Chem 201 – Day 5
WTh, Sept 12-13

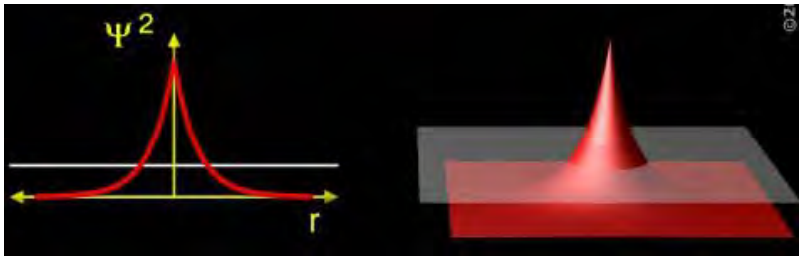
Bond Orbital Model

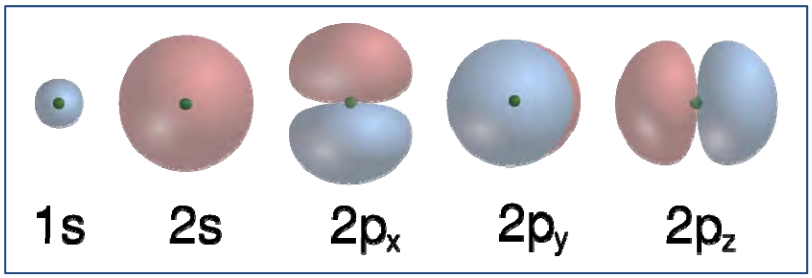
Hybrid Orbitals

Polar Bonds II

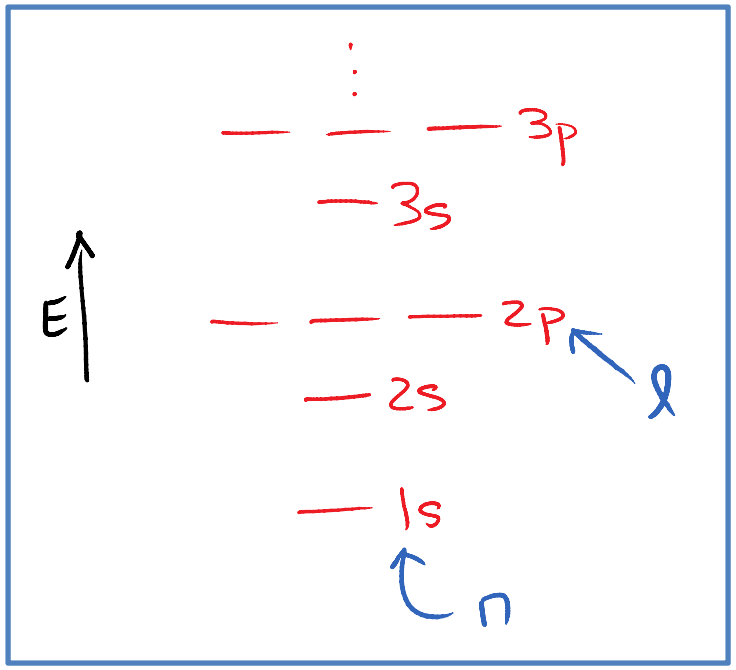
Things You Already **Know**

- Atomic Orbitals
  - Amplitudes
  - Probability = Amp^2



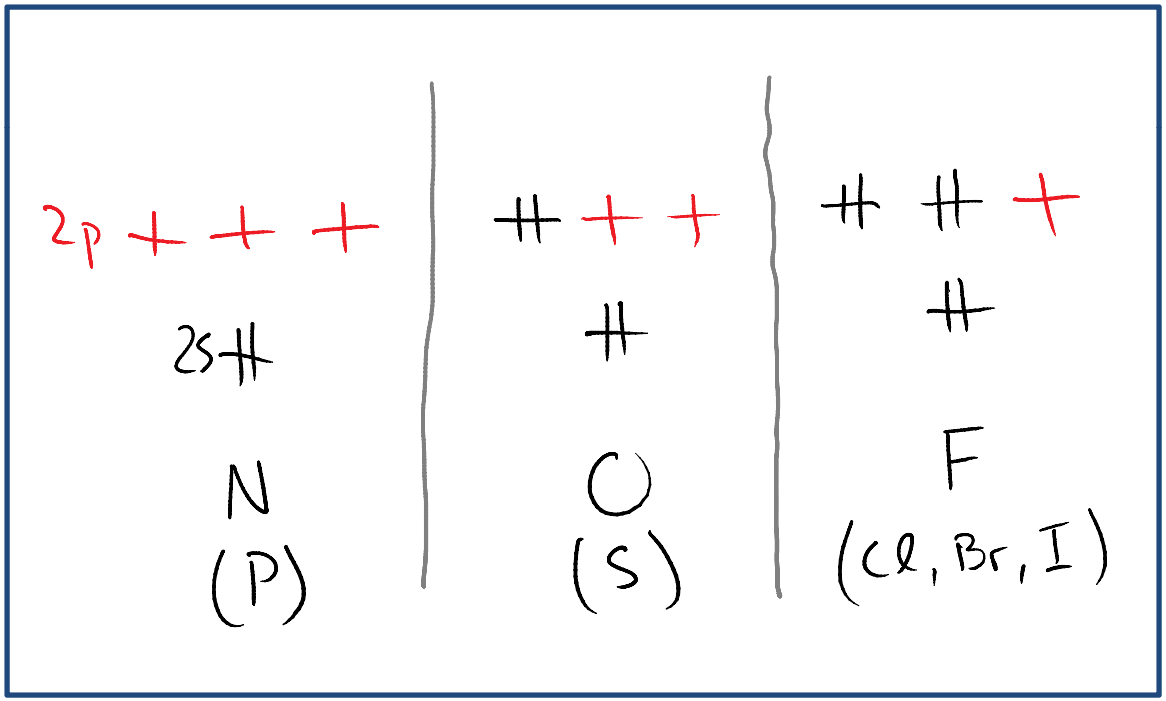


- Atomic Orbital Energies
  - *n* (principal) Q#
    - *Distance*
  - *l* (ang. momentum) Q#

