Chemical Bonding 4.8

Valence Bond Theory

Hybrid Orbital Theory

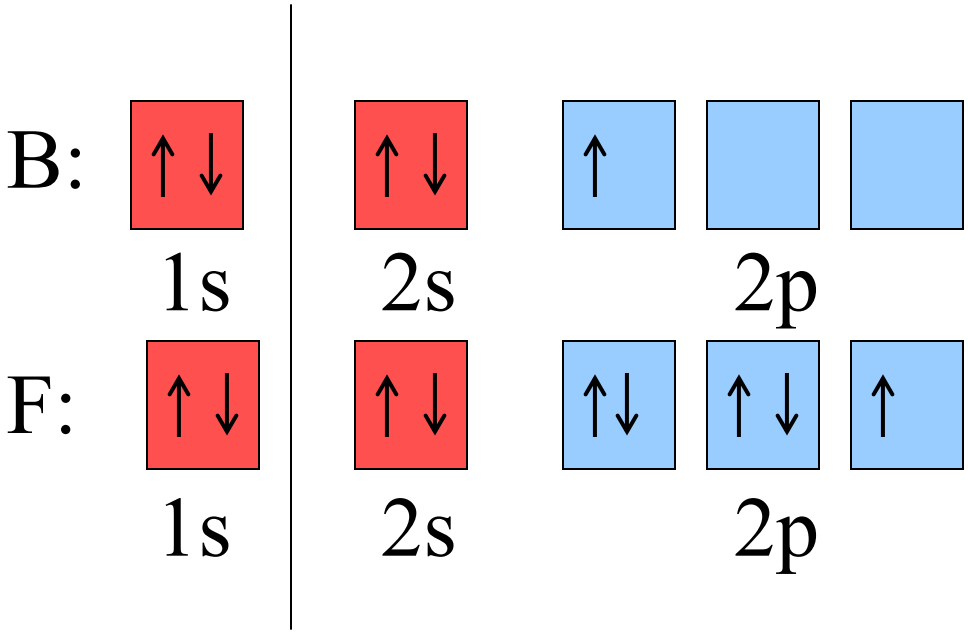
Multiple Bonds

Valence Bond Theory

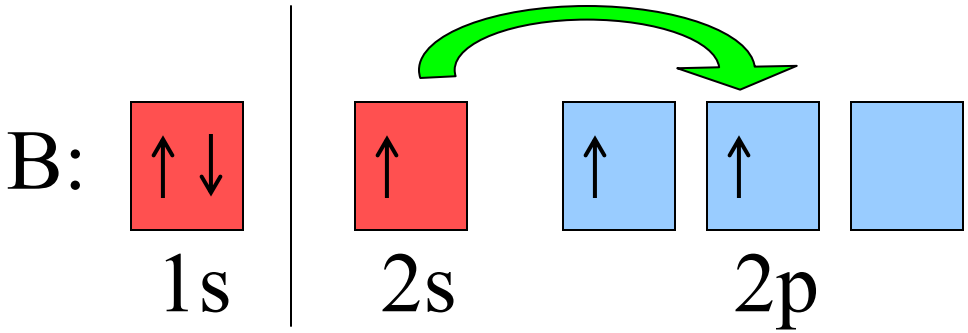
- Combines Lewis' theory of filling octets by sharing pairs of electrons with the electron configuration of atomic orbitals.

- Valence Bond Theory states that bonding occurs when atomic orbital overlap.

Building BF_3 with Valence Bond Theory

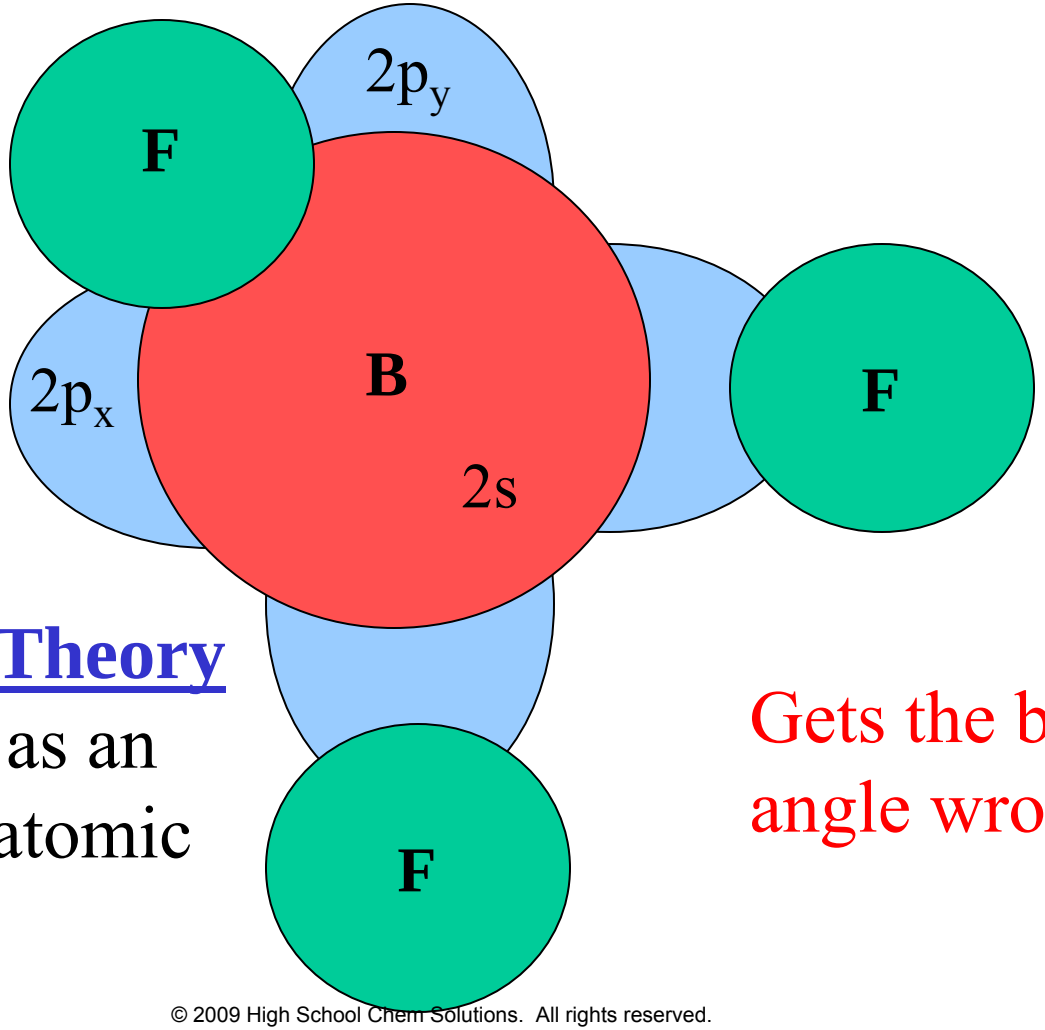


Building BF_3 with Valence Bond Theory



Boron enters an excited state where an electron from the 2s orbital is promoted to the $2p_y$ orbital.

