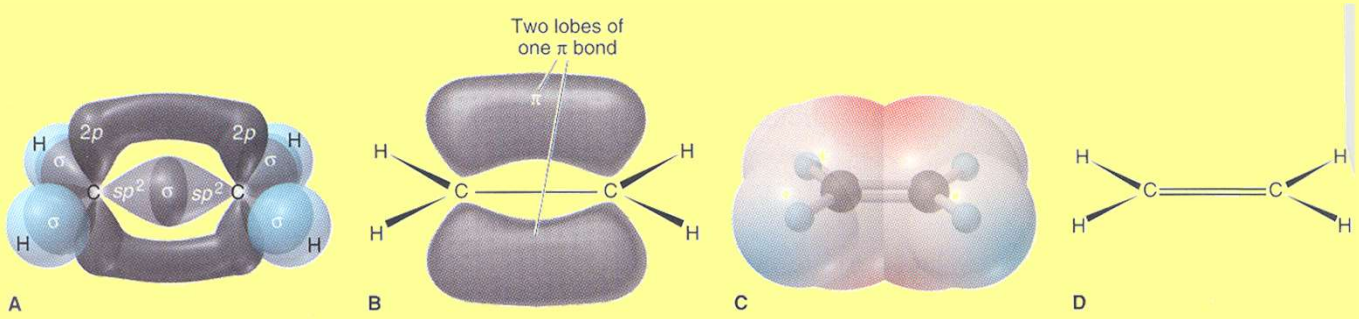
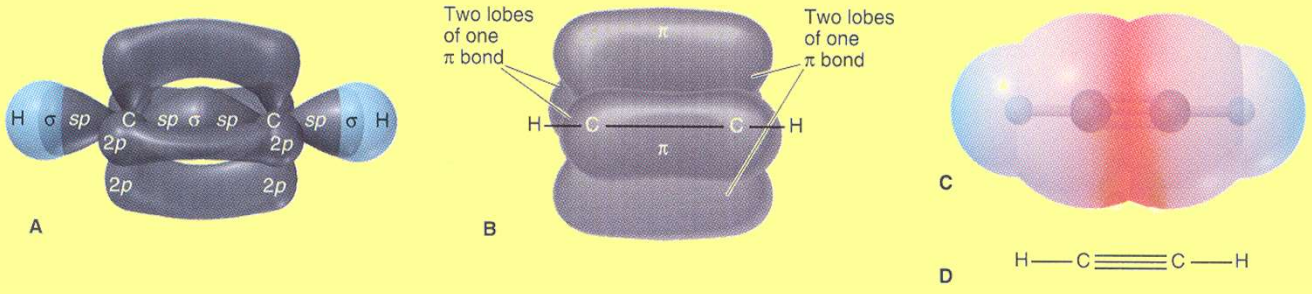


Chapter 11

Sections 11.1 & 11.2

Valence Bond Theory

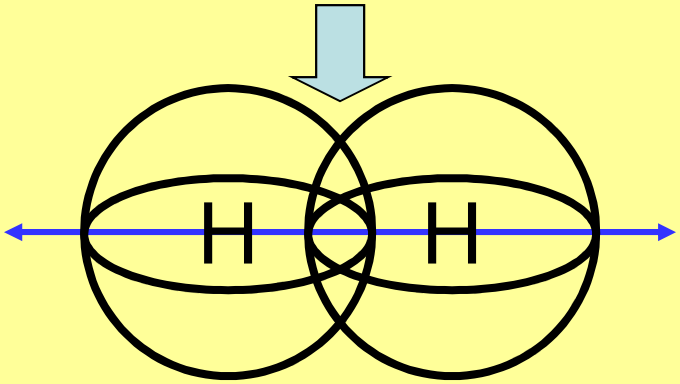
No assigned problems
substitute molecular modeling lab activity



Sigma(σ) Bonds: On-axis Overlap

H_2

Sigma (σ) Bond
1s – 1s overlap on axis.