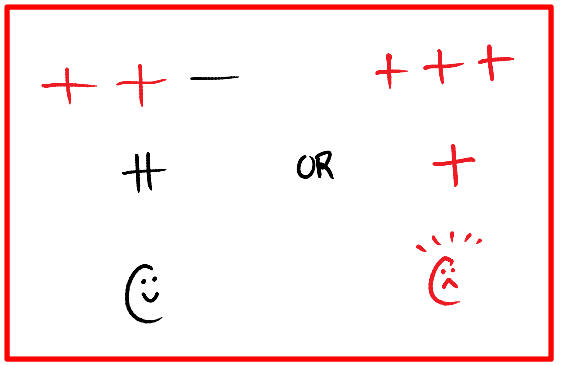


Things You **Already** … Pt. 2

- Bonds result from half-filled AOs

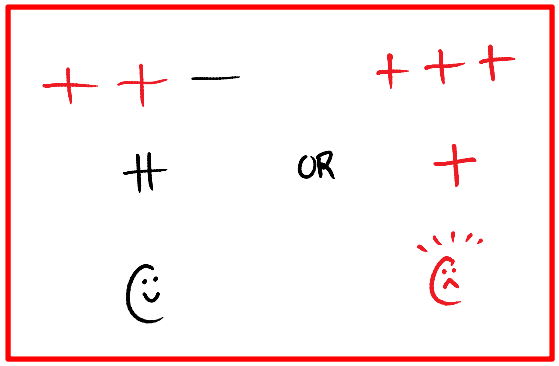


but not C doesn't fit the paradigm?



Things **You** … Pt. 3

- If C makes only 2 bonds
  - 2 downhills
- If C "promotes" electron (uphill) then makes 4 bonds
  - 4 downhills

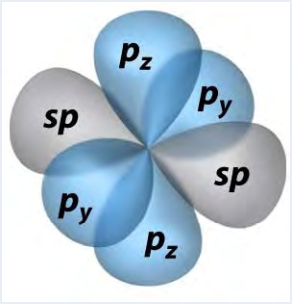
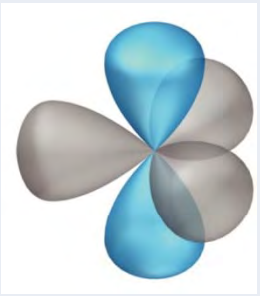
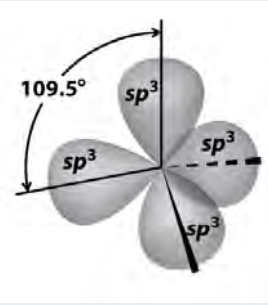


Things … Pt. 4

- C (and others) use hybrid orbitals
  - Choose hybrids to fit geometry (#ED, steric#)
  - 4 ED → sp^3 hybridized atom
  - 3 ED → sp^2 hybridized atom → *pictures*
  - 2 ED → sp hybridized atom

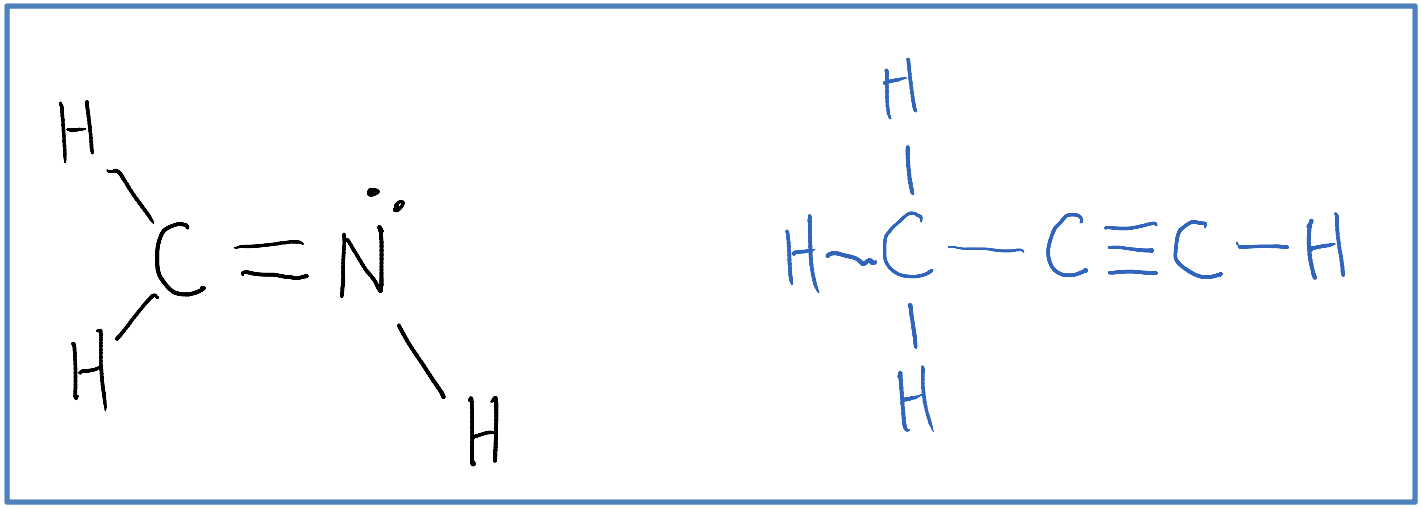
Hybrid Orbital (3 Options)