Valence Bond Theory has problems with the shape



Valence Bond Theory

Views bonding as an overlapping of atomic orbitals.

Gets the bond angle wrong

Problems with Valence Bond Theory and BF_3

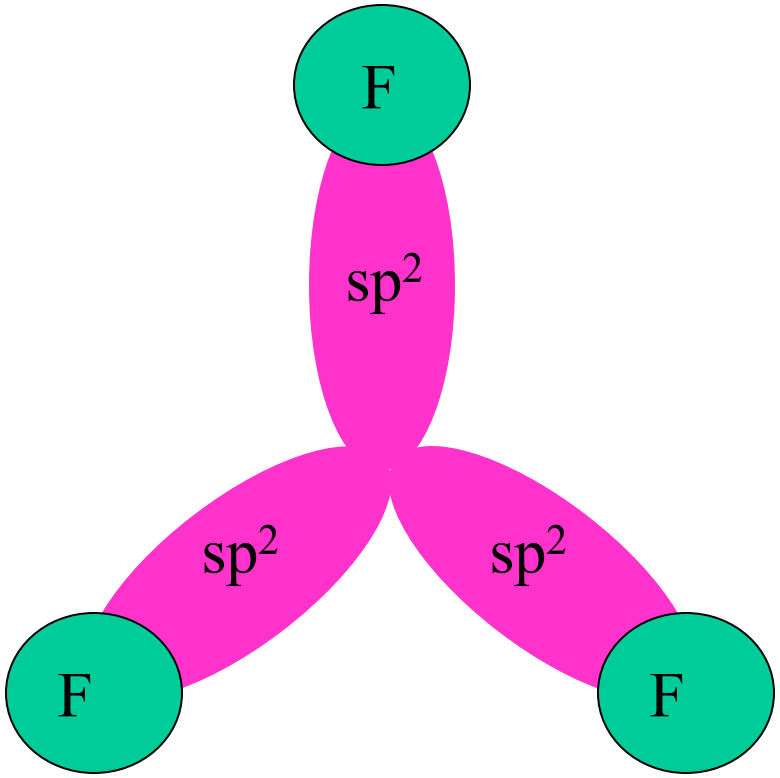
Problem (the bond angle is wrong)

- Valence Bond Theory says 90^o and a random angle for the fluorine bonded to the s-orbital.
- VSEPR theory says 120^o

Solution (Hybrid Orbitals)

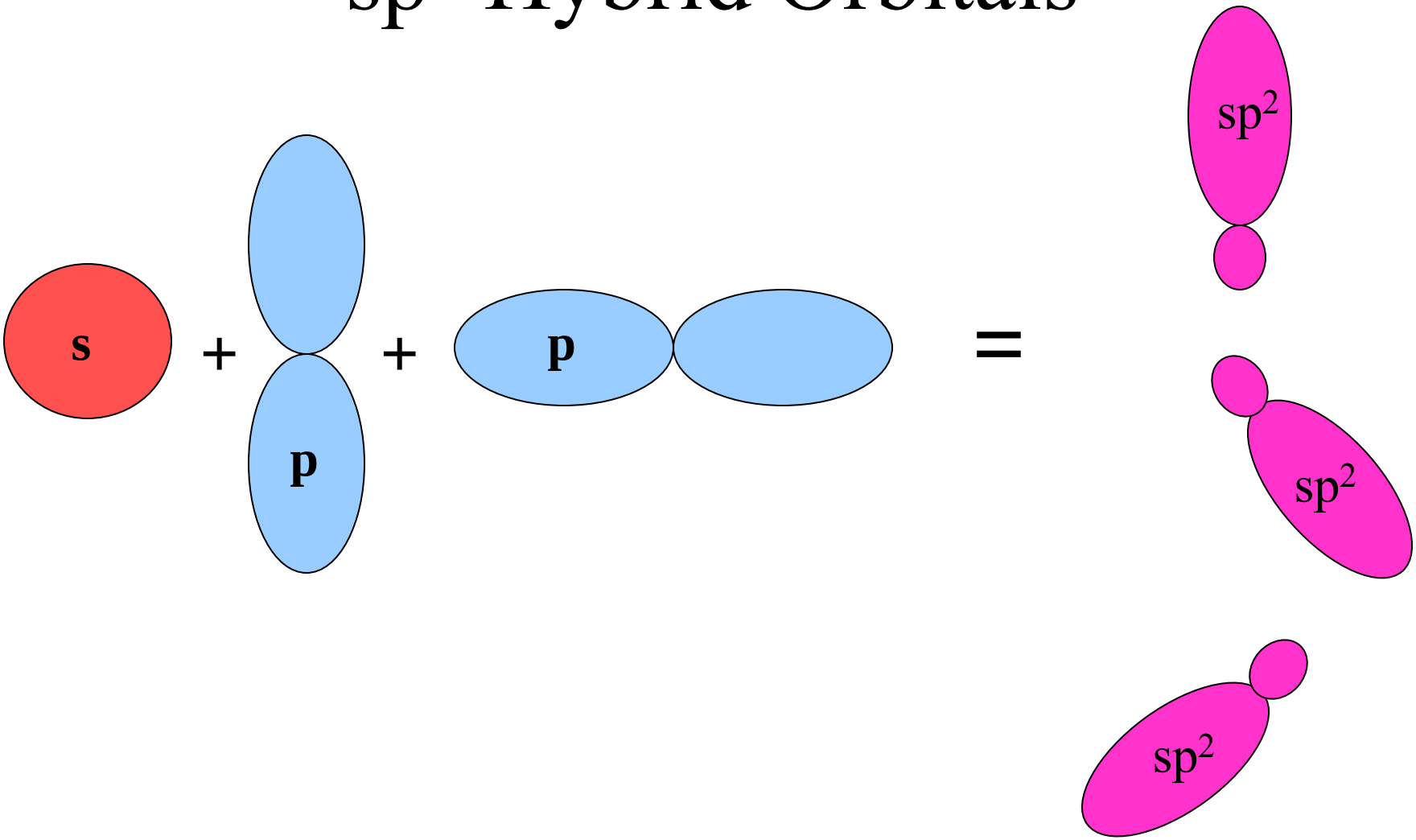
- When the electron is promoted, the 2s, $2p_x$, and $2p_y$ orbitals of boron morph into three separate **sp^2 hybrid orbitals** that are identical in shape and size.

