Chem 111

Lecture 33

Announcement

- Exam 3: Dec. 6th in class

→Same deal as before

  - No Makeups
  - Pyramid
  - Bring pencils, calculator, ID card and a good erasers

- Practice Exam:

http://courses.umass.edu/chem111-bbotch/

- Breanne has a recitation session HASA 126 – 12/1 (5-6pm)

Announcement Part 2

- SI sessions

- Sunday 4 – 6 PM, ISB 135, Prof. Vachet

- Spark discussion extra credit should show on Owl grades.

- Owl homework: if you did something during grace period and it hasn't checked off and it has been longer than a month contact me.

→You did the module correct.
→You did ALL parts of the module correct.
→You FINISHED ALL part of the module within grace period.

Exam

filling up
mole geometery

- Chapter 6: Dia/Paramagnetism
- Chapter 7: Everything
- Chapter 8: Everything
- Chapter 9: What I cover today

- No Equation Sheet

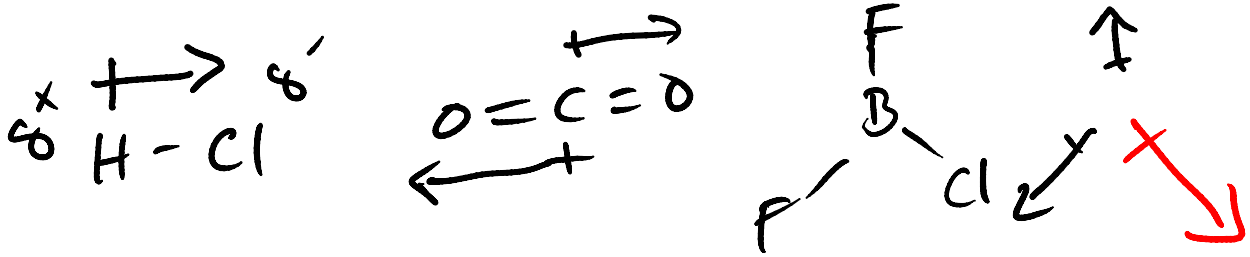
Know Formula Charge
B. O.
$\Delta H_r =$

- Need to know concepts from earlier chapters.

Homework

- Start Reading Chapter 9
- Owl Homework

Recap



- Polar Molecules
- Electroneutrality
- Bond Order — single bond = B.O. = 1
- Bold Length
- Bond Enthalpy

↑ Bond Order

↕ Bold Length

> size

Orbital Overlap

Lewis Structures and VSEPR doesn't get everything "correct".

Quantum Mechanics – valence-bond theory

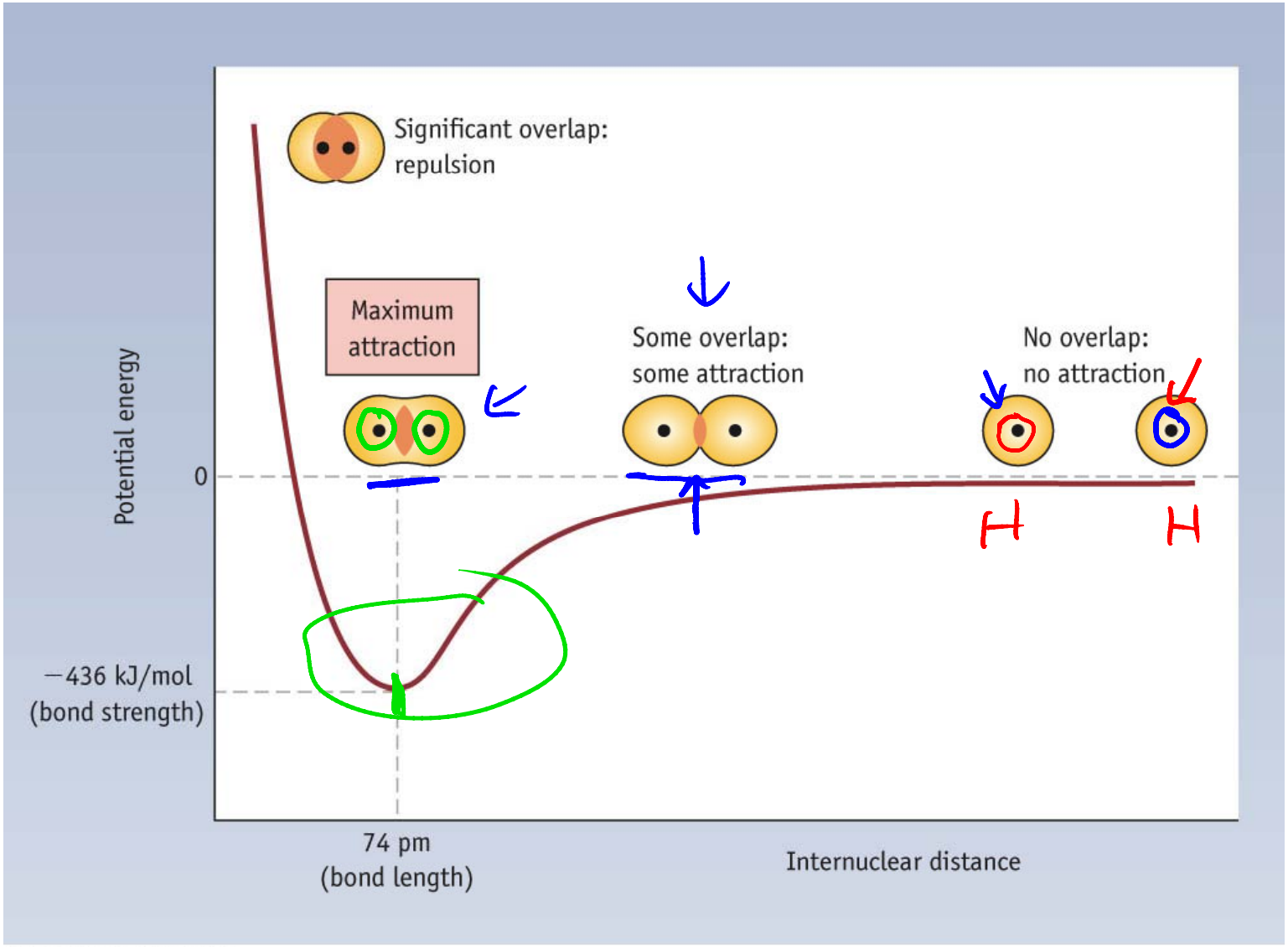
• Lewis Structures – bonds happen when atoms share electrons

