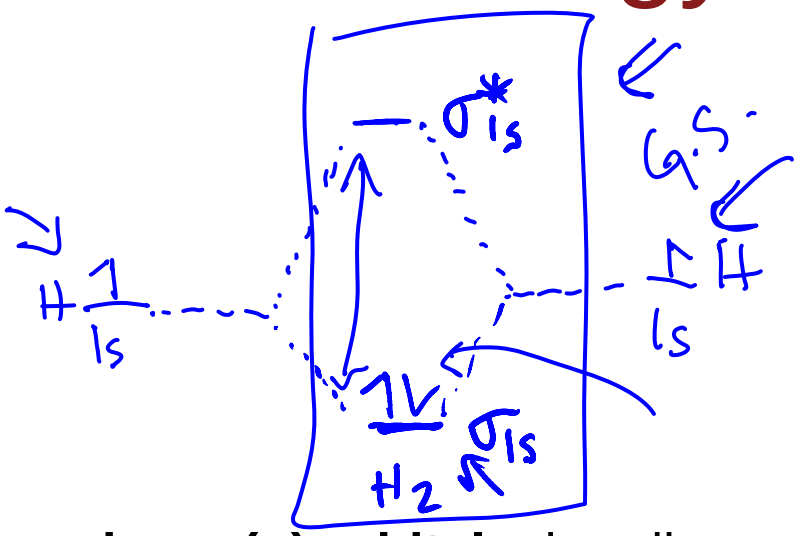


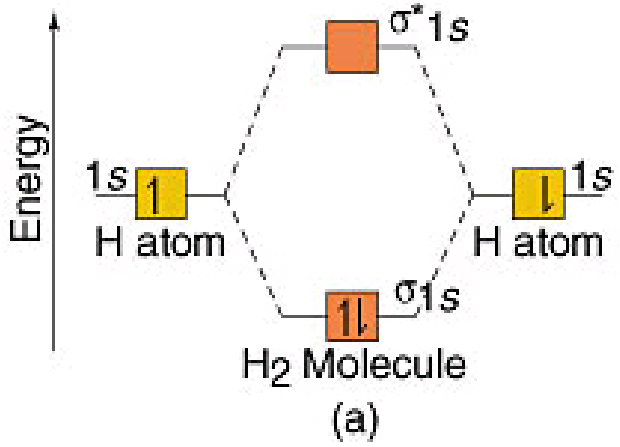
The total number of molecular orbitals created equal the total number of atomic orbitals used.

Bonding orbital – lower energy orbital (than atomic orbitals) that concentrate electron density between the atoms.

Antibonding orbital – higher energy orbital (than atomic orbitals) that have little electron density between the atoms.

MOT Energy Level Diagram





sigma (σ) orbital – bonding molecular orbital centered around internuclear distance.

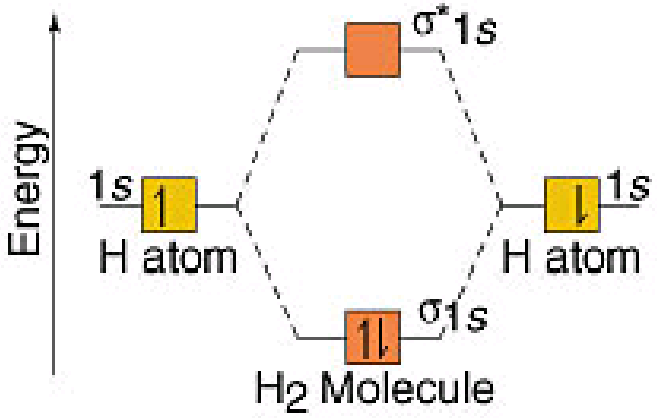
sigma-star (σ*) bond – anitbonding molecular orbital centered around internuclear distance.

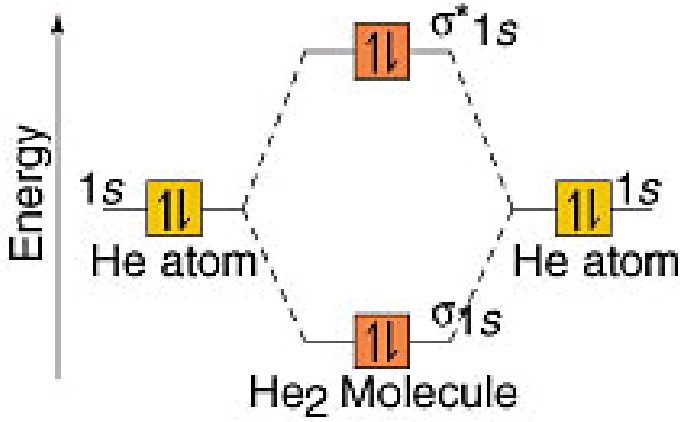
1s – denotes the character of the atomic orbitals that make up the molecular orbitals.