sp^2 Hybrid Orbitals

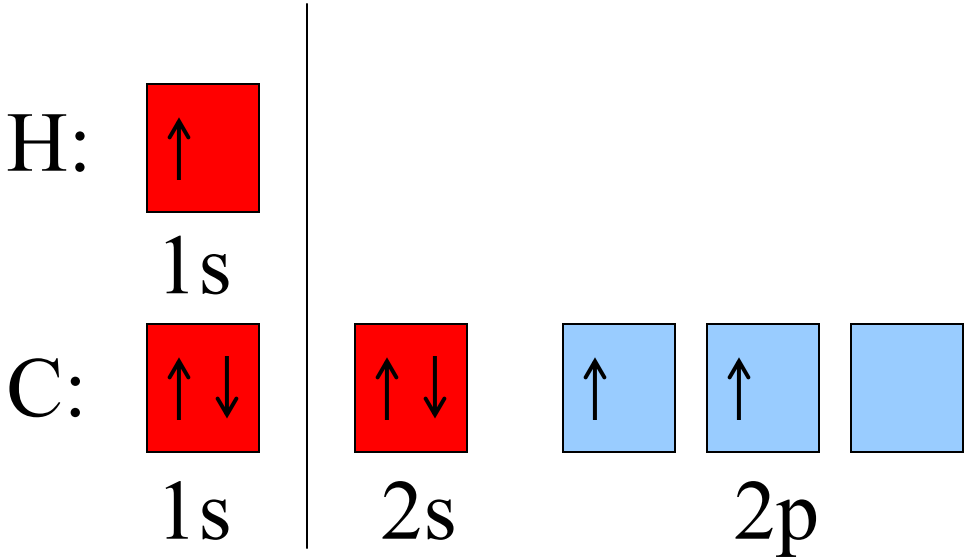


The 2s and two 2p orbitals morph into three identical sp^2 hybrid orbitals

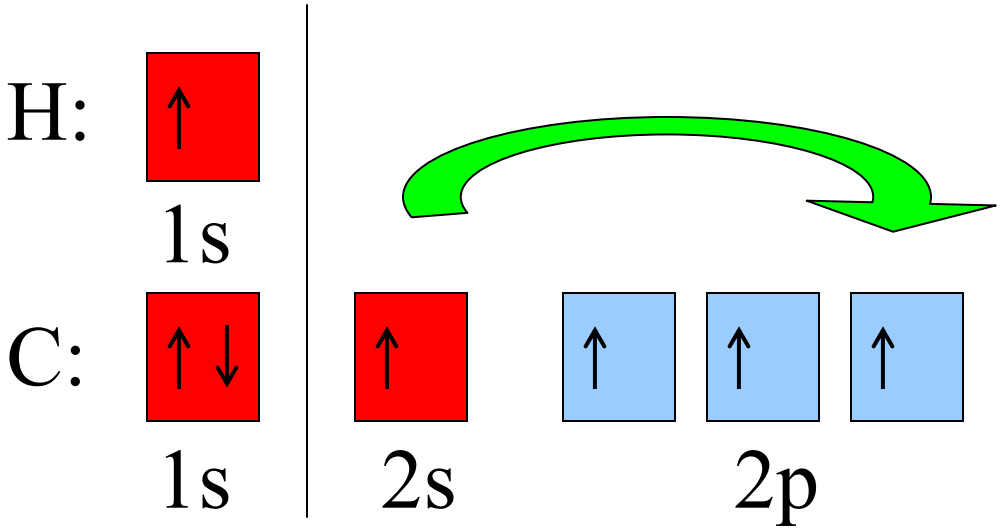
sp^2 Hybrid Orbitals



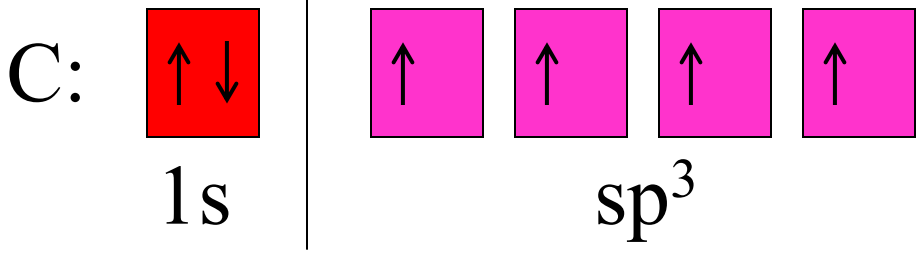
sp^3 Hybrid Orbitals (e.g. CH_4)