• **VB Theory -** electron density builds up between two nuclei when valence atomic orbitals merge with each other.

• This merger (or mixing) results in the orbitals occupying the same space called an **overlap.**

• **Overlap –** allows electrons of opposite spin to share the common space between the nuclei forming a bond.

Orbital Overlap

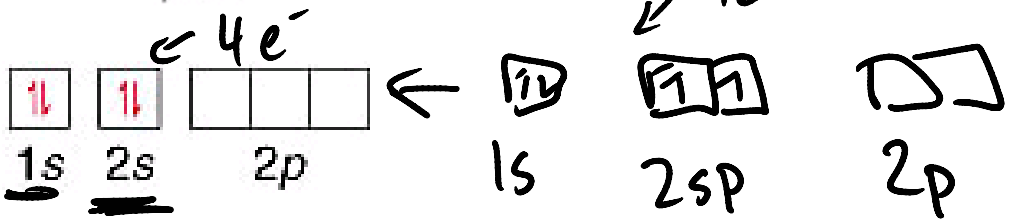


Hybridization

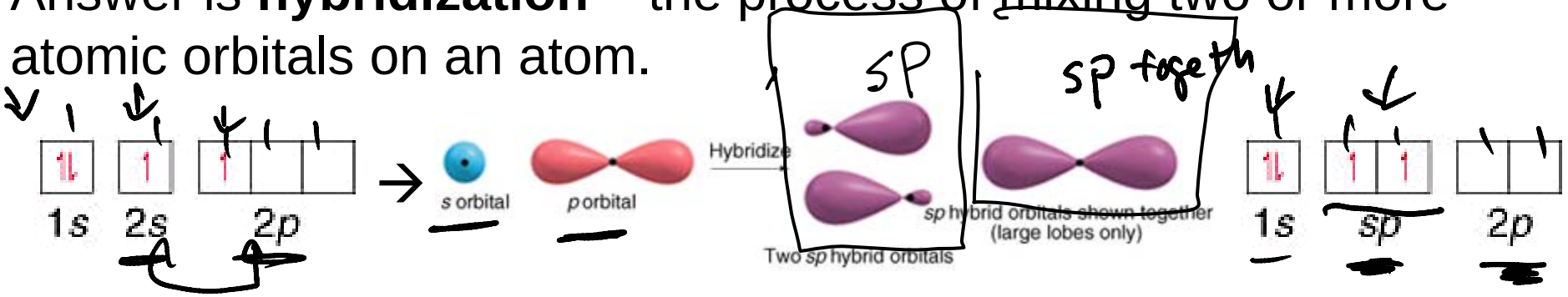
Consider BeF_2

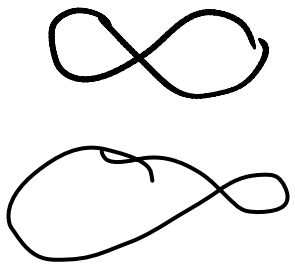
F ($1s^2 2s^2 2p^5$) – so p orbital

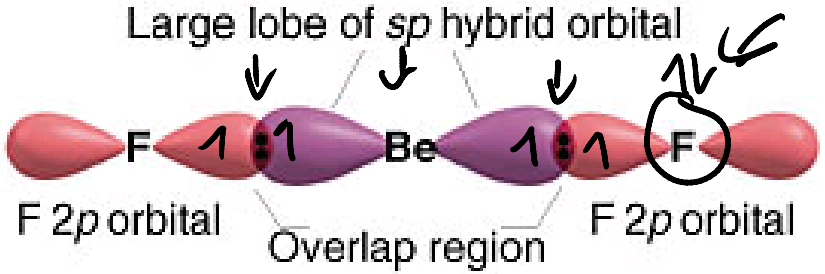
What about B ($1s^2 2s^2$)?

