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.

1. **Rules for making MO diagrams:** Please review the three rules for making MO diagrams:

   (a) In a minimal basis set MO diagram, the number of MOs equals the number of AOs.

   (b) When two orbitals combine, they combine to make two new orbitals. The original orbitals combine to make the lowest and highest energy combinations possible.

   (c) 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.

2. **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.

![Unhybridized N2 MO Diagram](image)

3. **Yesterday’s diagrams are not the final MOs.** Further orbital mixing will lower energies further. Which orbitals need to be mixed?

   (a) Please mix the \(\pi_x\) and \(\pi_y\) orbitals. Do they mix in a worthwhile way?

   (b) Please mix the \(\pi_x^*\) and \(\pi_y^*\) orbitals. Do they mix in a worthwhile way?

   (c) Please mix the \(\pi_z\) and \(\pi_z^*\) orbitals. Do they mix in a worthwhile way?

   (d) Please mix the \(\sigma^*_s\) and \(\sigma_s\) orbitals. Do they mix in a worthwhile way?

   (e) Please mix the \(\sigma^*_p\) and \(\sigma_p\) orbitals. Do they mix in a worthwhile way?

   (f) Please mix the \(\sigma_p\) and \(\sigma_s\) orbitals. Do they mix in a worthwhile way?
Please mix the $\sigma_p^*$ and $\sigma_s$ orbitals. Do they mix in a worthwhile way?

Please mix the $\sigma_p^*$ and $\sigma_s^*$ orbitals. Do they mix in a worthwhile way?

4. **Drawing the true N$_2$ MO diagram:** we complete the making of the hybridized orbital N$_2$ 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 N$_2$ 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>
<thead>
<tr>
<th>Element</th>
<th>Valence $s$ energy</th>
<th>Valence $p$ energy</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>-13.6 eV</td>
<td>–</td>
</tr>
<tr>
<td>Li</td>
<td>-5.4 eV</td>
<td>-3.5 eV</td>
</tr>
<tr>
<td>Be</td>
<td>-10 eV</td>
<td>-6 eV</td>
</tr>
<tr>
<td>B</td>
<td>-15.2 eV</td>
<td>-8.5 eV</td>
</tr>
<tr>
<td>C</td>
<td>-21.4 eV</td>
<td>-11.4 eV</td>
</tr>
<tr>
<td>N</td>
<td>-26.0 eV</td>
<td>-13.4 eV</td>
</tr>
<tr>
<td>O</td>
<td>-32.3 eV</td>
<td>-14.8 eV</td>
</tr>
<tr>
<td>F</td>
<td>-40.0 eV</td>
<td>-18.1 eV</td>
</tr>
<tr>
<td>Ne</td>
<td>-41.0 eV</td>
<td>-21.6 eV</td>
</tr>
</tbody>
</table>

(b) Going across the row, from Li to Ne, does shielding increase faster for the 2s or the 2p 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.