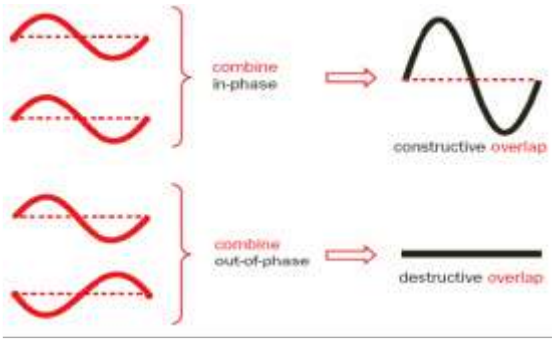
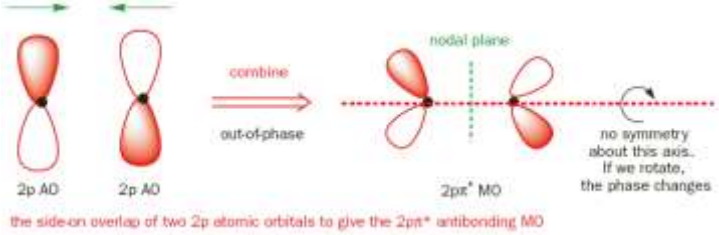
CH 101Fall 2018
Discussion #13
Chapter 10

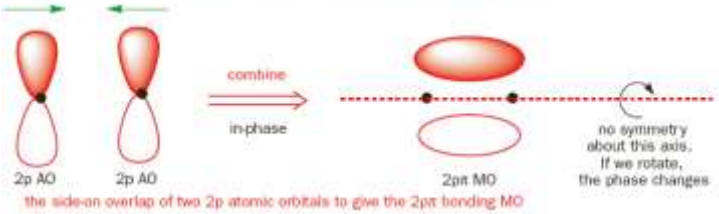
Your name: _____ TF's name:_____ Discussion Day/Time: _____

Things you should know when you leave Discussion today

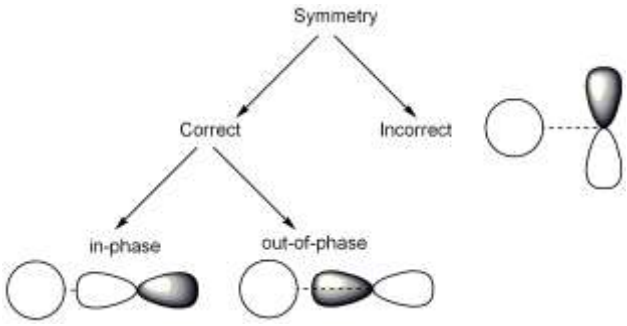


- Atomic orbitals (s, p, d, f) vs. molecular orbitals (σ, σ*, NB, π, π*, π_{nb})
- Total Number of MO =Total Number of AO
- Constructive and destructive interference (in phase and out-of-phase interaction)
  - Sigma bond is achieved by head–on–overlap
  - Bonding MO (σ, π) - Constructive interference **in-**phase interaction
  - Antibonding MO (σ*, π*) - Destructive interference **out-of-**phase interaction
  - π formed from side-by-side overlap of available p AO
    - π* is out-of-phase overlap of available p AO
    - π is in-phase side-by-side overlap of available p AO



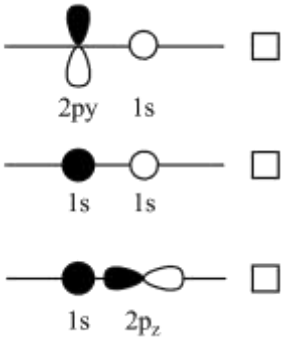


- Factors that affect the formation of MOs from AOs: S.O.E.
  - **Symmetry** AOs must have a compatible orientation to achieve an overlap.
  - **Overlap:** valence orbitals of correct symmetry.
  - **Energy:** If the pair of AO's has the correct symmetry and greatest overlap, and closest in energy



1. If you have two atoms that together have 5 atomic orbitals, when those atoms combine to form a molecule, how many molecular orbitals are you going to have?