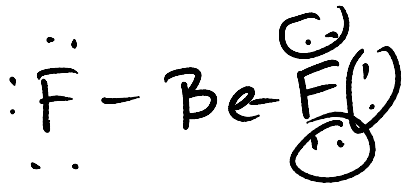


Answer is **hybridization** – the process of mixing two or more atomic orbitals on an atom.





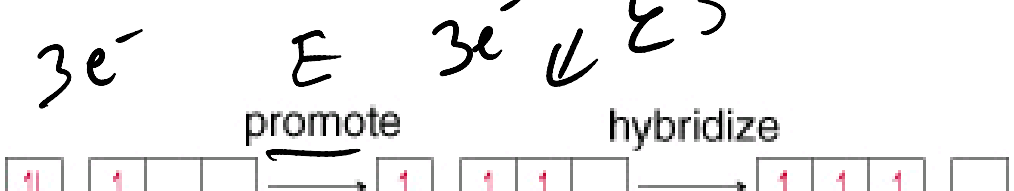


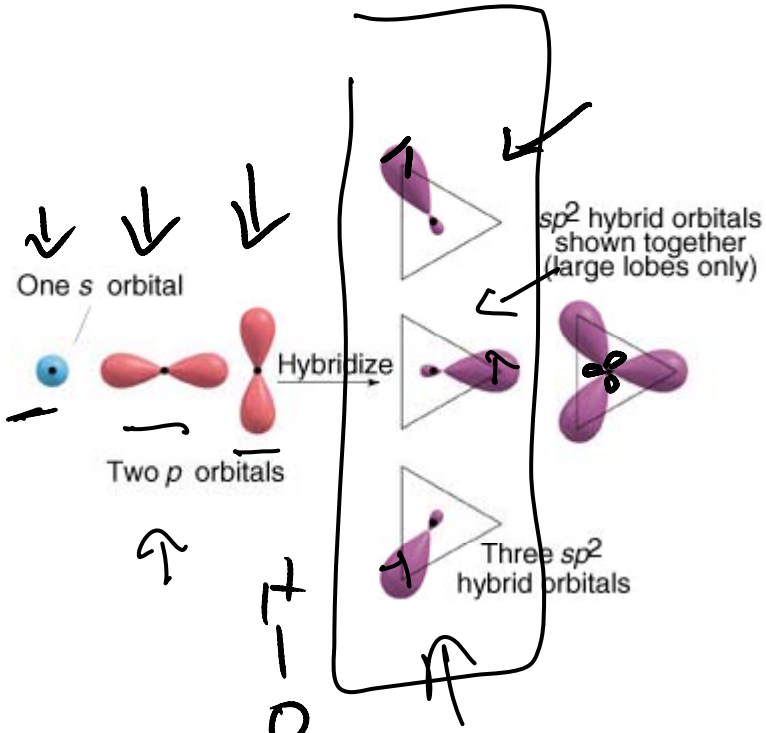


sp^2 Hybridization

atomic orbitals = # hybrid orbitals

Consider BF_3

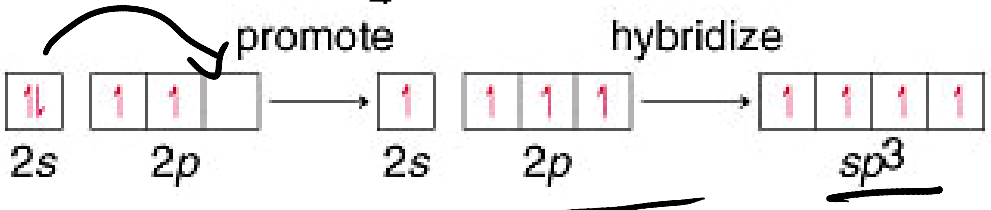


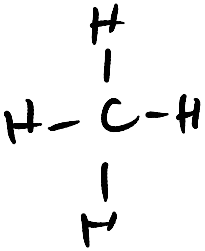


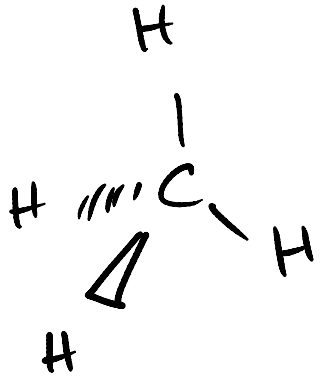
sp^2 and sp^3 Hybridization

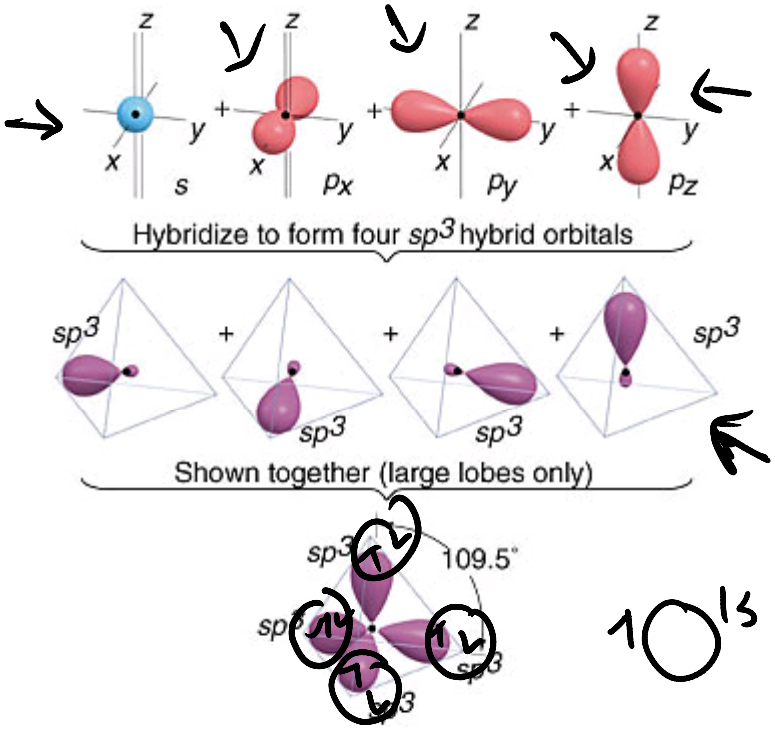
atomic orbitals = # hybrid orbitals