- Hybrid orbital direction → good overlap

AO	sp HO	sp^2 HO	sp^3 HO
2p ↑ ↑ ↑ 2s ↑	2p ↑ ↑ sp ↑ ↑ 50% p ⇧	2p ↑ sp^2 ↑ ↑ ↑ 67% p ⇧	sp^3 ↑ ↑ ↑ ↑ 75% p ⇧
			

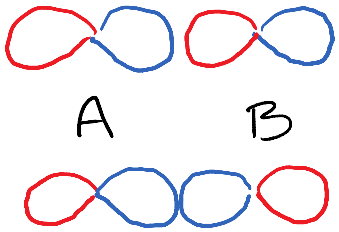
Examples

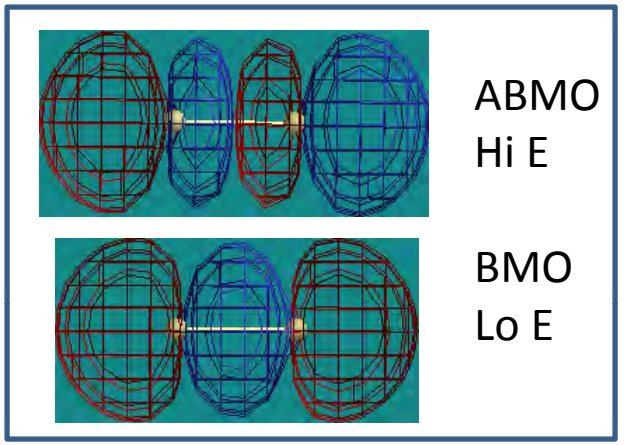
- Atom hybridizations
- Orbitals that overlap to make bonds
- Orbitals that hold lone pairs



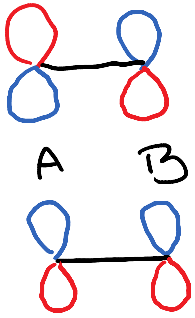
Combining 2 AO Gives Bonding (BMO) and Antibonding (ABMO)

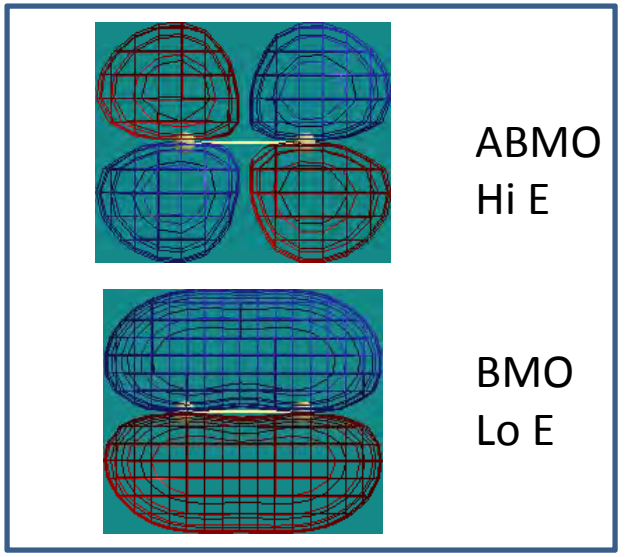
- Sigma





- Pi





- electron location
- nodes

New Stuff:
AO overlap/energy → MO energy

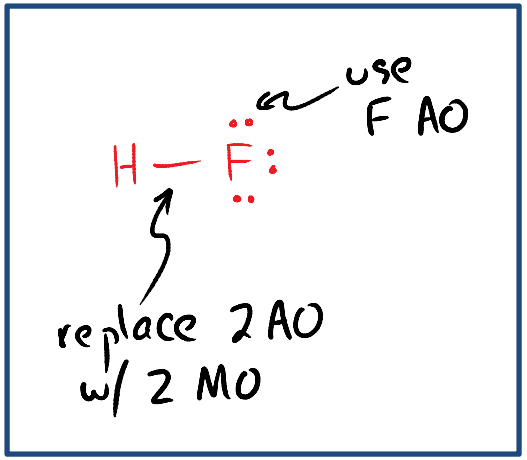
- How does electron energy change?
  - Electrons in BMO vs. ABMO
  - Good vs. bad AO overlap
  - Good vs. bad match in AO energies
- How is this connected with
  - Lewis Octet, 2-electron bond
  - Geometry
    - angles + distances + dihedral angles
    - stiffness & flexibility
  - Polarity
  - Partial Bonds (Resonance)

Electrons Have Lower PE in Molecules

- A▪ + B▪ → A-B + energy
  - bond making is always downhill
- Electrons in AO → Electrons in MO + energy
  - Replace “hi E” AO with “low energy” MO

MO Building Strategy
Molecules w/ Localized Bonds & Charges

- Build MO model for each electron pair
- Bonds
  - Model **combines** 2 AO (1 AO from each atom)
  - 2 AO **replaced** by 2 MO (BMO + ABMO)
- Lone pairs
  - Use existing AO on atom