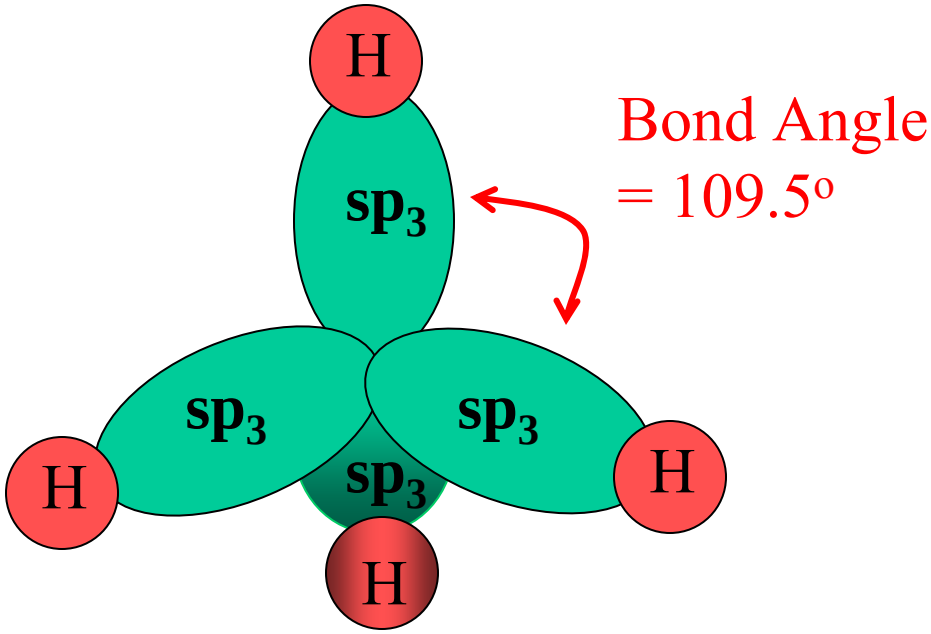
sp^3 Hybrid Orbitals (e.g. CH_4)



Hybridization of Carbon

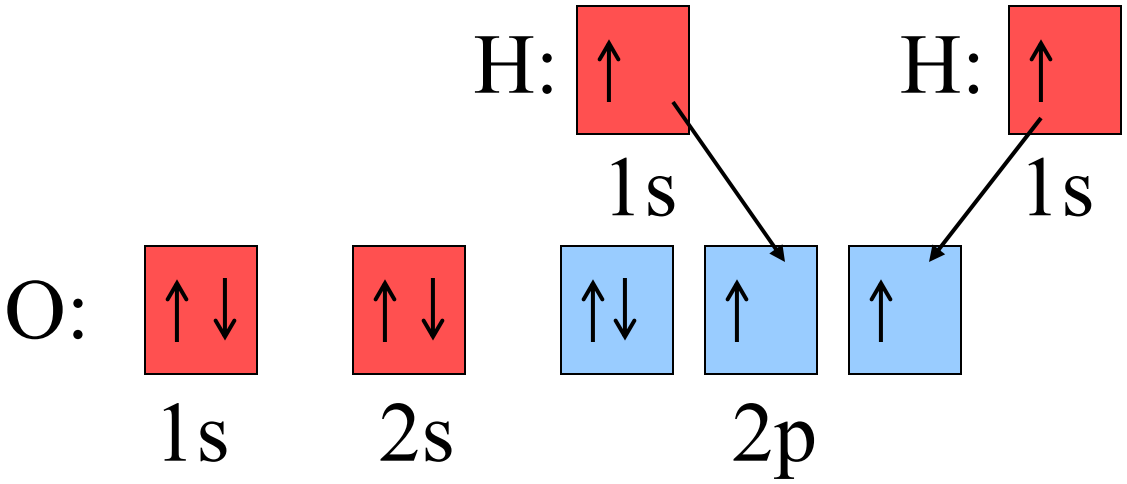


sp^3 Hybrid Orbitals (e.g. CH_4)



Valence Bond Theory and Lone Pairs (e.g. H_2O)

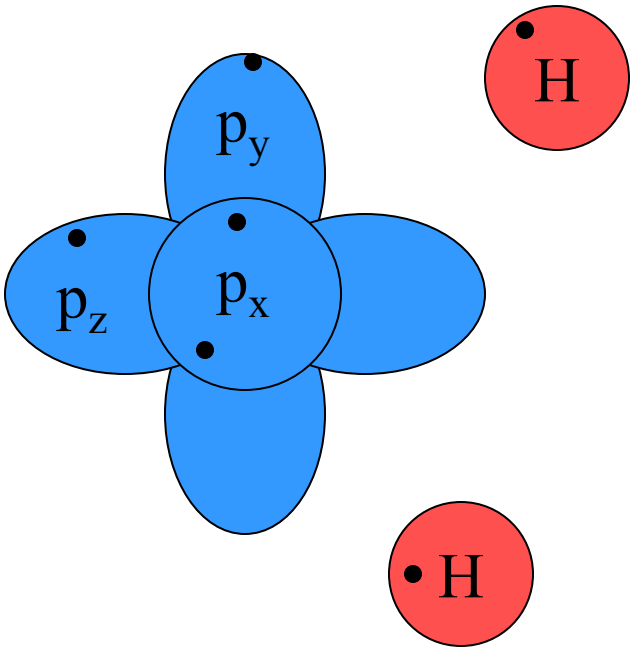
Building H_2O with **Valence Bond Theory**

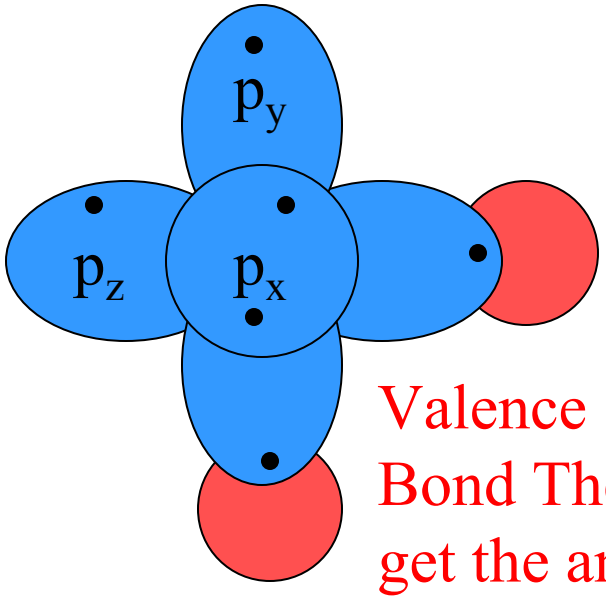


Oxygen could accept one electron from one Hydrogen in its p_y orbital and another from the other Hydrogen in its p_z orbital.

Valence Bond Theory and Lone Pairs (e.g. H_2O)

- Valence Bond Theory views bonding as an overlapping of atomic orbitals.