Electron fill like atomic orbitals, low energy first & spin paired.

Bond Order (Using MOT)

Bond order = ½ (# of bonding electrons - # of nonbonding electrons)



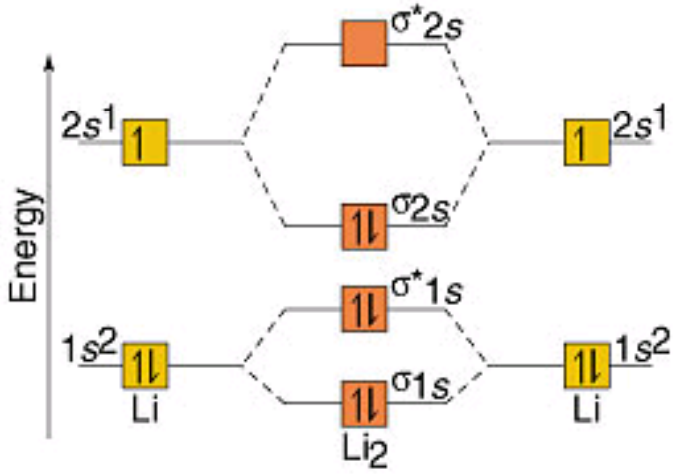


Let’s Practice

Draw the molecular energy level diagram of He_2^+? What is the bond order?

MO of Li_2

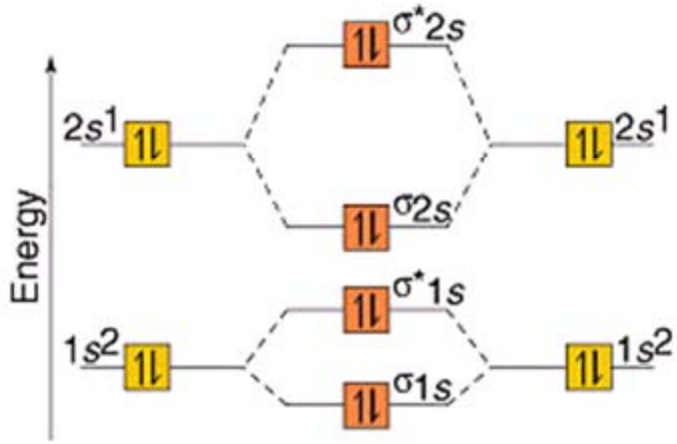
Atomic orbitals must be of similar energy to form molecular orbitals.



Core electrons usually don't do not contribute significantly to bonding in the molecule formation.

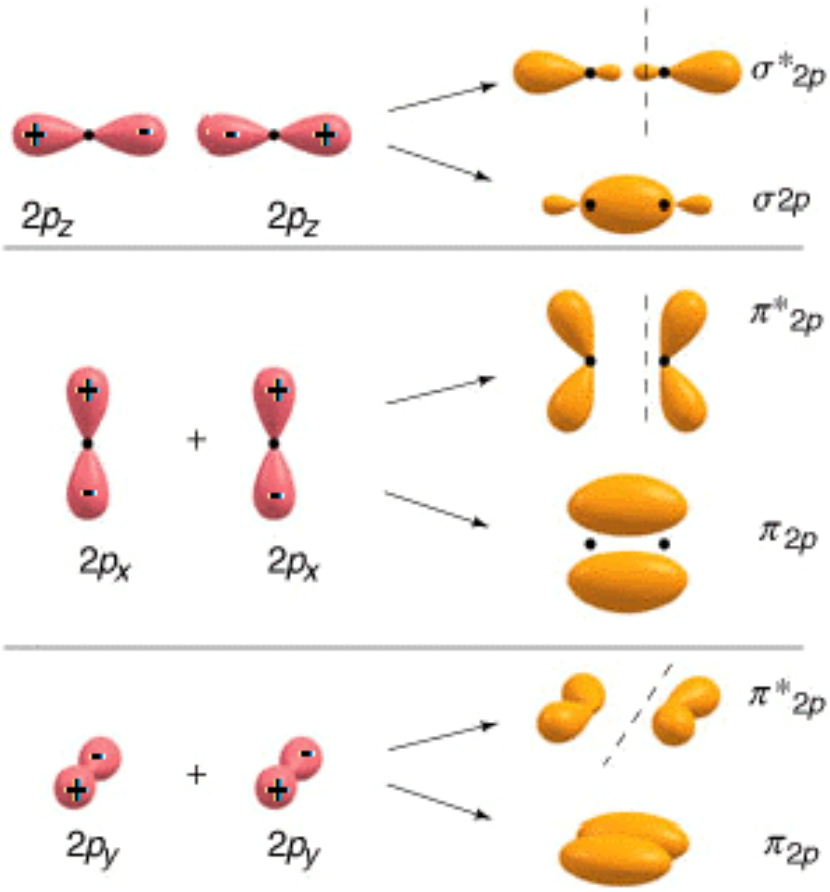
Li_2 MO Configuration = $(\sigma_{1s})^2(\sigma^*_{1s})^2(\sigma_{2s})^2$