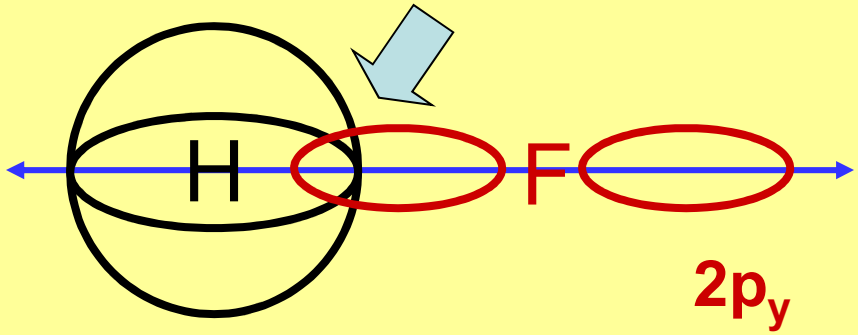


1 s orbital **1 s orbital**

$H \overset{\sigma}{—} H$

HF

Sigma (σ) Bond
1s – 2p overlap on axis.



axis

1 s orbital

$2p_y$ orbital

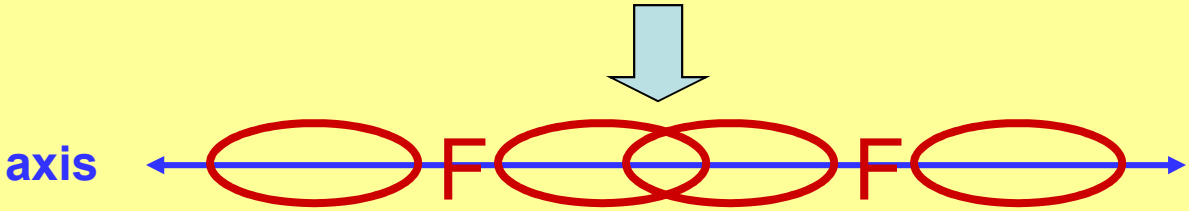
$H \overset{\sigma}{—} F$

Sigma Bonds: On Axis Overlap

F_2

Sigma (σ) Bond

2p – 2p overlap on axis.