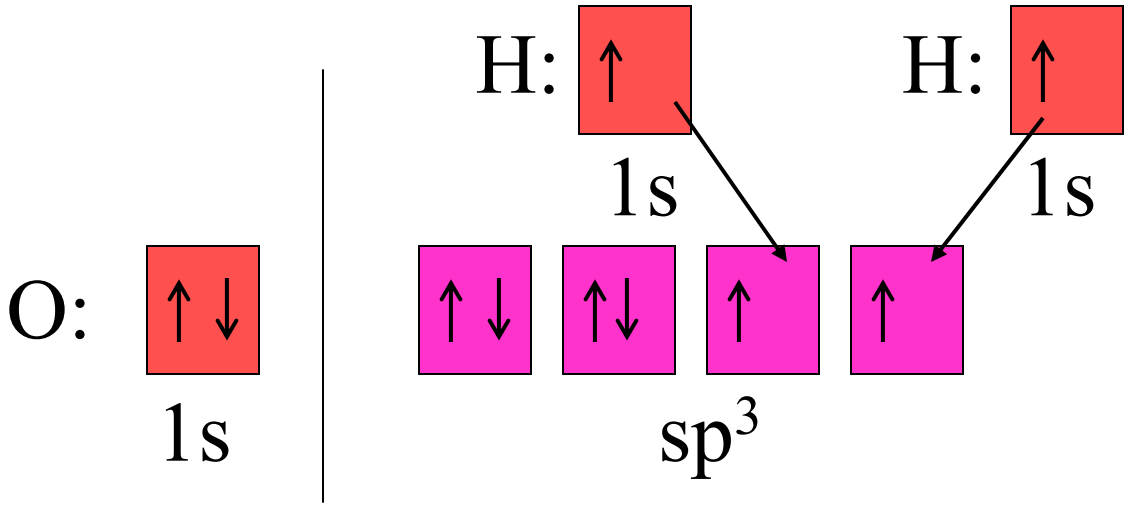


Valence Bond Theory get the angle wrong again!

Problems with Valence Bond Theory in the H_2O Example

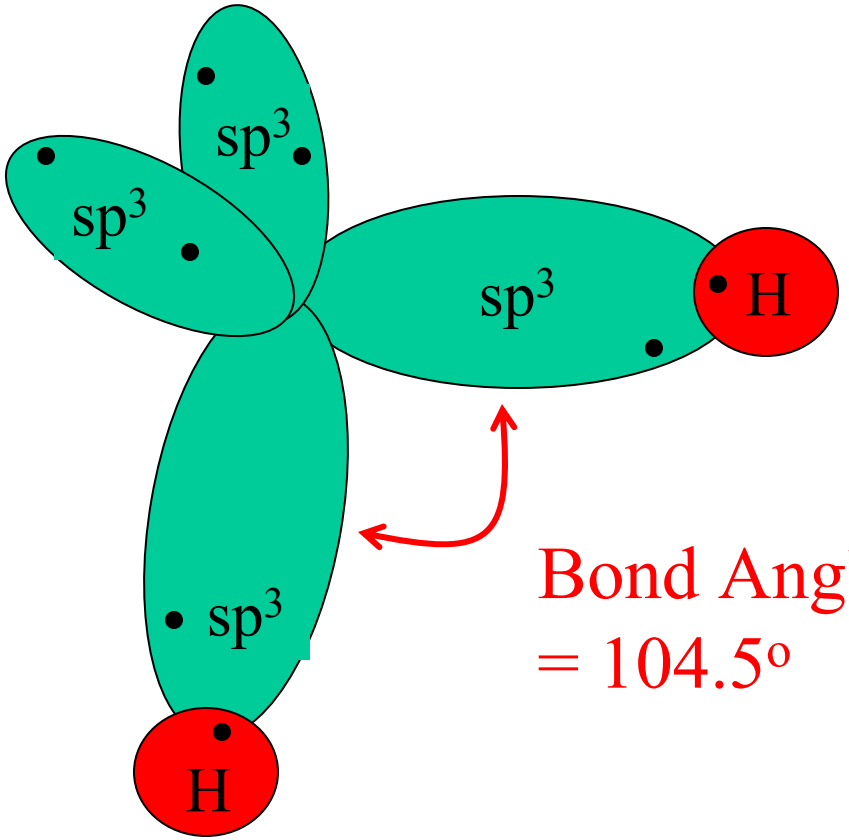
- The bond angle is wrong.
  - Valence Bond Theory predicts 90^o
  - VSEPR Theory predicts 104.5^o
- The orbital shape must be wrong.
  - Shared electrons are not spending enough time with the Hydrogen.

Hybrid Orbital Theory and Lone Pairs (e.g. H_2O)



Electrons are not promoted here, but every orbital in the $n = 2$ energy level becomes hybridized.

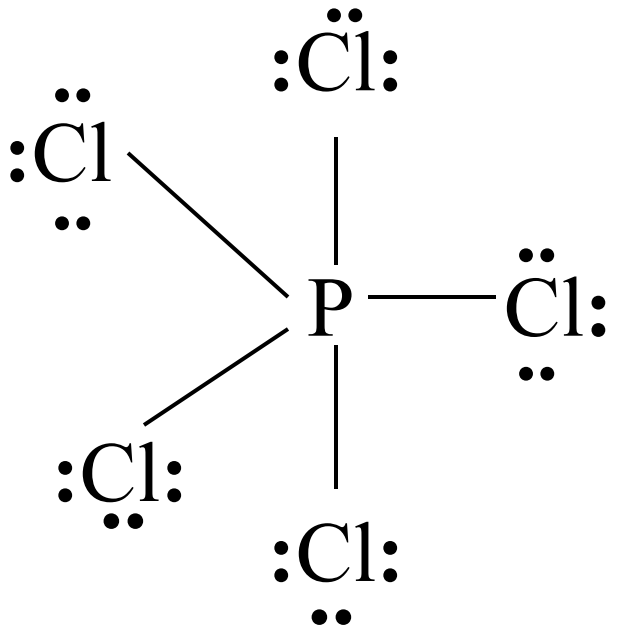
sp^3 Hybrid Orbitals (H_2O)