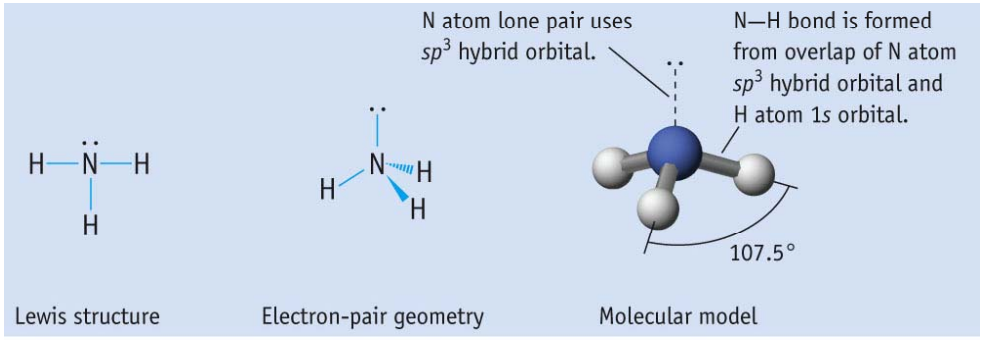
Consider CH_4

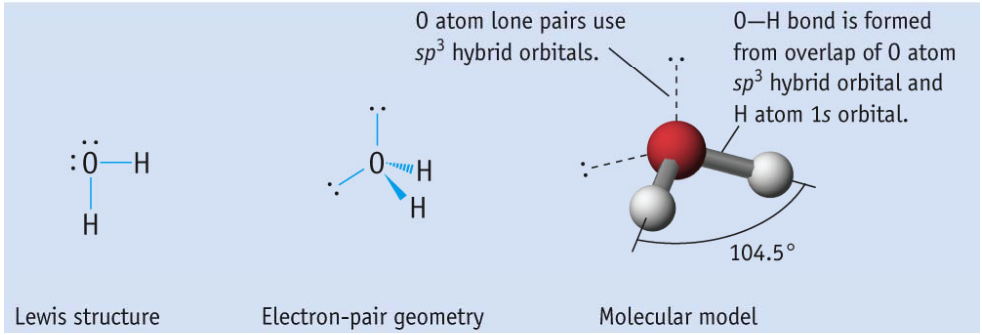




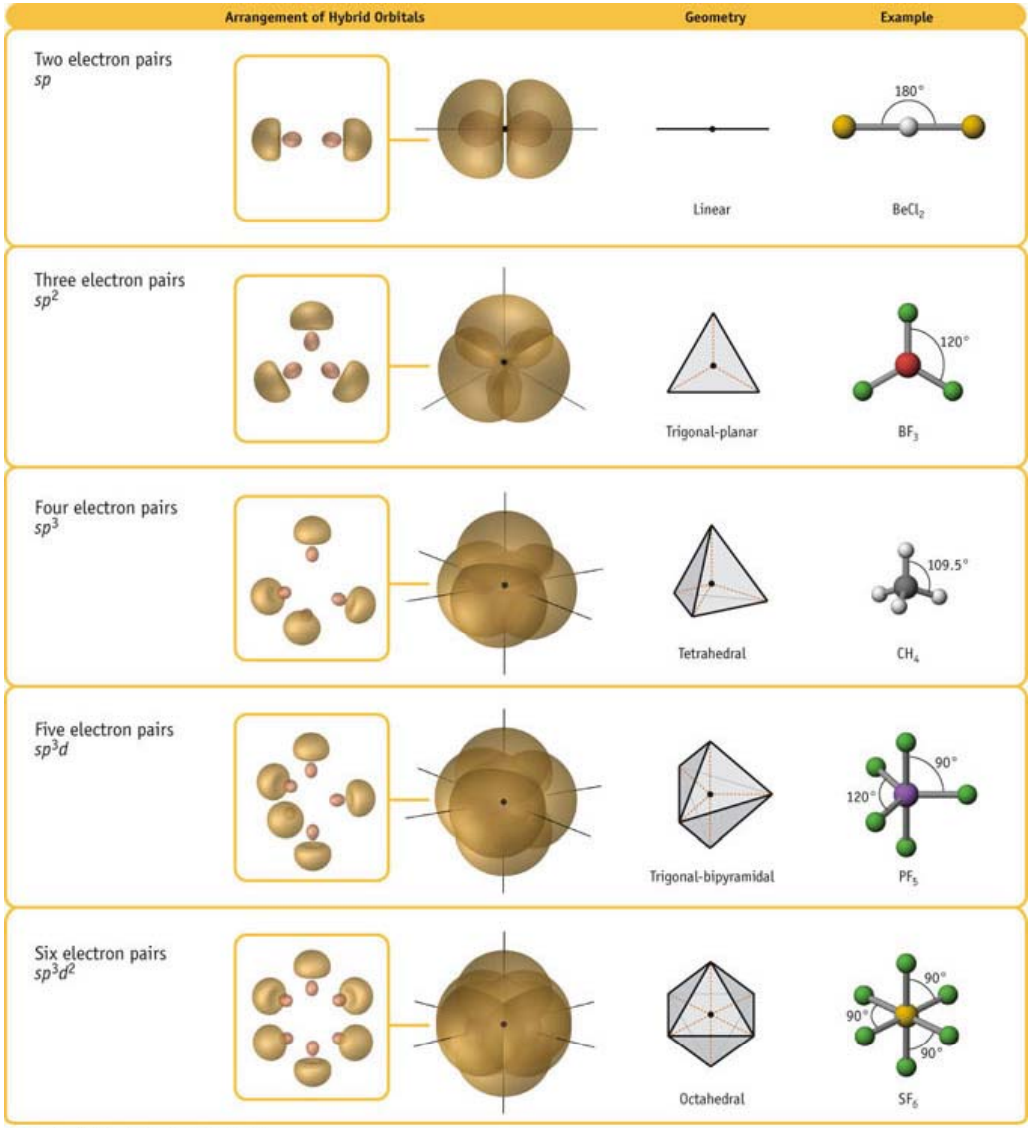


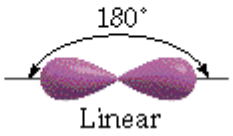
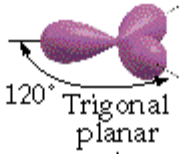
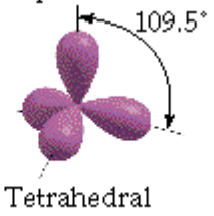
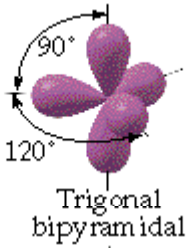
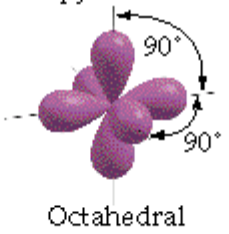






Hybridization



Atomic Orbital Set	Hybrid Orbital Set	Geometry	Examples
s,p	Two *sp*		BeF_2, $HgCl_2$
s,p,p	Three sp^2		BF_3, SO_3
s,p,p,p	Four sp^3		CH_4, NH_3, H_2O
s,p,p,p,d	Five sp^3d		PF_5, SF_4, BrF_3
s,p,p,p,d,d	Six sp^3d^2		SF_4, ClF_3, XeF_4

Summary for Hybridization

1. Draw the Lewis structure for the molecule or ion
2. Determine the electron-pair geometry using VSEPR model.
3. Specify the hybrid orbitals needed to accommodate the electron pairs based on their geometrical arrangement.

Let’s Practice

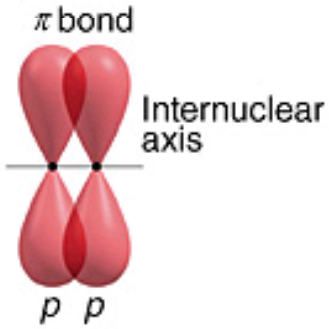
Indicate the hybridization of orbitals employed by the central atom in each of the following: NH_2^- and SF_6.