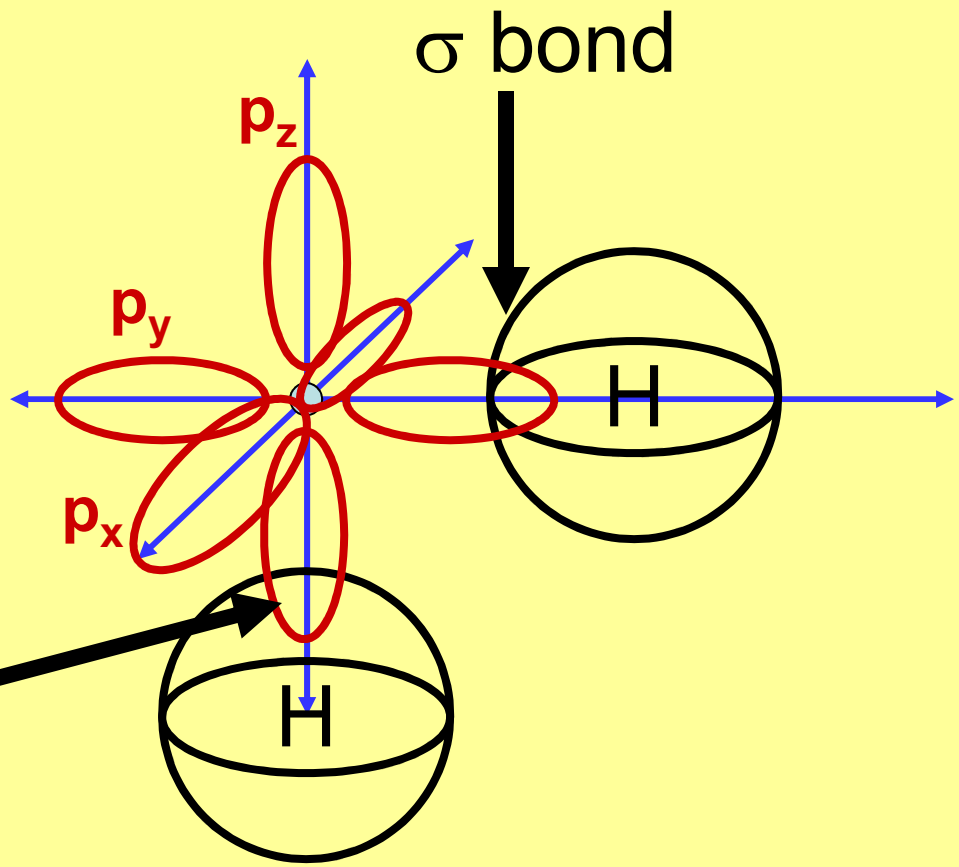
2 p_y orbital **2 p_y orbital**

F — σ — F

Sigma Bonds: On Axis Overlap

H_2O

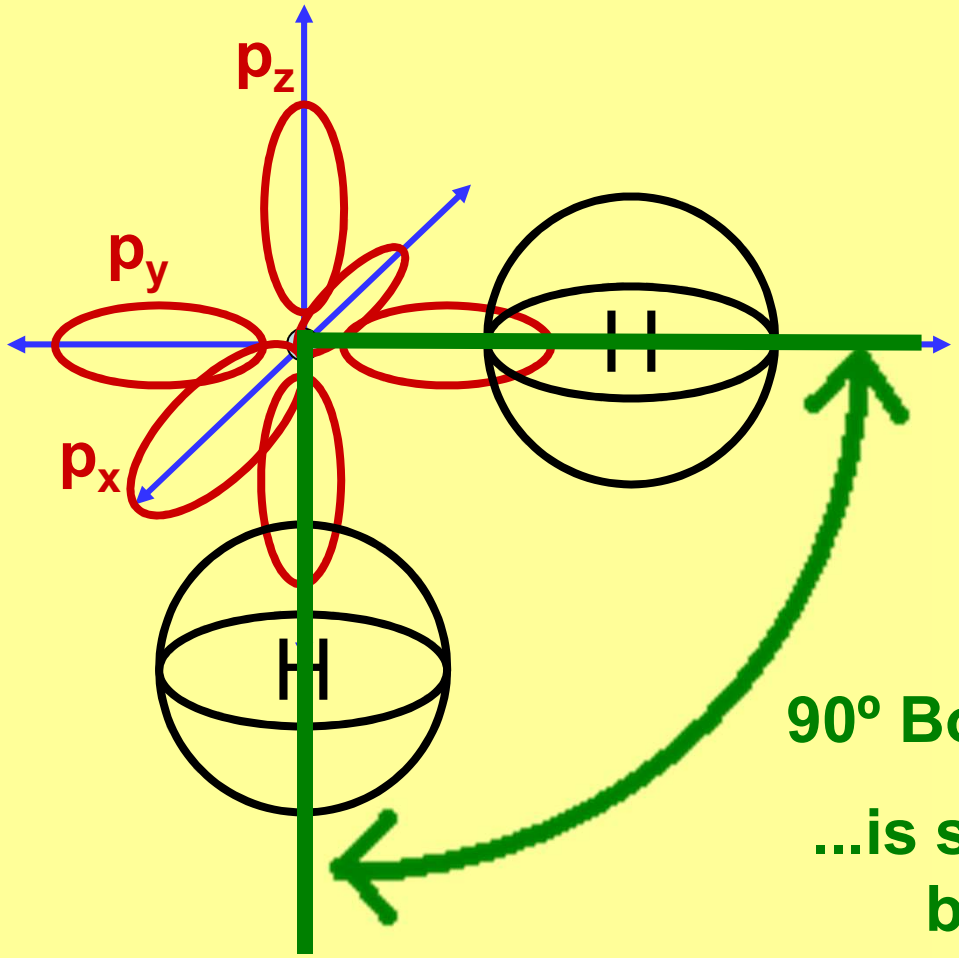
Oxygen p orbitals



...but something is wrong here!!!