Four sp^3 hybrid orbitals are formed

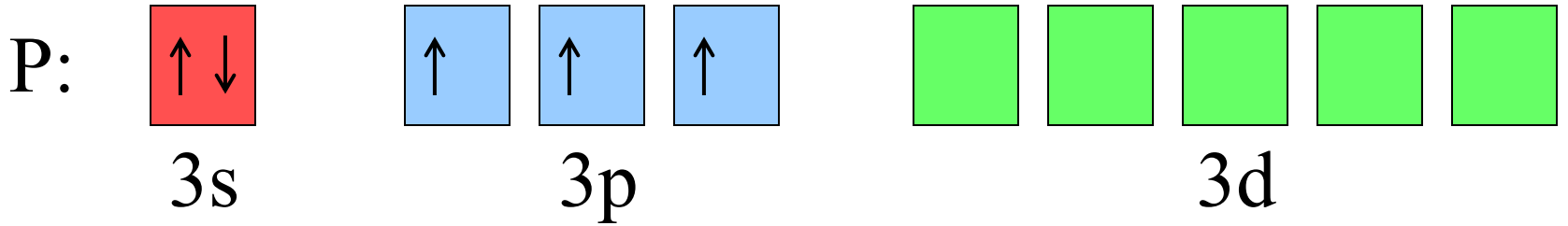
Bond Angle = 104.5°

Hybrid Orbital Theory and 5 Charge Clouds! (e.g. PCl_5)

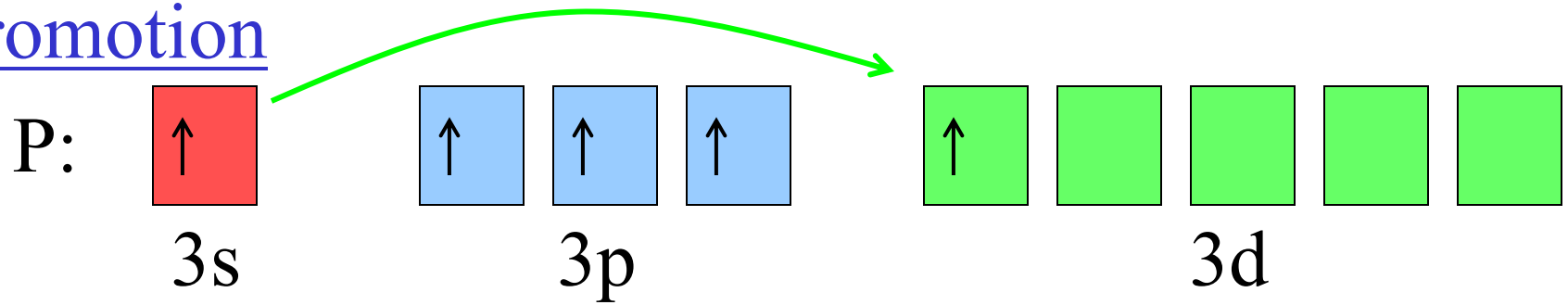


sp^3d Hybrid Orbitals

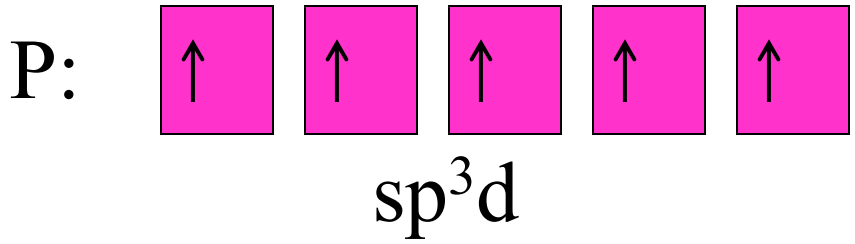
Atomic Orbitals



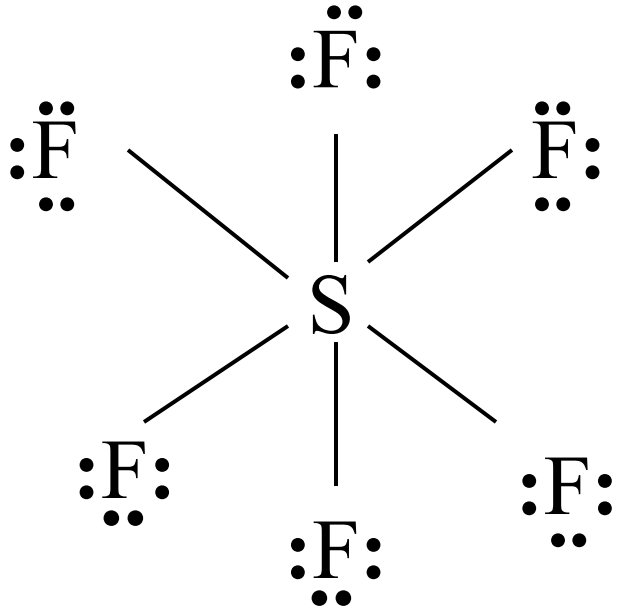
Promotion



Hybridization

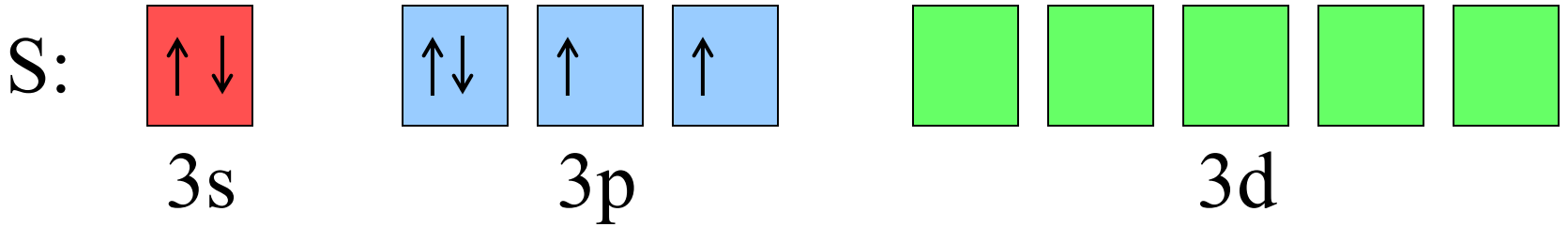


Hybrid Orbital Theory and 6 Charge Clouds! (e.g. SF_6)