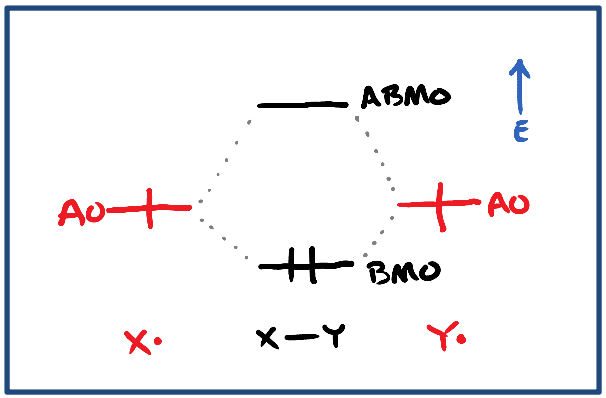


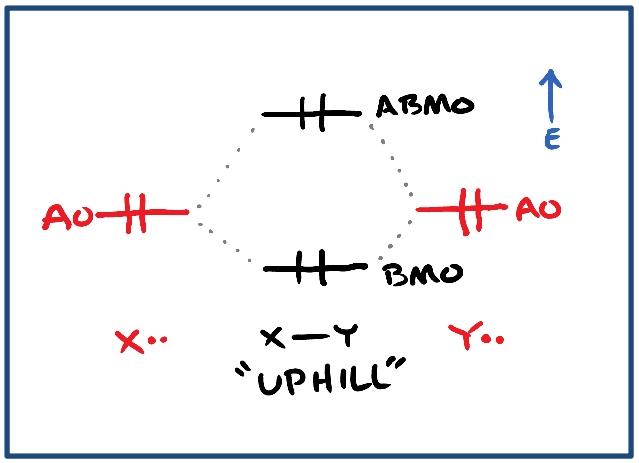
Two Conditions for **Combine/Replace**

- For 2 AO to **combine/be replaced** they
  - must **overlap**
    - Large amplitudes in same regions of space
      - **Core** AO too small
      - **Valence** AO just right
    - Must pay attention to ‘positive’ & ‘negative’ overlap
  - must have **similar energies**
    - **Valence** orbitals have similar energies
    - **Core & valence** orbitals do not

Energy Properties of New MO

- **Orbital Mixing Diagram**
  - Atomic orbital models in red
  - Molecular orbital models in black