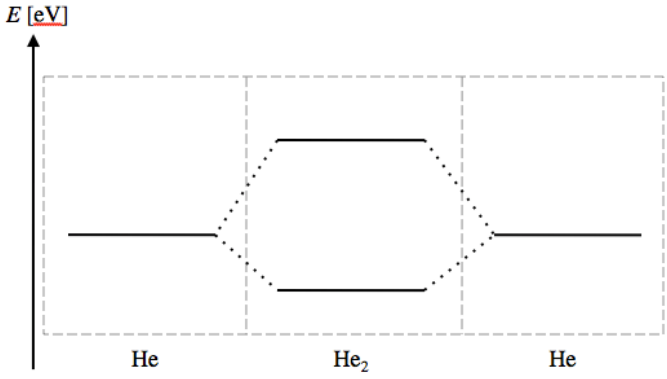
2. For each of the AO combinations below, draw the resulting MO. What do we call that resulting MO?
   a. Discuss any axes of symmetry the MO may have.
   b. Is this MO destructive or constructive interference (or neither or both)?

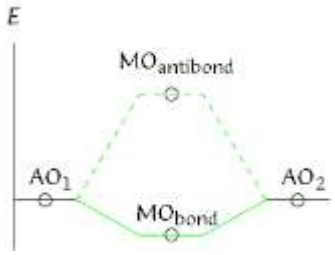


   c. (at home) Draw as many other combinations of AOs that give σ and σ* MOs as you can, using only s and p AOs. Discuss the relative energies of the resultant MOs you just drew.

   d. (at home) Draw as many other combinations of AOs that give π and π* MOs.

3. Draw correlation diagram for He_2^+. *Hint: 1sσ* is more unstable than 1sσ is stable.*





Bond Order (BO): $B.O. = \left[\frac{(\#\text{of } e^- \text{ on the bonding orbitals}) - (\#\text{of } e^- \text{on the antibonding orbitals})}{2}\right]$

   a. What is the bond order of He_2^+?

   b. Put in the order of increasing bond length H_2; H_2^+ and He_2^+. Hint: find the bond orders for all the molecules or molecular ions.

4. (at home) Draw the correlation diagram for the HeH molecule. Which molecule or molecular ion will have the shortest bond HeH^{3+},HeH^{2+}, HeH^+, HeH, HeH^-?

5. Consider the ionization energies for H, Na, and F. Assume z is along the bond axis.

Element		IE (eV)
H	**1s**	**13.6**
F	**2s**	**25.0**
F	**$2p_z$**	**17.4**
Na	**3s**	**5.1**

   a. Draw the correlation diagram for NaF and HF:

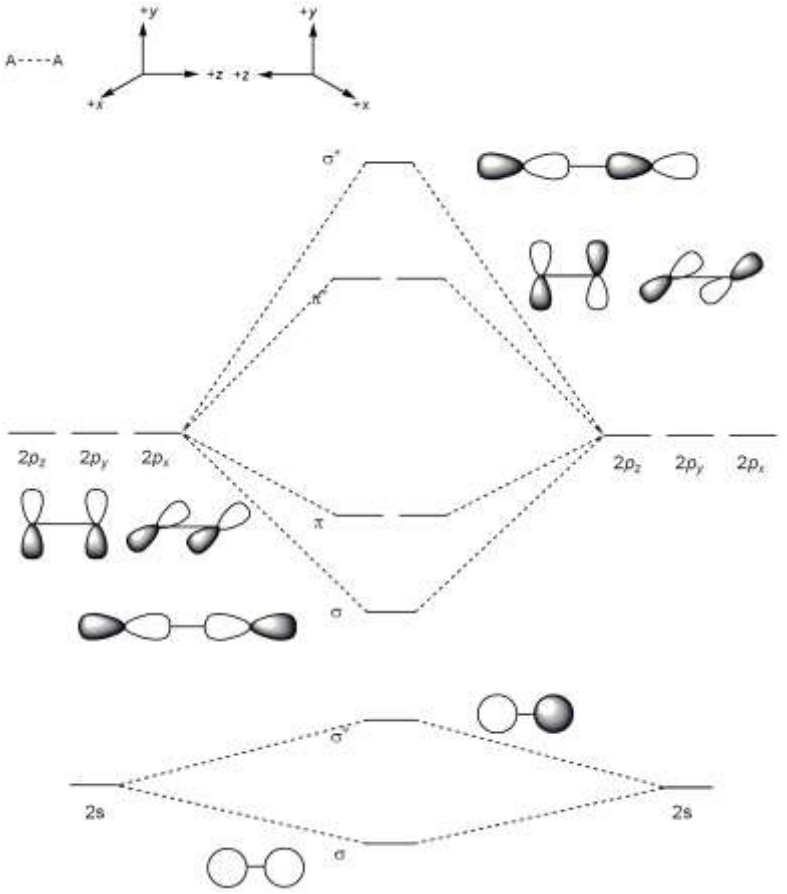
HF NaF

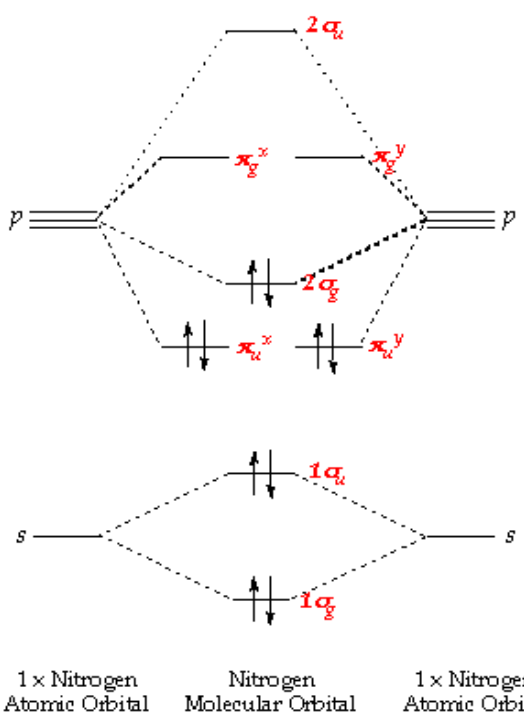
   b. Discuss the relative ionic and covalent character of NaF verses HF.

6. Generally, the valence electrons on different atoms, rather than the core electrons, interact with one another. Choose the best explanation:
   a. Adjacent valence electron waves have the greatest overlap.
   b. Adjacent valence electron waves have the same energy.
   c. Core electron clouds have the wrong symmetry.
   d. Core electron clouds move with the wrong frequency.

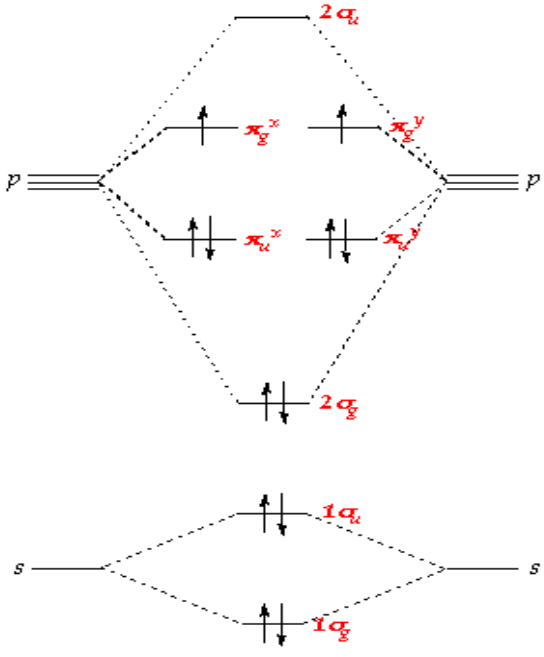
7. When is the interaction of two AO orbitals most favored?

