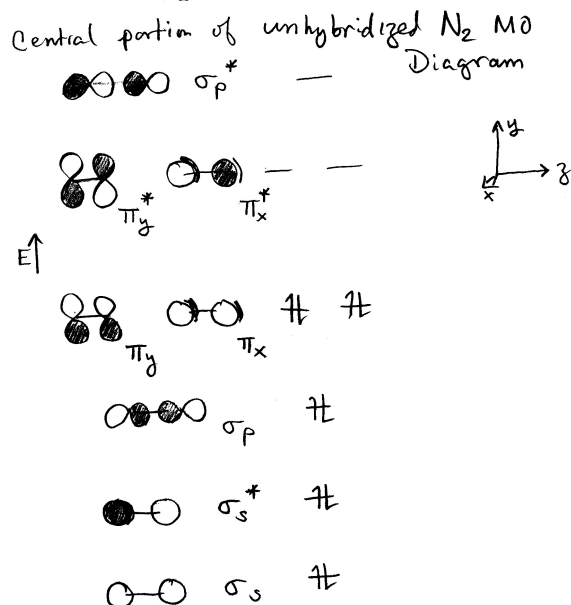


1 Morning class week 5 day 2: Diatomic MOs with sp hybridization

The goal of today's lecture is to generate the hybridized diatomic MO diagram. In deriving this diagram we will also deduce why the MO energy ordering in O_2 and F_2 MOs differs from that of the other second row main group diatomic molecules.

- Rules for making MO diagrams:** Please review the three rules for making MO diagrams:
 - In a minimal basis set MO diagram, the number of MOs equals the number of AOs.
 - When two orbitals combine, they combine to make two new orbitals. The original orbitals combine to make the lowest and highest energy combinations possible.
 - Orbitals which are initially close in energy interact stronger than orbitals which are initially far apart in energy. When two orbitals of different energy combine, the resultant low energy combination resembles more the initially lower energy orbital; the resultant high energy combination resembles more the initially high energy orbital. Two orbitals of equal initial energy combine to make two new orbitals with equal contributions from the two starting orbitals equally.
- The unhybridized N_2 MO diagram:** Please review that using the above rules that you are able to generate the unhybridized N_2 MO diagram shown below.



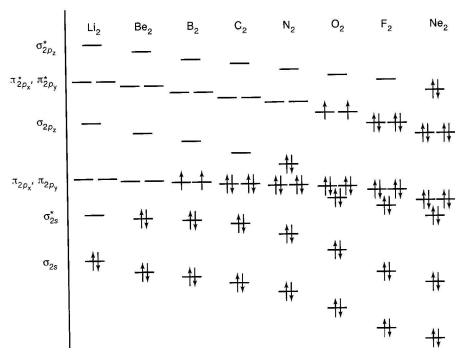
- Yesterday's diagrams are not the final MOs.** Further orbital mixing will lower energies further. Which orbitals need to be mixed?
 - Please mix the π_x and π_y orbitals. Do they mix in a worthwhile way?
 - Please mix the π_x^* and π_y^* orbitals. Do they mix in a worthwhile way?
 - Please mix the π_x and π_x^* orbitals. Do they mix in a worthwhile way?
 - Please mix the σ_s^* and σ_s orbitals. Do they mix in a worthwhile way?
 - Please mix the σ_s^* and σ_p orbitals. Do they mix in a worthwhile way?
 - Please mix the σ_p and σ_s orbitals. Do they mix in a worthwhile way?

- (g) Please mix the σ_{p^*} and σ_s orbitals. Do they mix in a worthwhile way?
- (h) Please mix the σ_{p^*} and σ_s^* orbitals. Do they mix in a worthwhile way?
4. **Drawing the true N₂ MO diagram:** we complete the making of the hybridized orbital N₂ MO diagram using the unhybridized MO diagram, which we derived yesterday, as a starting point.
- (a) What is the lowest possible energy MO we can imagine? We wish to generate an MO with the longest de Broglie wavelength possible.
- (b) Which two orbitals in the unhybridized MO diagram need to be mixed to generate this orbital? Please mix these two orbitals.
- (c) What is the highest possible energy MO we can imagine? We wish to generate an MO with the shortest de Broglie wavelength possible.
- (d) Which two orbitals in the unhybridized MO diagram need to be mixed to generate this orbital? Please mix these two orbitals.
- (e) We have generated the final N₂ MO diagram. Please review what you have learned.
5. **Second row diatomic MOs:** In this last item we derive the remaining second row diatomic MO diagrams.
- (a) In the table below the energies of all the second row main group valence atomic orbitals are given. Please plot these orbital energies on a graph.

Table 1: Energies of hydrogen and second row main group AOs.

Element	Valence <i>s</i> energy	Valence <i>p</i> energy
H	-13.6 eV	–
Li	-5.4 eV	-3.5 eV
Be	-10 eV	-6 eV
B	-15.2 eV	-8.5 eV
C	-21.4 eV	-11.4 eV
N	-26.0 eV	-13.4 eV
O	-32.3 eV	-14.8 eV
F	-40.0 eV	-18.1 eV
Ne	-41.0 eV	-21.6 eV

- (b) Going across the row, from Li to Ne, does shielding increase faster for the 2*s* or the 2*p* orbitals?
- (c) Recall Rule 3 for making MO diagrams. How can we use the above table to rationalize the figure shown below, taken from your textbook? This figure shows all the second row diatomic MO energy diagrams.



- (d) Please review everything you have learned.