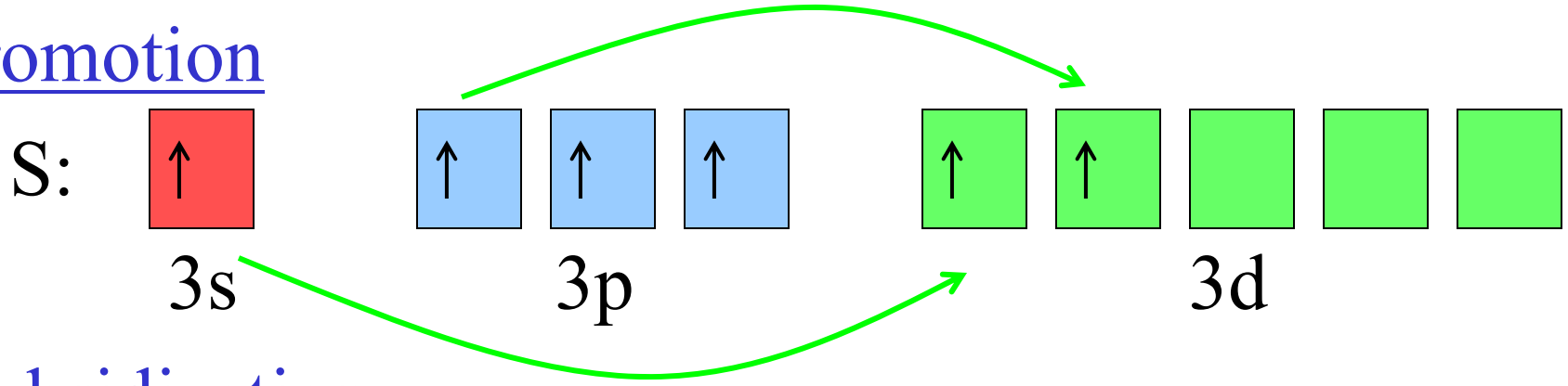


sp^3d^2 Hybrid Orbitals

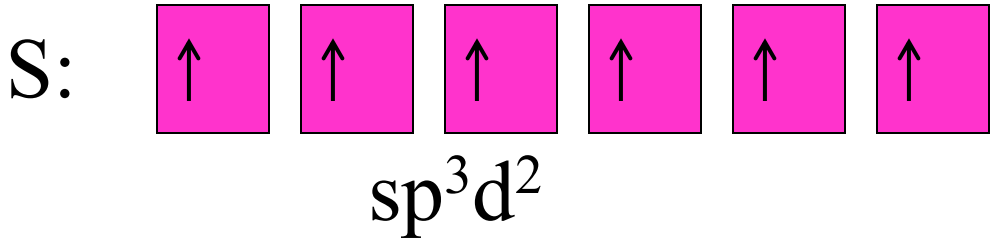
Atomic Orbitals



Promotion



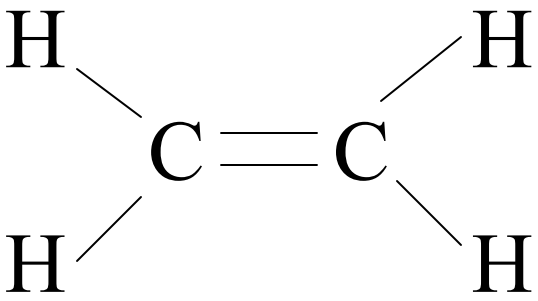
Hybridization



Summary

Charge Clouds	Hybridization
2	sp
3	sp^2
4	sp^3
5	sp^3d
6	sp^3d^2

Double Bonds (e.g. C_2H_4)

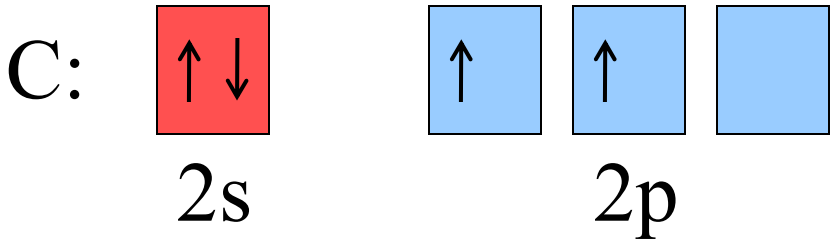


Each carbon has 3 charge clouds.

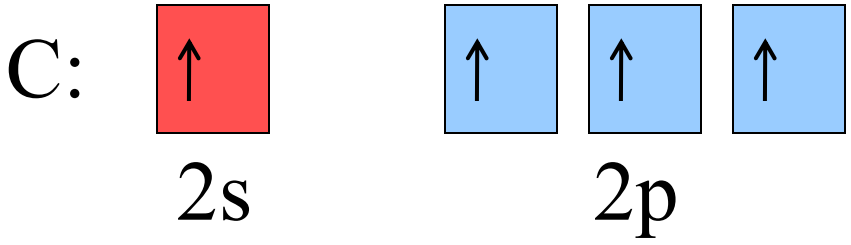
sp^2 hybrid orbitals

Double Bonds (e.g. C_2H_4)