- Below: General MO Correlation Diagram for second row in the periodic table. *Note: This diagram is correct for O and F; for correlation diagrams involving B, C, and N, the σ and π bonding orbitals are inverted*





1 × Nitrogen Atomic Orbital | Nitrogen Molecular Orbital | 1 × Nitrogen Atomic Orbital



1 × Oxygen Atomic Orbital | Oxygen Molecular Orbital | 1 × Oxygen Atomic Orbital

8. Draw two AO energy diagrams for the atoms in CN^- one atom on the left and one atom on the right, leaving space in the middle. Draw a picture of each AO. Draw the MO energy diagram and pictures of the resulting MOs in between and fill them with the electrons for the molecule.
    a. Draw the MO diagram *Hint: count how many valence electrons and AOs you start with.*

    b. Calculate the bond order.

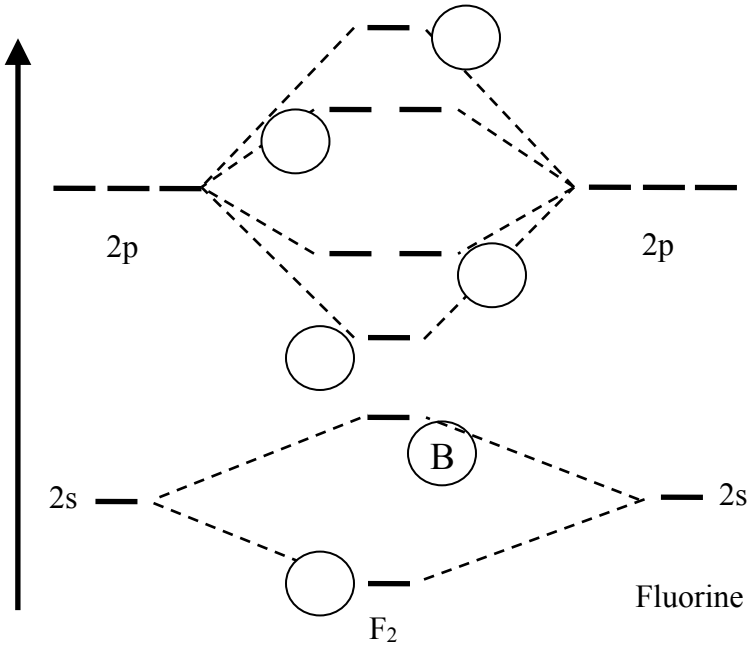
    c. Is CN^- diamagnetic or paramagnetic?

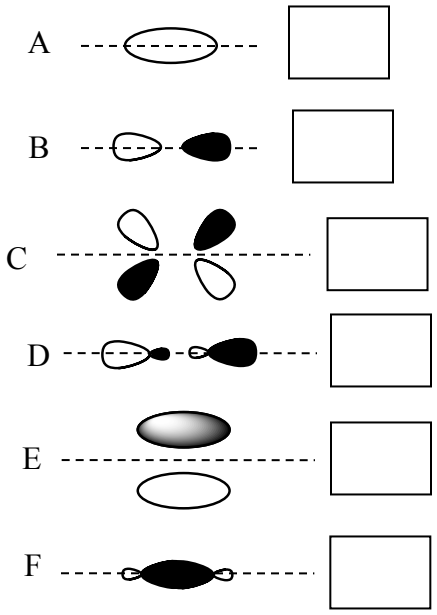
    d. Are the electrons centered more on C or on the N?

    e. If an electron is removed, will this make the bond longer or shorter?