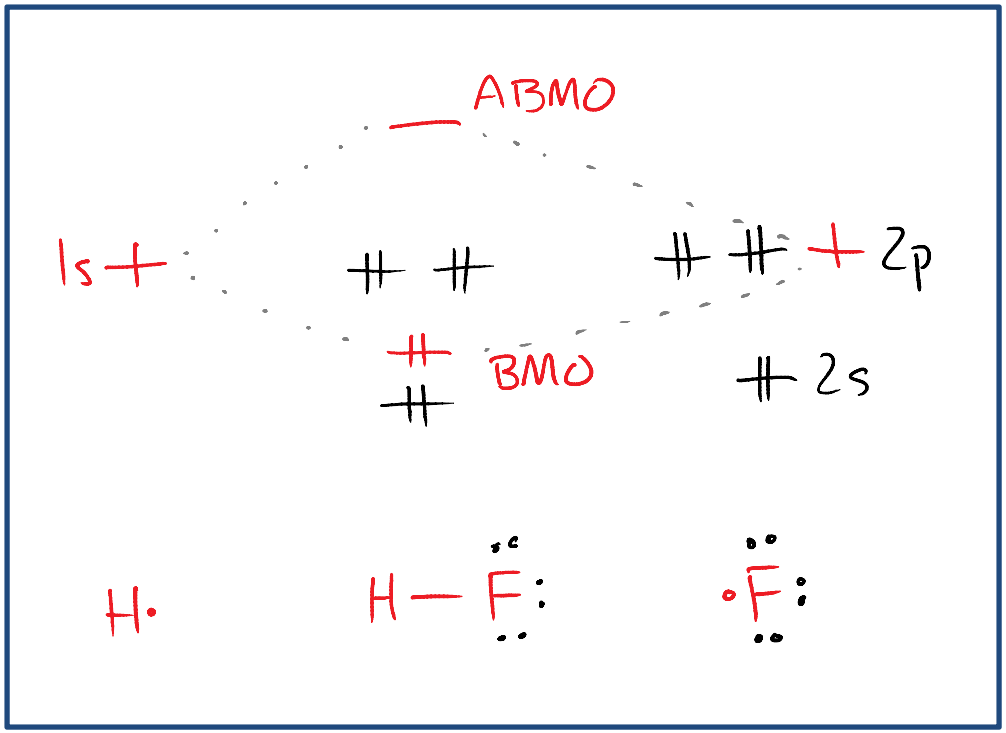




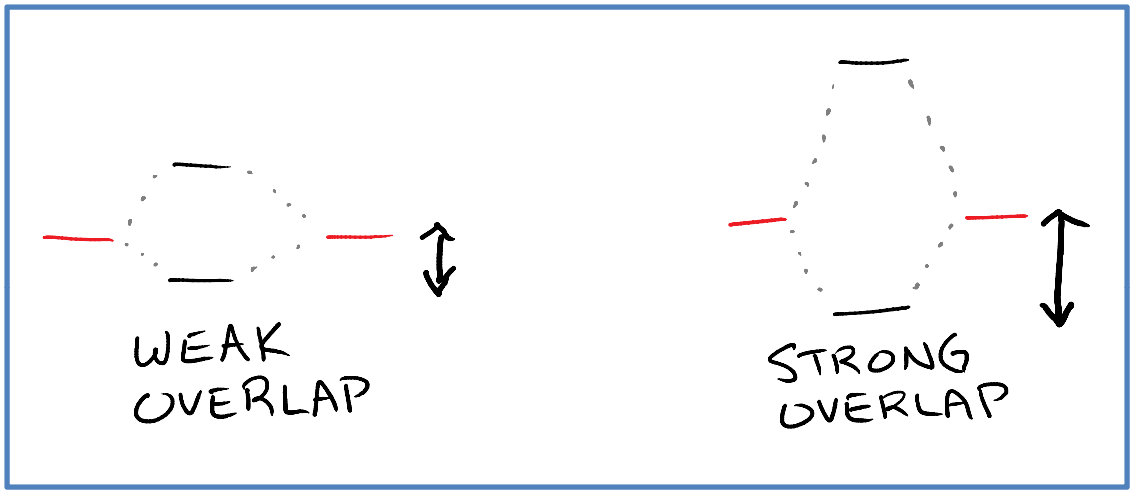
- **MO Bond** = combining half-filled AO makes filled BMO + empty ABMO

Connect with Electron Count

- H = $1s^1$
- F = $2s^2\ 2p_x^2\ 2p_y^2\ 2p_z^1$



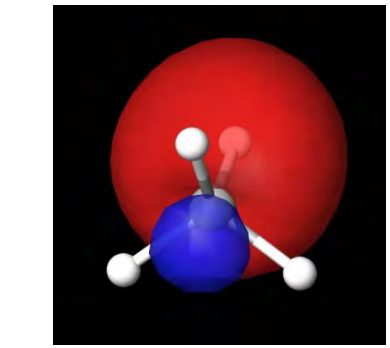
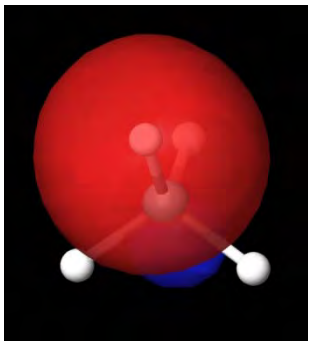
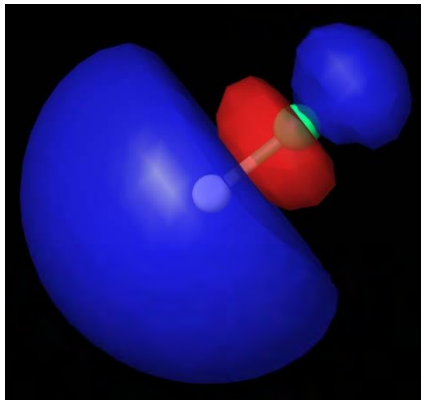
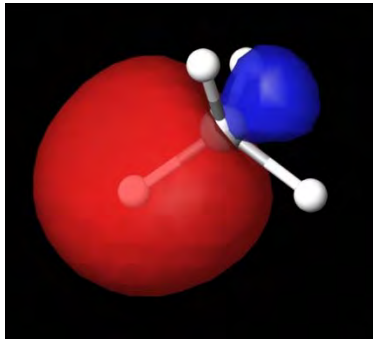
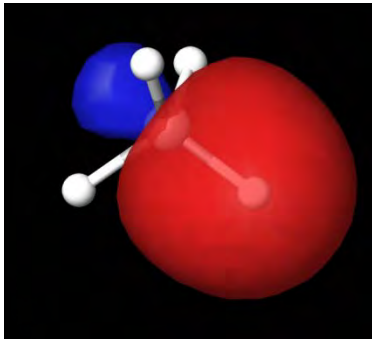
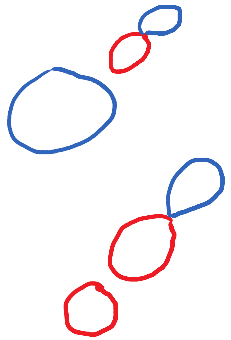
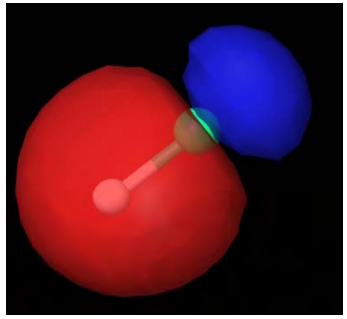
Connect with Geometry



- Rationalize experimental facts
  - Choose hybrid orbitals that give good overlap
- Predicting geometries
  - Position atoms to get good overlap