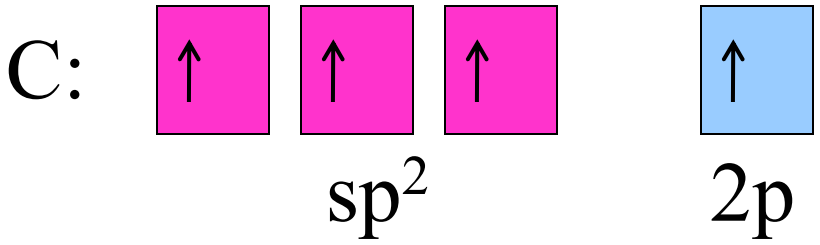
Atomic Orbitals



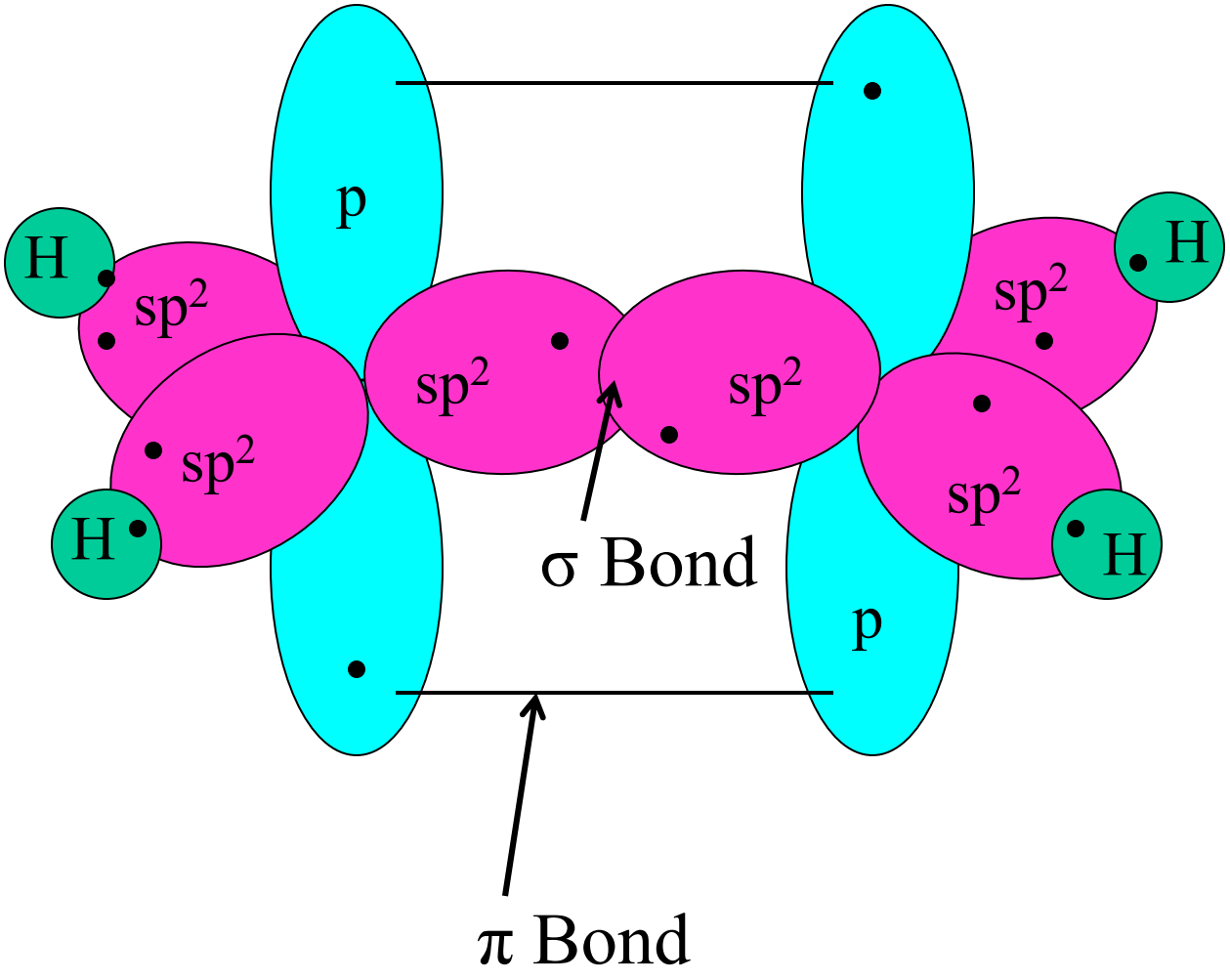
Promotion



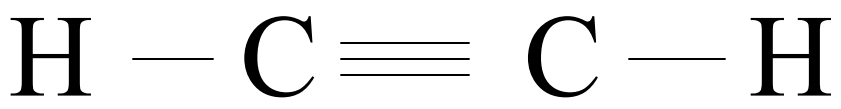
Hybridization



Double Bond (C_2H_4)



Triple Bonds (e.g. C_2H_2)

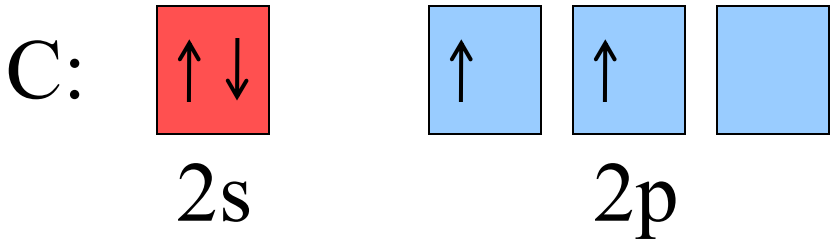


Each carbon has two charge clouds.

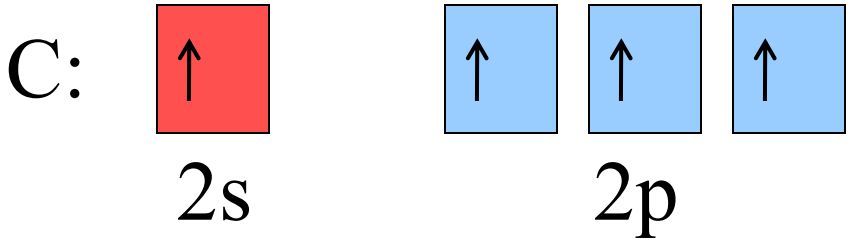
sp hybrid orbitals

Triple Bonds (e.g. C_2H_2)

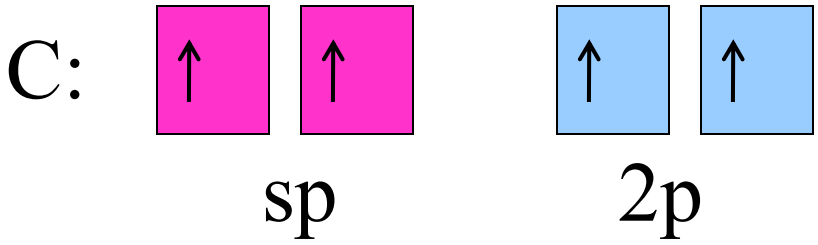
Atomic Orbitals



Promotion



Hybridization



Triple Bond (C_2H_2)