MO of Be_2



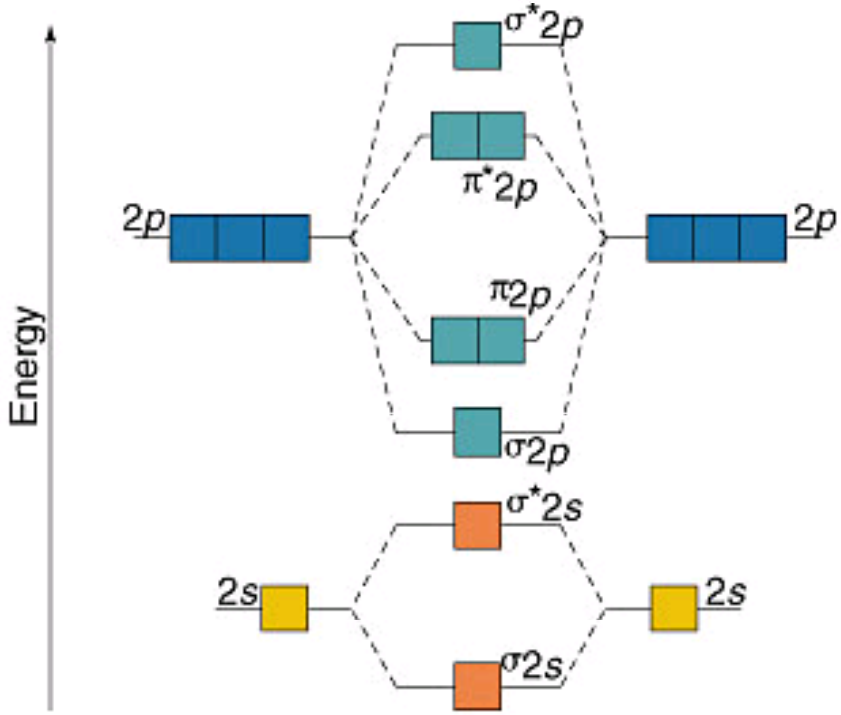
Be_2 MO Configuration = $(\sigma_{1s})^2(\sigma^*_{1s})^2(\sigma_{2s})^2(\sigma^*_{2s})^2$