Sigma Bonds: On Axis Overlap

H_2O

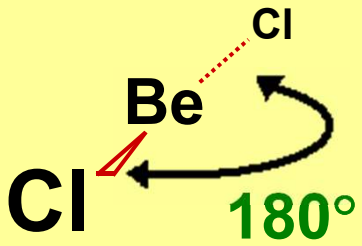


90º Bond Angle!

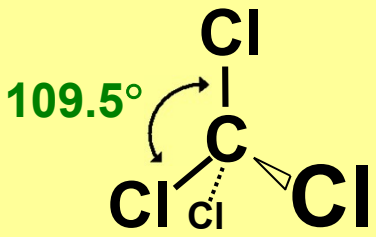
...is supposed to be 104.5º

We can't get ALL of the molecular geometries from atomic orbital overlap!

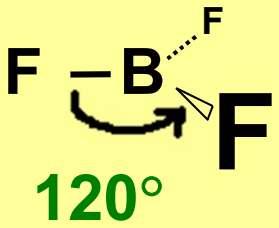
How can the required geometries be obtained using atomic orbitals?



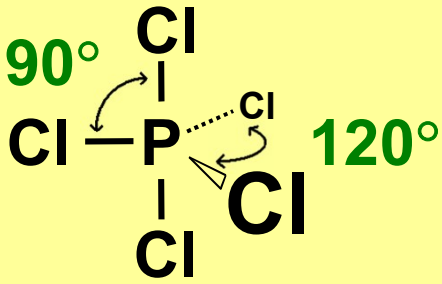
Linear



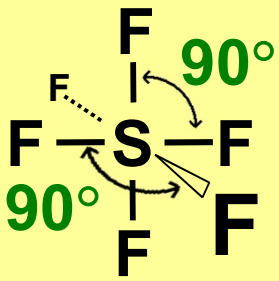
Tetrahedral



Trigonal Planar



Trigonal Bipyramidal

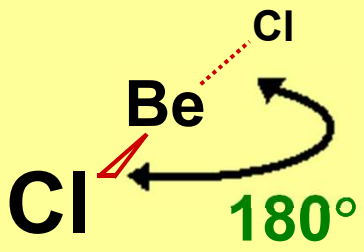


Octahedral

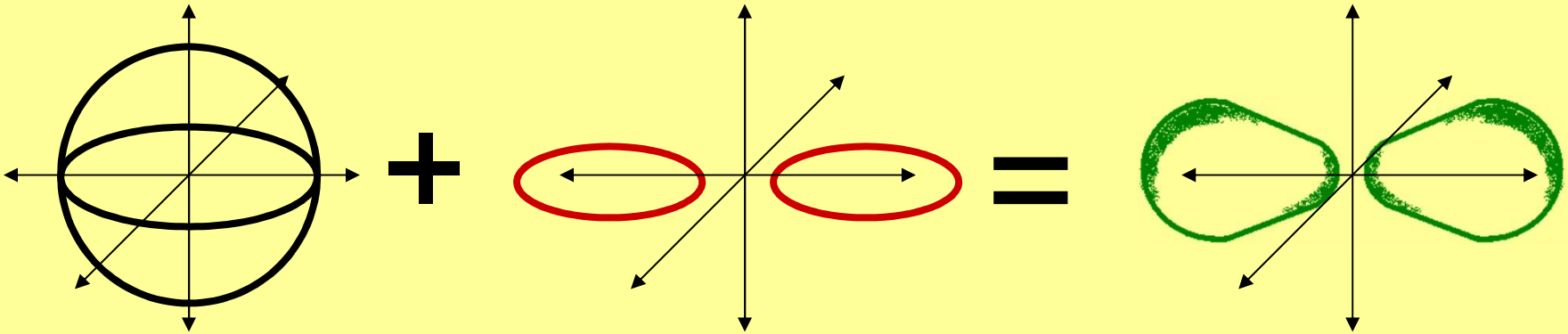
Valence Bond Theory:

New Geometries From *Blended* Atomic Orbitals

$BeCl_2$:



Linear



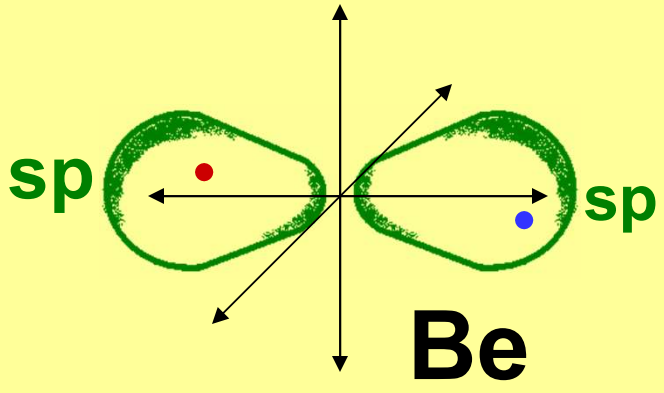
Be
2 s orbital

Be
2 p_y orbital

Be
sp hybrid orbital

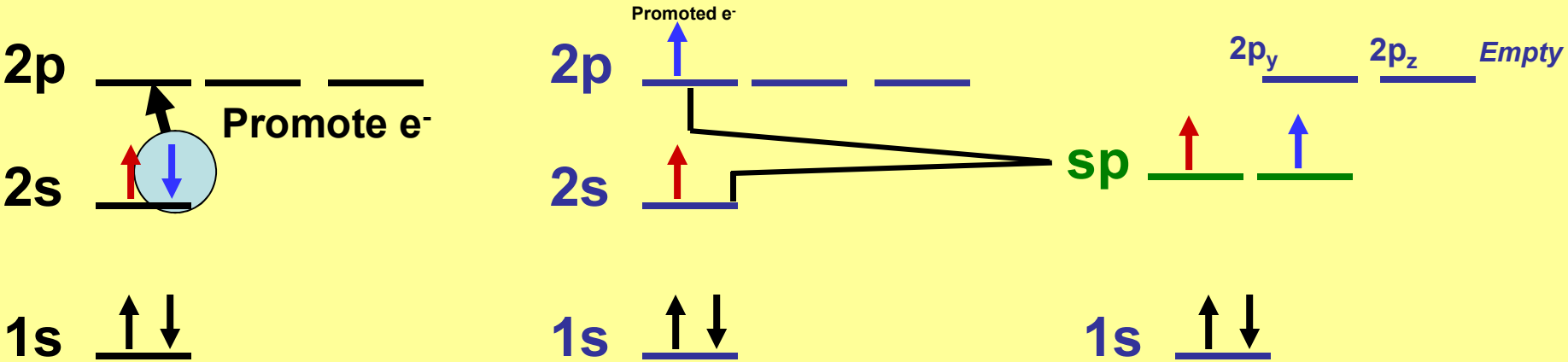
Valence Bond Theory:

ENERGIES



$BeCl_2$: ***Linear (sp)***

Be: e^- configuration: $1s^2 2s^2$



Ground State E-Level Diag

No unpaired e^- ⇒ No possible bonds!