BMO CH_4
BMO + ABMO HF

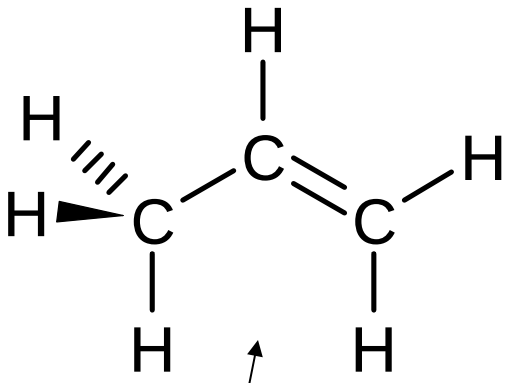
HF ABMO

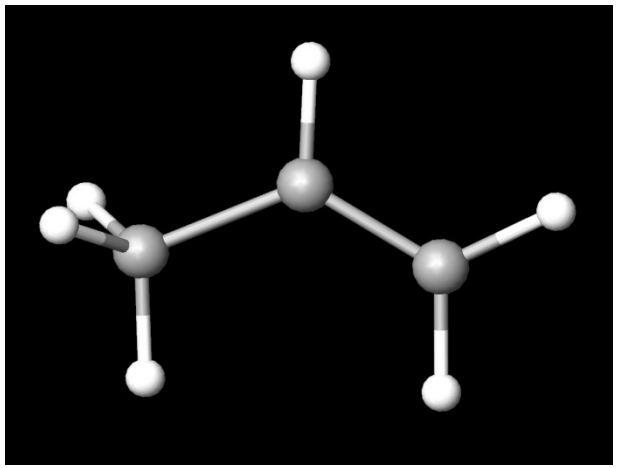
CH_4 BMO = C sp^3 + H 1s

HF MO = F 2p ± H 1s

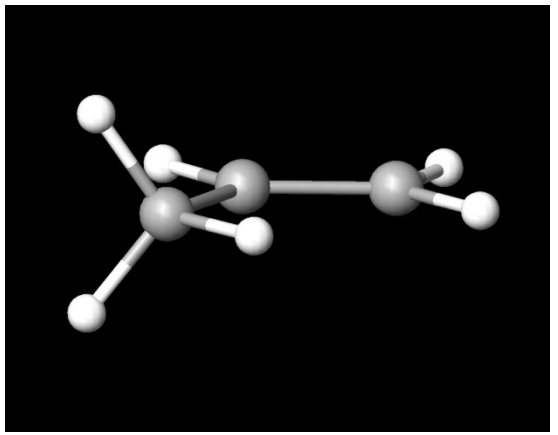
Propene - Orientation



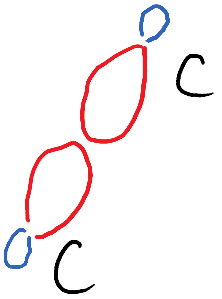
FACE view

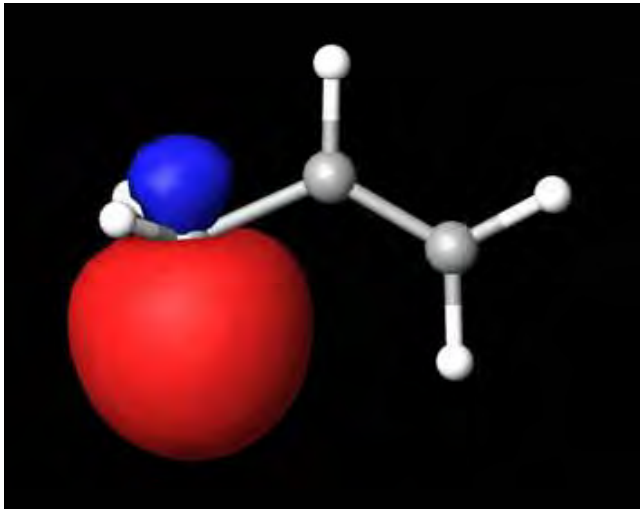


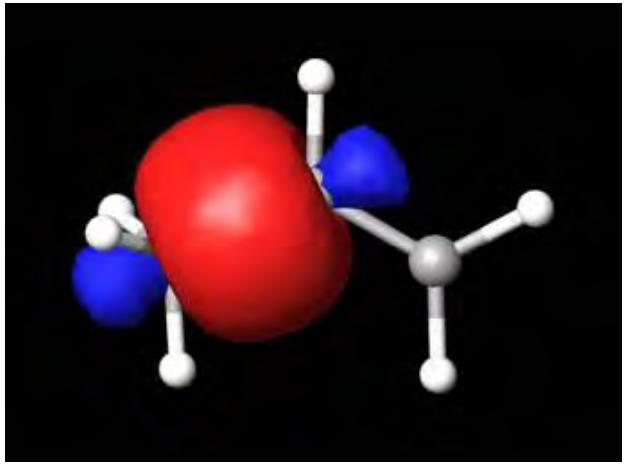