9. (At home on a separate piece of paper) Draw two AO energy diagrams for the following atoms in [C_2, N_2, O_2, O_2^-,F_2, HF, BF, HB^+, HO^+], one atom on the left and one atom on the right, leaving space in the middle. Draw a picture of each AO. Draw the MO energy diagram and pictures of the resulting MOs in between and fill them with the electrons for the molecule.
    a. Calculate the bond order for each molecule.
    b. Discuss which of the molecular orbitals are responsible for single, double bonds, etc.
    c. Discuss the relative length, reactivity and 'strength' of these bonds.
    d. What are the magnetic properties of these molecules?
    (Which are diamagnetic and which are paramagnetic.)

10. Below on the left is an empty molecular orbital diagram of F_2. Below to the right are various molecular orbitals, with the inter-nuclear axes shown with a dotted line. Fill in the boxes next to the molecular orbitals in part (a). Fill in the circles on the molecular orbital diagram in part (b). <u>Carefully follow the instructions below</u>.





a. In the box to the <u>right</u> of the molecular orbitals formed in F_2 above, provide the proper name of each molecular orbital (e.g. σ_{2s}, π^*, etc).

b. Match each molecular orbital on the right to the molecular orbital diagram on the left. Show your answer by placing the <u>letter</u> in the circle beside the molecular orbital. Letter "B" is filled in for you.

c. In the molecular orbital diagram above, populate both the atomic and molecular orbitals with electrons by putting arrows on the horizontal lines for F_2 and the fluorine atoms. All three systems are in the ground state.

d. Using the diagram above to guide you, calculate the bond orders for the following species.

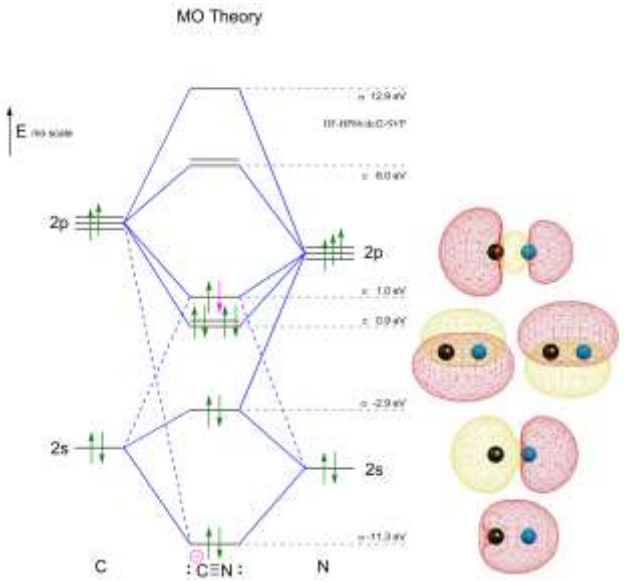
F_2^+ : _____ F_2^{2-} : _____

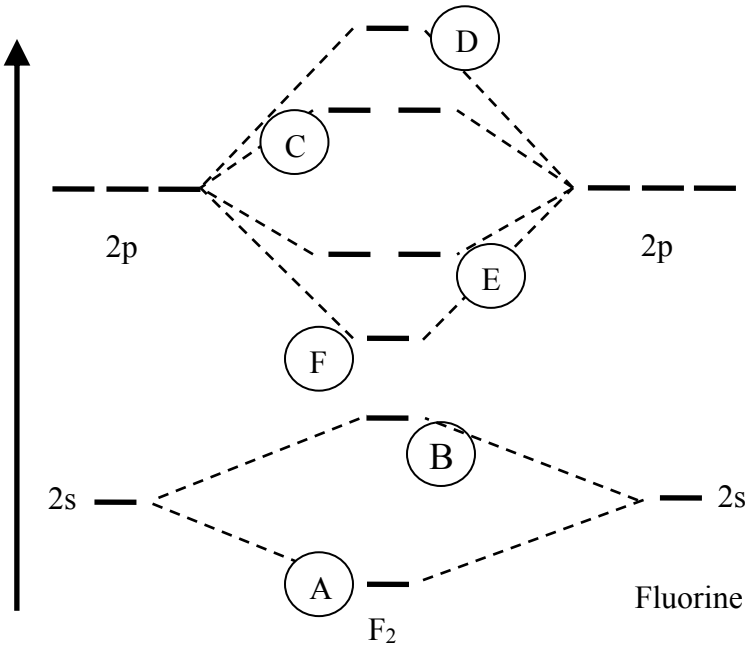
e. Naturally Fluorine is a diamagnetic molecule. Let say in the planet far, far away we found a fluorine that is paramagnetic: proposed and draw the molecular orbitals that Fluorine must have to be paramagnetic.