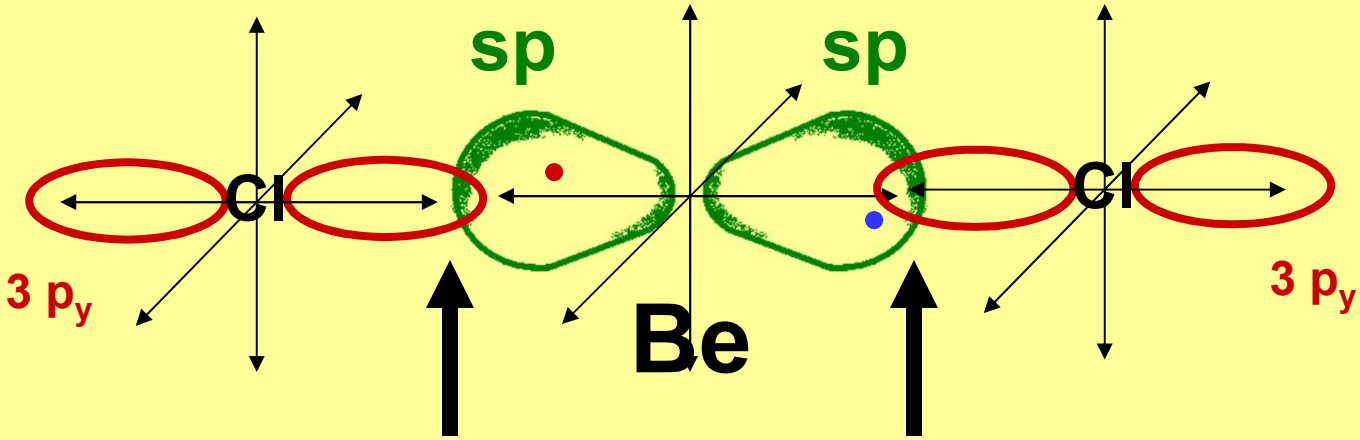
Promoted State E-Level Diag

2 unpaired e^- ⇒ 2 possible bonds

Hybrid State E-Level Diag

2 sp hybrid levels form 2 bonds

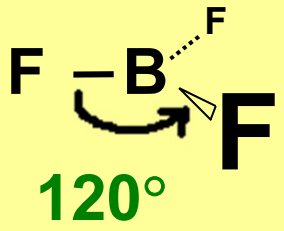
$BeCl_2$: Two σ Bonds

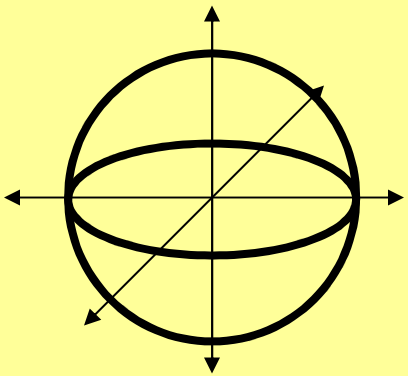


Valence Bond Theory:

Getting New Geometries From Atomic Orbitals

BF_3: ***Trigonal Planar***

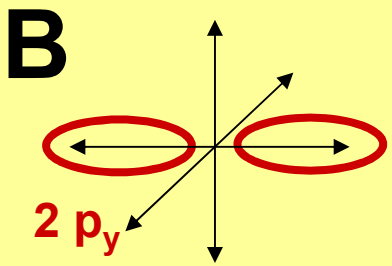


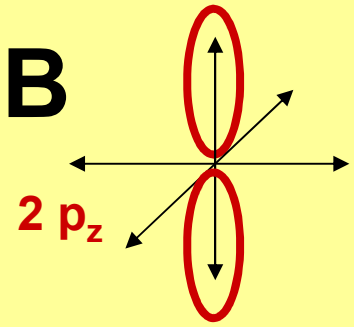


B

2 s orbital

+





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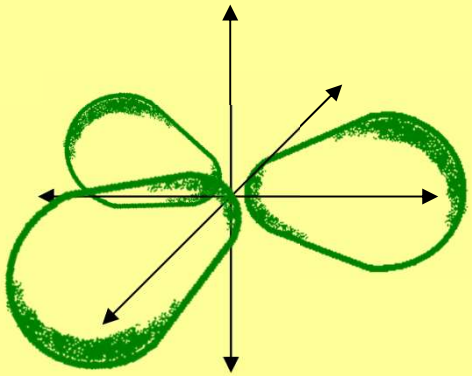