EDGE view

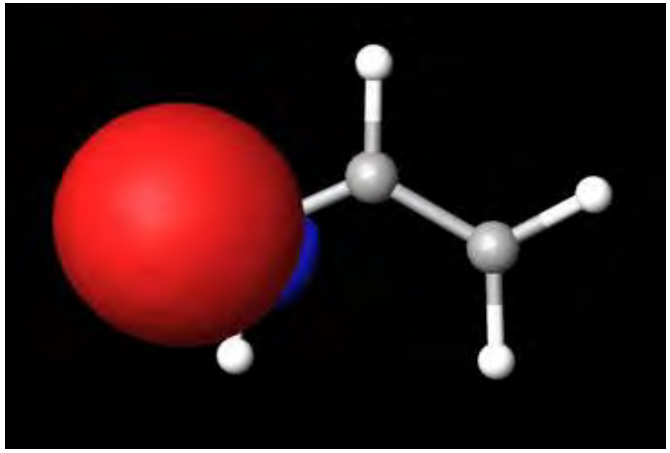


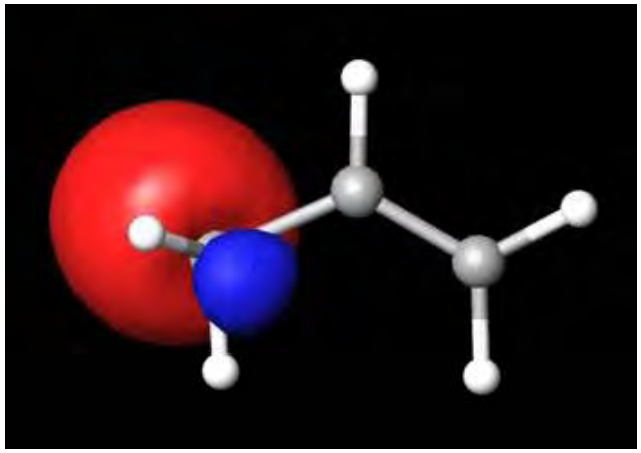
CH_3C 4σ Bonding LMO



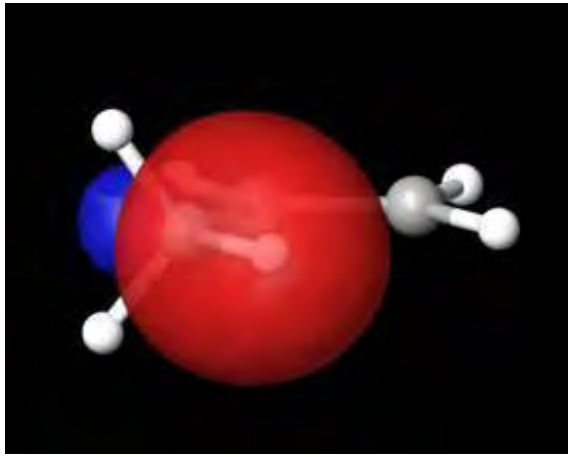


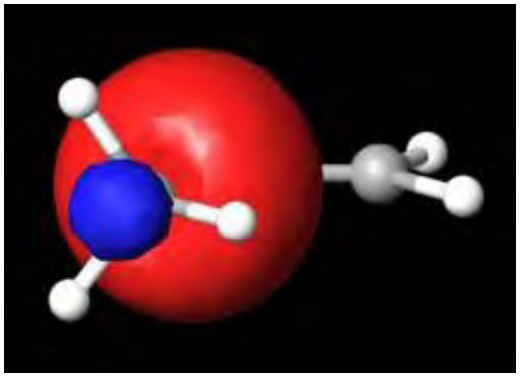


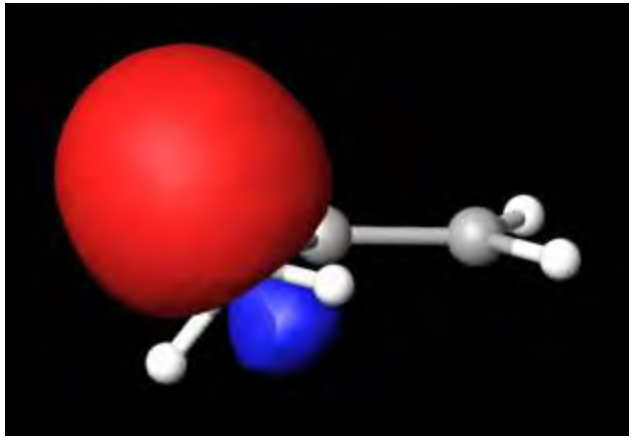


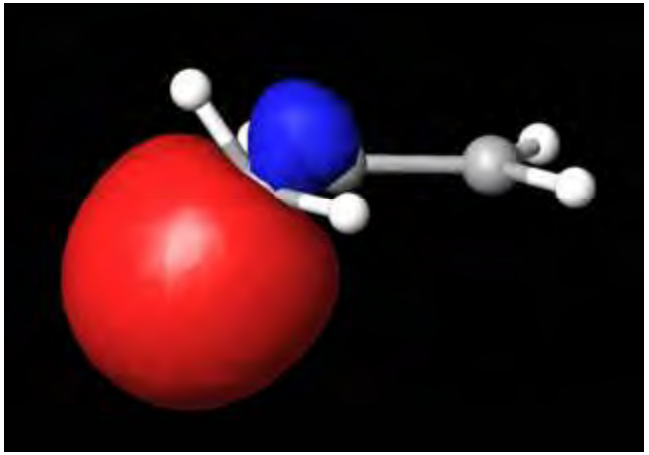


CH_3C 4σ Bonding LMO
(EDGE view)