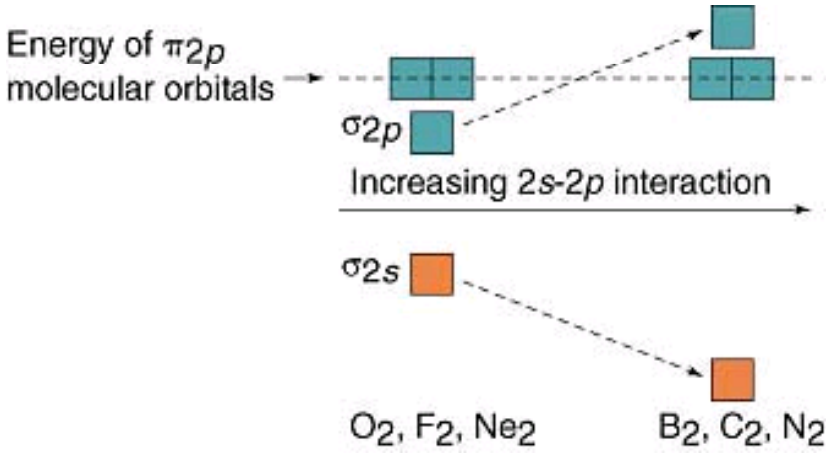
Molecular orbitals from P orbitals



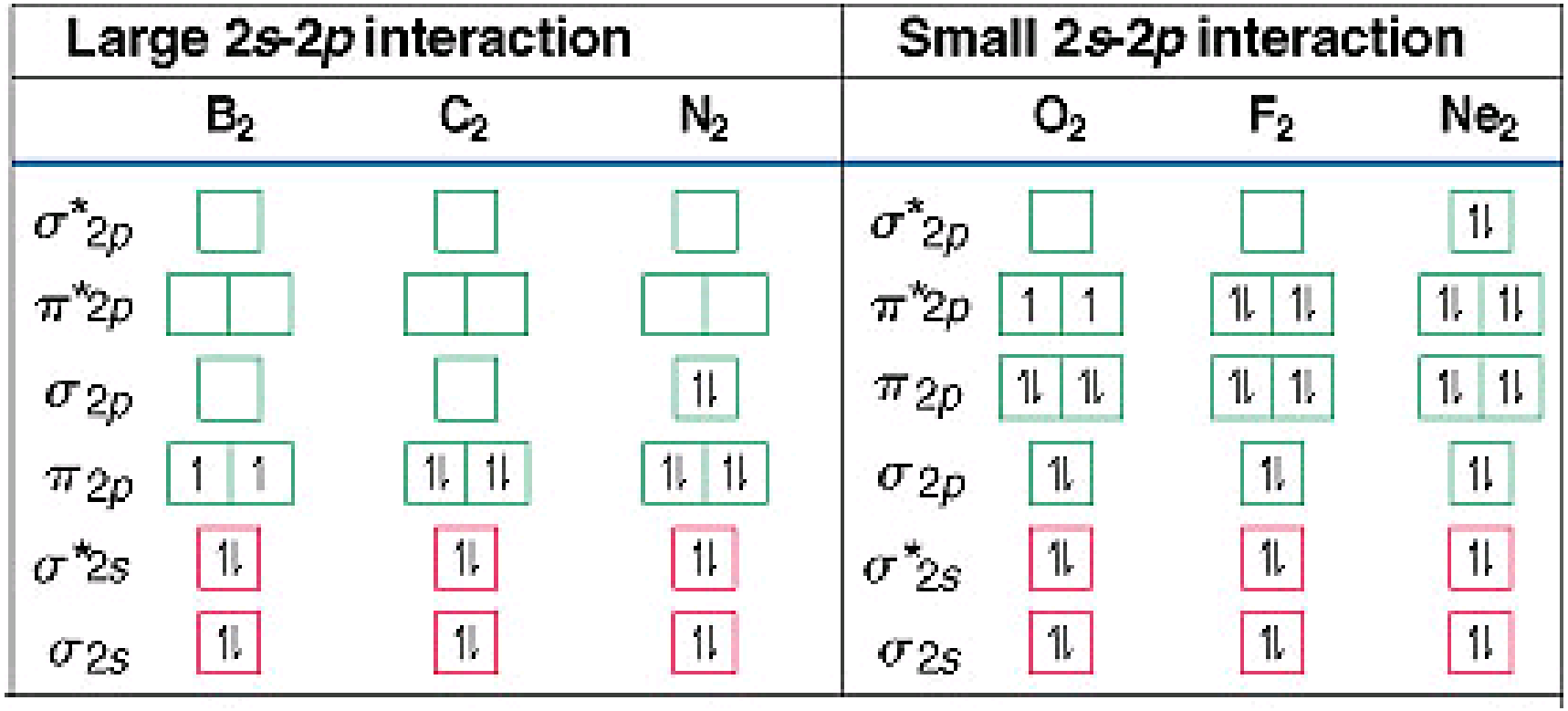
Note the amount they can mix and their relation to internuclear axis