B

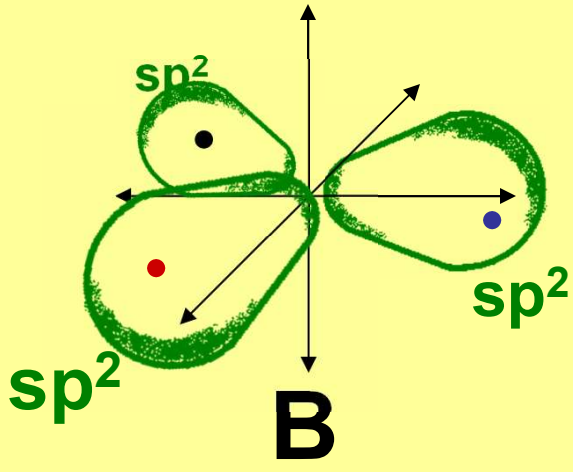
sp^2 hybrid orbital

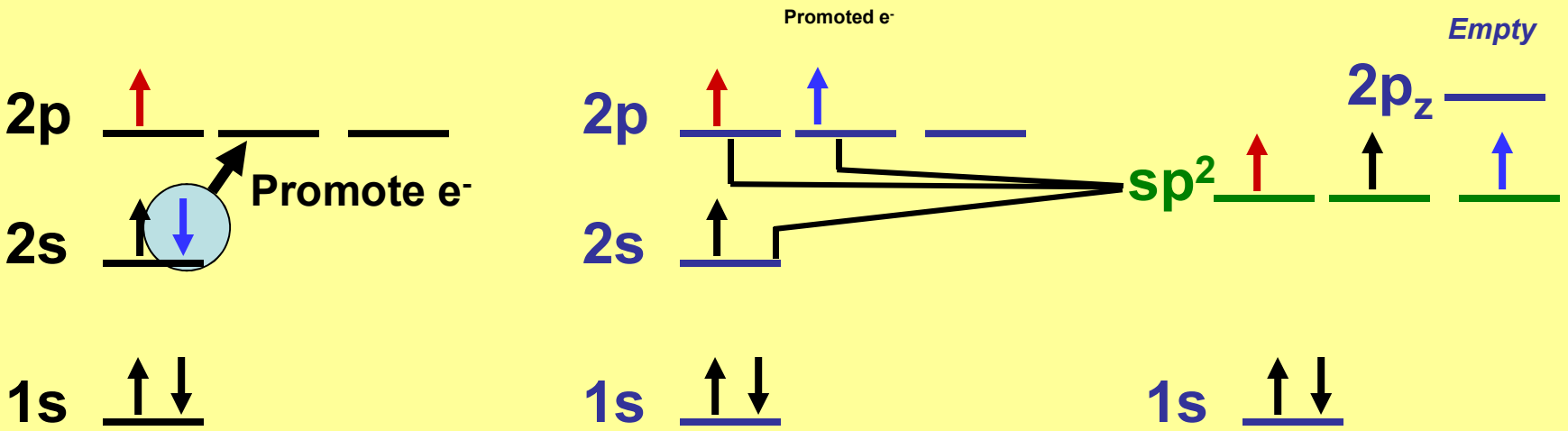
Valence Bond Theory:

ENERGIES

BF_3: ***Trigonal Planar (sp^2)***

B: e^- configuration: $1s^2 2s^2 2p^1$





1s ↑↓

Ground State E-Level Diag

1 unpaired e^- ⇒ 1 possible bond

1s ↑↓

Promoted State E-Level Diag

3 unpaired e^- ⇒ 3 possible bonds

1s ↑↓

Hybrid State E-Level Diag

3 sp^2 hybrid levels form 3 bonds

BF_3: Three σ Bonds