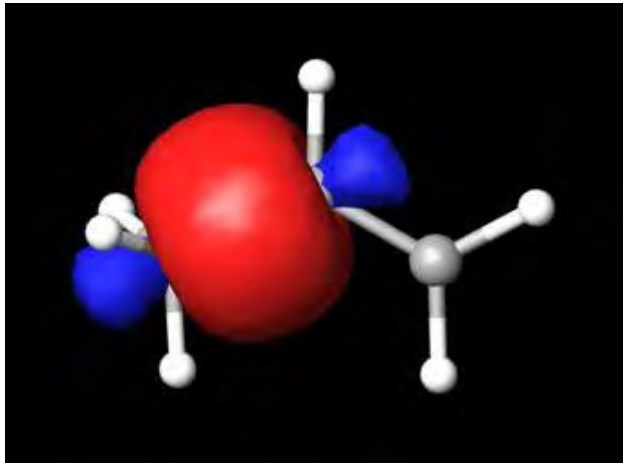


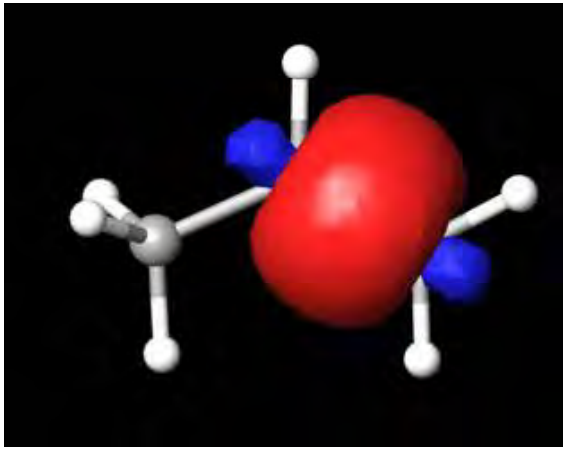


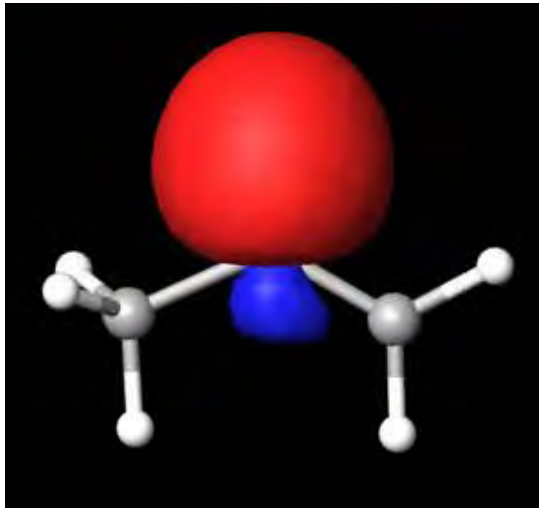


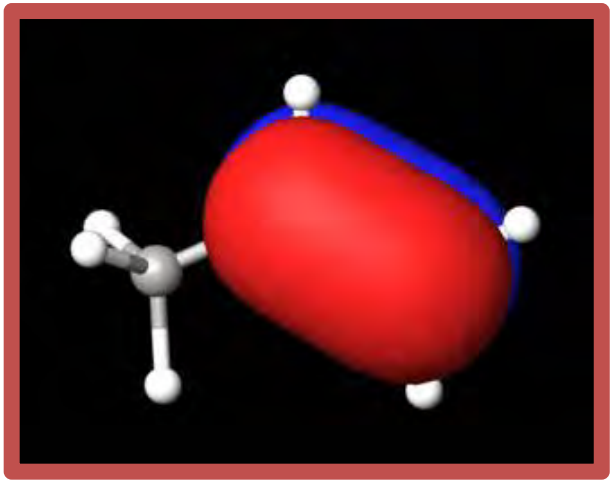


C*C*H=C 3σ + 1π bonding LMO

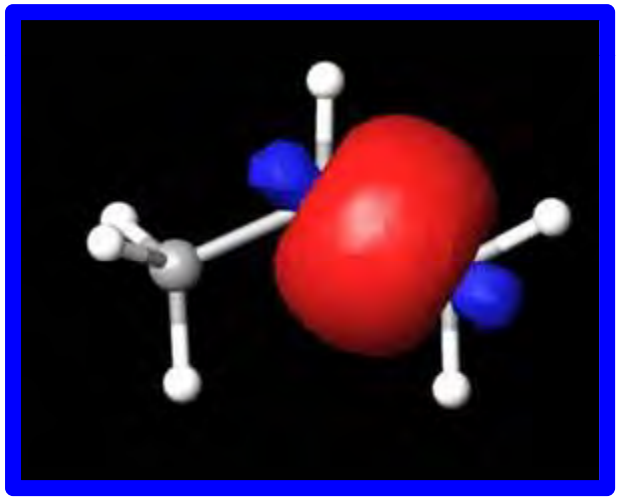


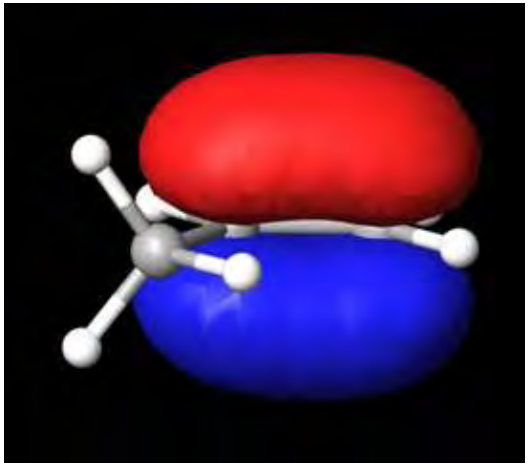


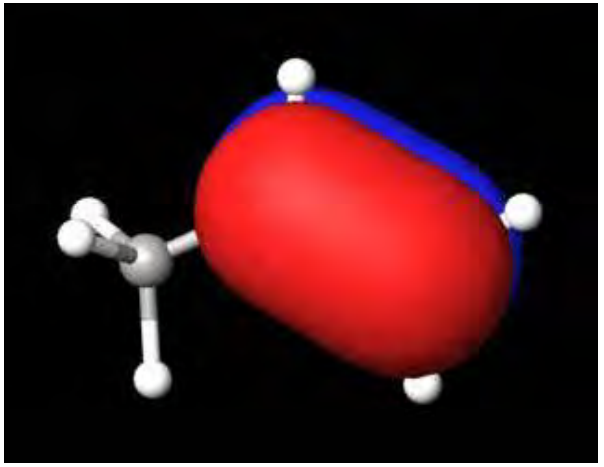




C=C 1σ + 1π







C=*C* both 3σ bonding LMO