Multiple Bonds

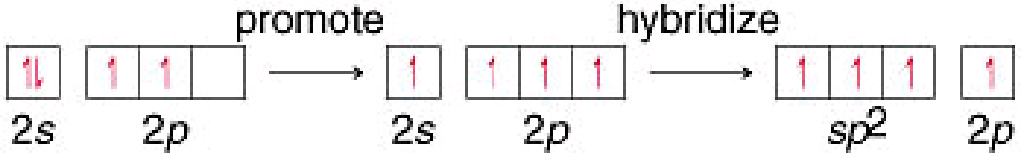
Internuclear Axis - Line connecting the nuclei of two bonded atoms

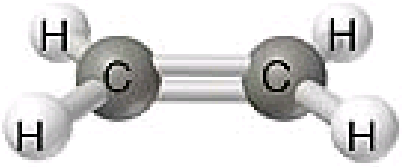
Sigma (σ) bond – is a covalent bond in which the overlap region lies along the internuclear axis.

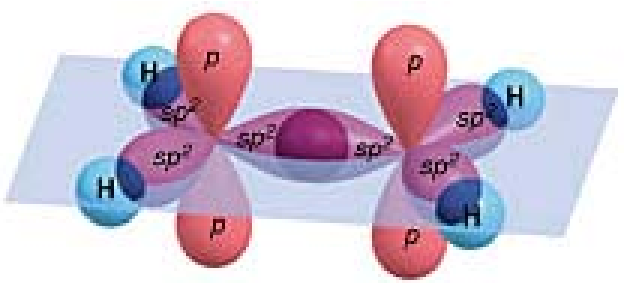
Pi (π) bonds – is a covalent bond in which the overlap regions lie above and below the internuclear axis.

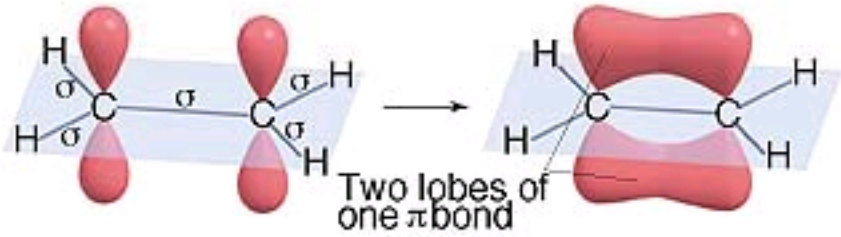


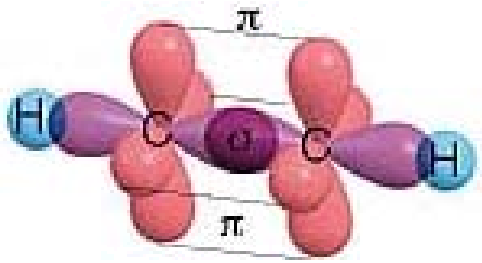
Multiple Bonds





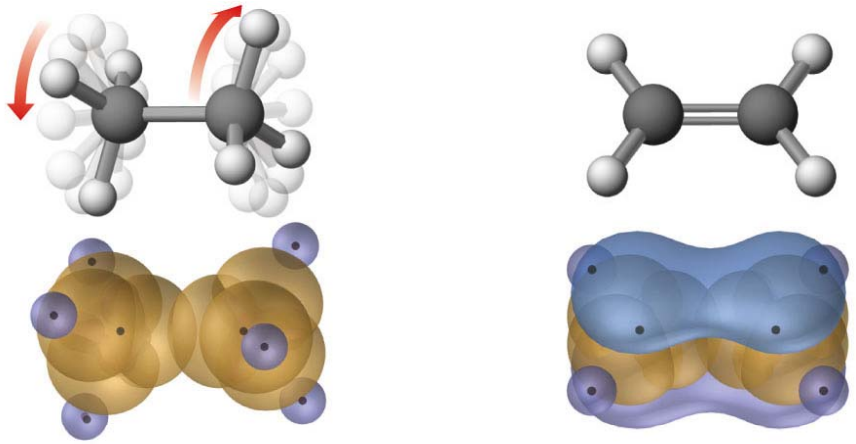




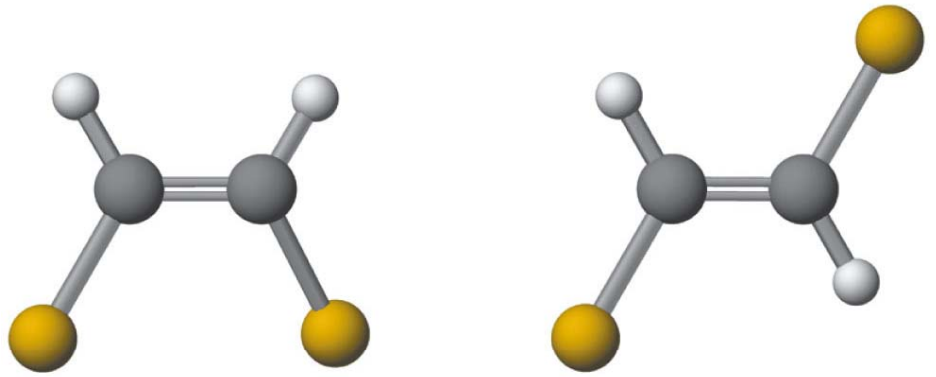


Double bond = 1 σ bond and 1 π bond
Triple bond = 1 σ bond and 2 π bond
πbond usually happen with unhybridized p orbitals, therefore sp and sp^2 hybridization.
πUsually C, O, N, and S