MO Diagram


Energy
σ*2p
π*2p
2p
2p
π2p
σ2p
σ*2s
2s
2s
σ2s

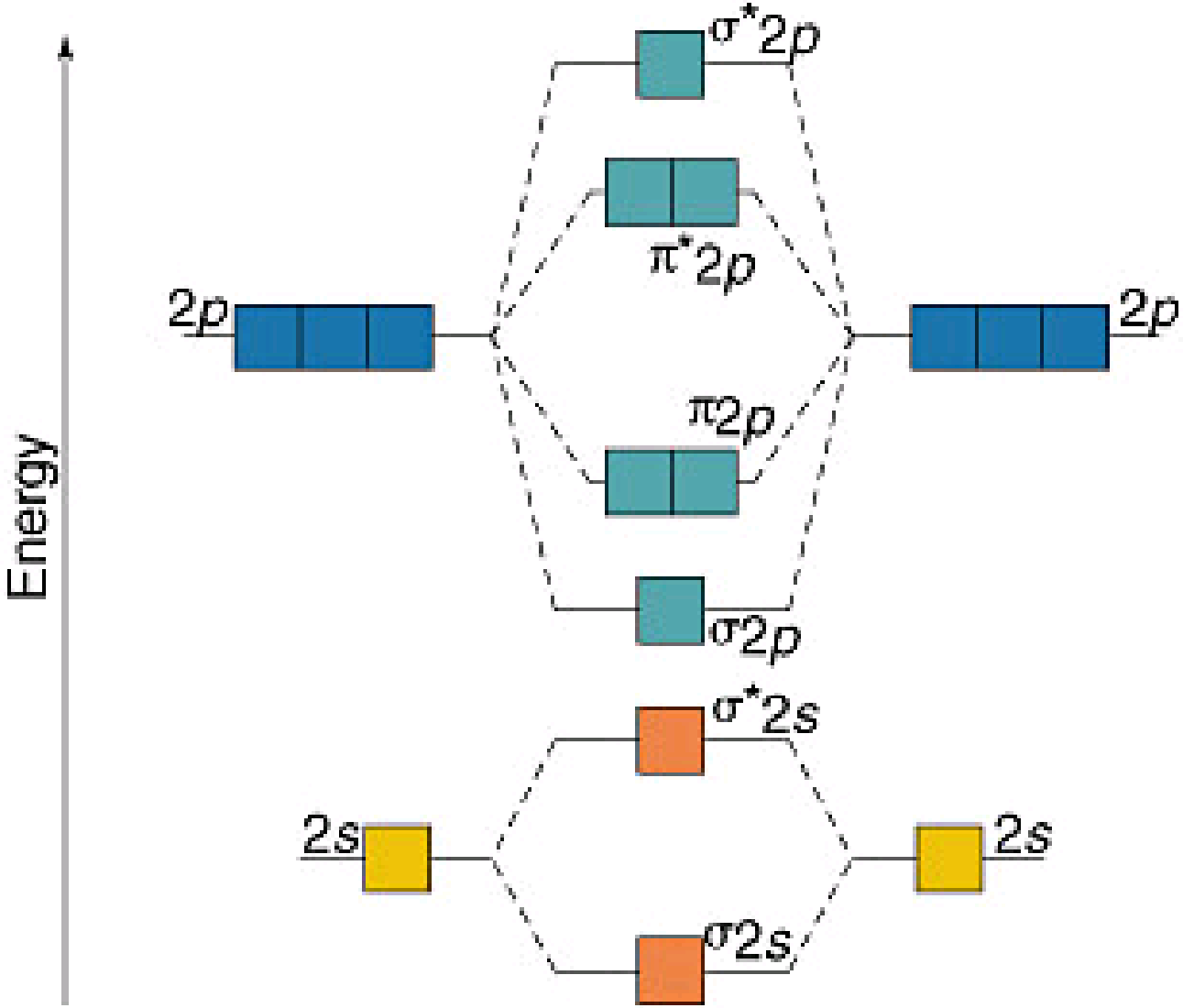

Energy of π2p
molecular orbitals
σ2p
Increasing 2s-2p interaction
σ2s
O2, F2, Ne2
B2, C2, N2

MOT P block


Large 2s-2p interaction
Small 2s-2p interaction
B2
C2
N2
O2
F2
Ne2
σ*2p
π*2p
σ 2p
π 2p
σ*2s
σ 2s

Let's practice

What is the Bond Order O_2, O_2^-, O_2^{2-}, O_2^+



MOT-Heteronuclear Diatomics

- Differences from Homonuclear case:
  - Electrons will be drawn to the more electronegative element . Thus bonding orbitals will have more of that element character and antibonding orbitals will have more character from the less electronegative element.
  - As a result of having more A character, the molecular orbital will be closer in energy to that elements atomic orbital.