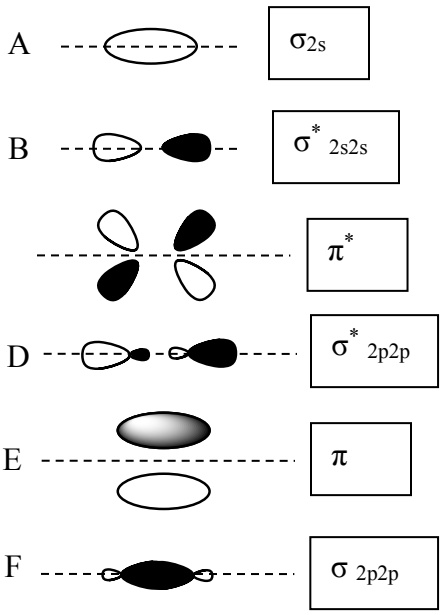
11. (at home) C_2 is naturally is diamagnetic and O_2 is paramagnetic. Propose and draw the molecular orbitals that will make C2 paramagnetic and O2 diamagnetic.

Handout Answers:

1. 5MOs
2. N
3.
   a. BO = 0.5
   b. bond length: $H_2 < H_2^+ < He_2^+$
      BO: 1 0.5 0.5
4. HeH^+
   molecule: HeH^{3+},HeH^{2+}, HeH^+, HeH, HeH^-
   BO: 0 0.5 1 0.5 0
5.
   a. draw correlation diagrams
   b. NaF-ionic; HF-covalent
6. A
7. SEO
8.
   a. 3
   b. diamagnetic
   c. N
   d. Longer(BO=2.5)
9.
10.
   d. F_2^+ BO=1.5; F_2^{2-} BO=0
   e. Switch the order of π^* and σ^*_{2p2p}







Final Exam OPTIONAL review session's schedule:
Thursday December 13.
Session 1 10am-11:50pm
Session2 1pm -2:50pm

1. **Exam1 / Chapter 2,3,4,5/ Dimensional analysis/ Stoichiometry/ Limiting Reagent / MS/IR / Intermolecular Forces/** **CAS 313**

2. **Chapter 6 /Vapor pressure/Gas phase verses Liquid phase verses solid phase/ Chemical reactions/Precipitation Reaction & Solubilit/ Acid-base, Redox /Molar calculations /Dimensional analysis/$\Delta_{vap}H$, $\Delta_{fus}H$/ /Heat capacity/Solubility of Ionic compounds/ ,Exam 2** **CAS 211**

3. **Chapter 8/ Light and 1 electron system / emission /absorption/ Energy of a photon/ KE/ Ionization/Hydrogen Family Album /Multi-electron Atoms / Quantum Numbers / Electron Configuration/ Trends/ Shielding/** **CAS 224**

4. **MOs Chapter 10/ Multi-electron Atoms Lewis Structures / FC/ ON / Electron Configuration/ Trends/ Shielding/** **CAS 522**

5. **Chapter 7/Enthalpy/ First law/ calorimeter/ Exam 3** **CAS B12**

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3. Comments in the text fields are valued and encouraged. Please try to answer all questions, but if a question is not applicable to you or you do not wish to answer it then simply skip it.

4. When you are done, please close your browser.