Cis-Trans Isomers



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



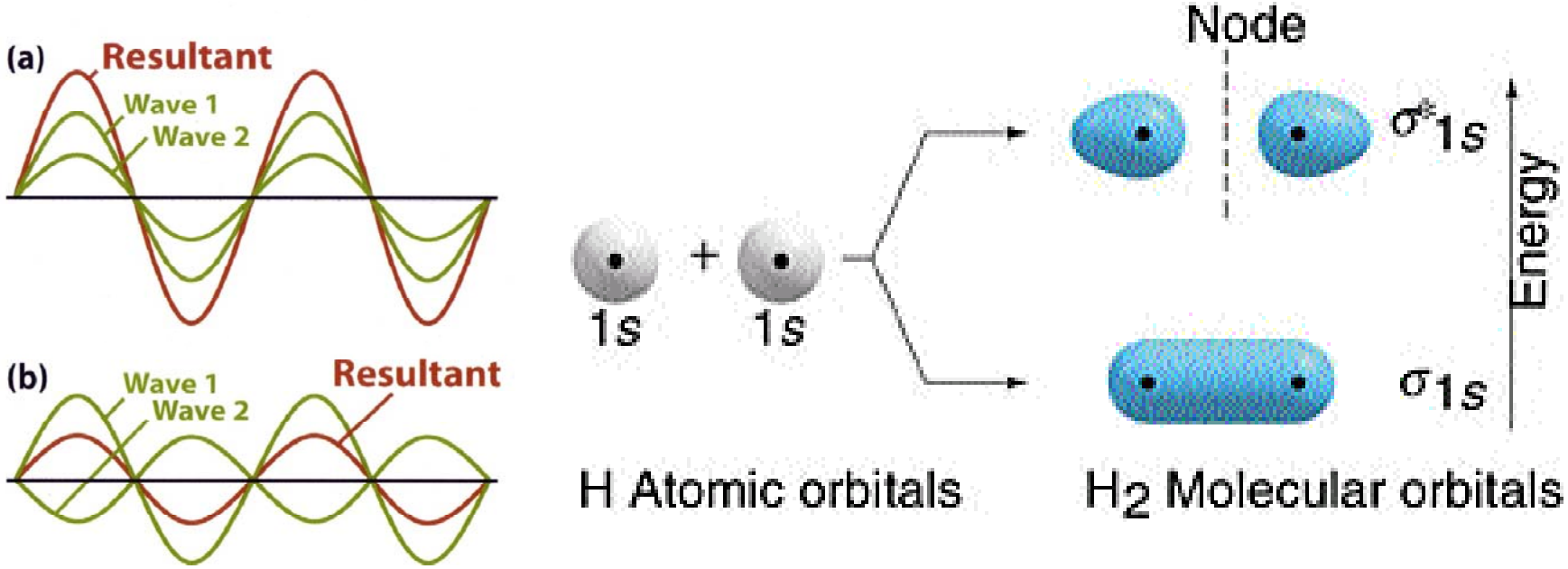
cis-1,2-dichloroethylene

trans-1,2-dichloroethylene

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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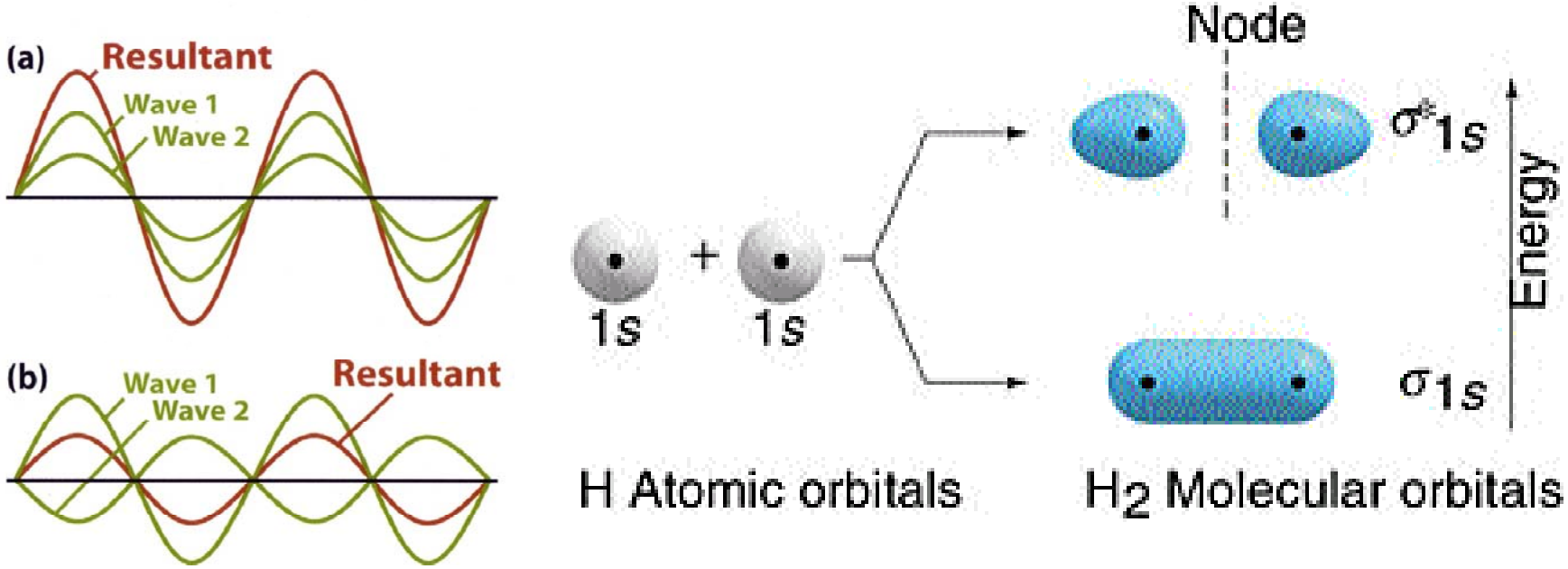
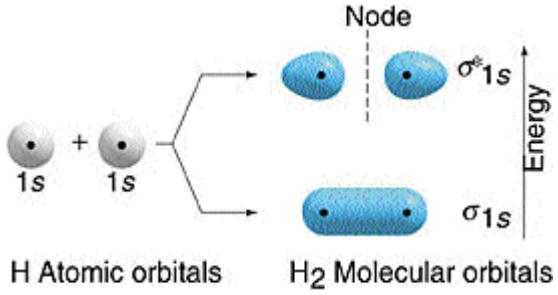
Consider H_2



Molecular Orbital Theory

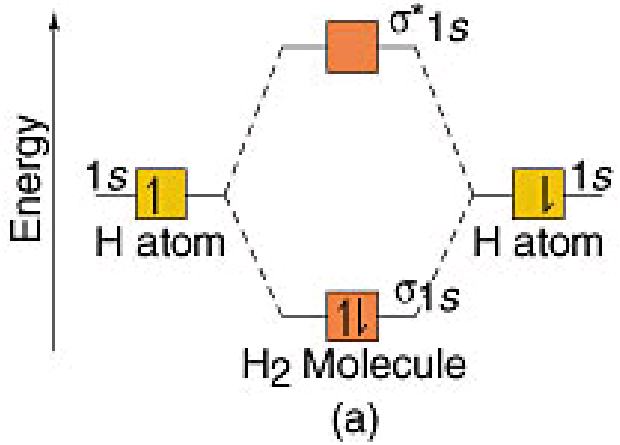


The total number of molecular orbitals created equal the total number of atomic orbitals used.

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.

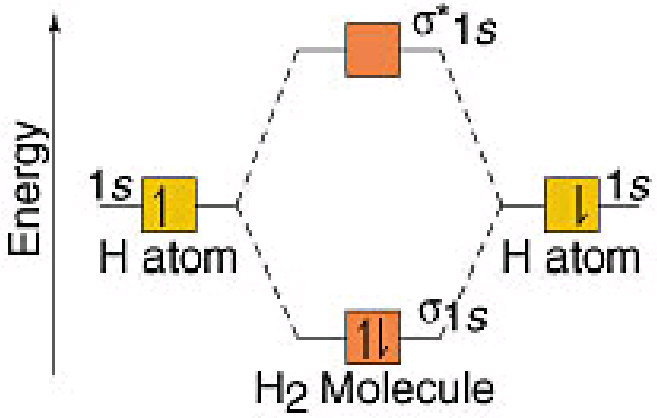
sigma-star (σ*) bond – anitbonding molecular orbital centered around internuclear distance.

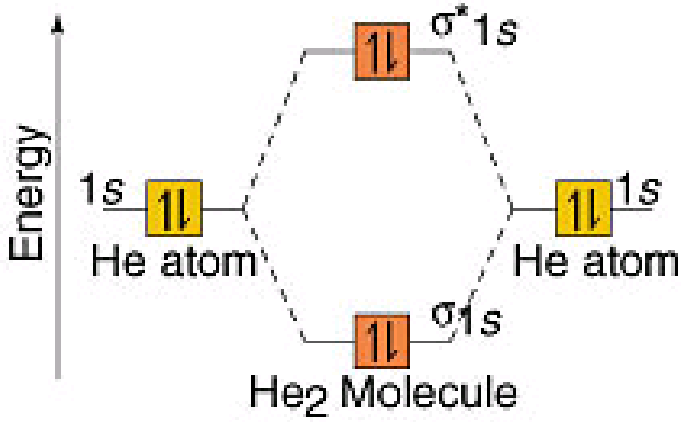
1s – denotes the character of the atomic orbitals that make up the molecular orbitals.

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?