1 Morning class week 5 day 1: Diatomic molecular orbital diagrams without *sp* hybridization

1. **Making MO diagrams**

   Making more traditional outside-to inside MO diagrams requires knowing two different things: the flow diagram by which MO diagrams are generated and the rules by which the flow-chart is processed.

   (a) **The flow chart:** There are four steps.

      i. Place the two atomic orbital (AO) energy diagrams on the two sides of the sheet of paper.

      ii. Based on the atomic electron configuration, place the correct electron fillings for the two AO energy diagrams, one on each side.

      iii. Mix pairs of AOs to derive two MOs. One of the MOs is more bonding, the other more antibonding. They are indicated by horizontal lines in the center of the page. MO balloon drawings are placed next to each of these central horizontal lines.

      iv. Follow the Aufbau principle and fill the central horizontal lines with the correct number of electrons.

   (b) **The rules:** There are three rules for the making of MO diagrams.

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

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

      iii. 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.

   (c) Examine the H_2 MO diagram you previously drew and detemine where the three rules were applied in the making of the diagram.

2. **We apply the above ideas to make MO diagrams for a variety of different diatomic molecules.**

   (a) Draw an MO diagram for Be_2^+ using only the $1s$ and $2s$ Be AOs.

   (b) Draw an MO diagram for Be_2^+ using only the $2s$ Be AOs.

(c) Draw an MO diagram for LiBe using only the $2s$ Be and Li AOs.

(d) Draw an MO diagram for Bi_2 using only the Bi $6p$ AOs. Place the Bi-Bi bond along the z-axis.

(e) Draw an MO diagram for N_2 using only the N $2s$ and $2p$ AOs. Place the N≡N bond along the z-axis. The N $2s$ and $2p$ orbitals are the nitrogen *valence orbitals*. *SIMPLIFICATION: DO NOT COMBINE* $2s$ *ORBITALS WITH* $2p$ *ORBITALS.*

(f) Draw an MO diagram for CO using only the C and O $2s$ and $2p$ AOs. Place the C≡O bond along the z-axis. The C and O $2s$ and $2p$ orbitals are the nitrogen *valence orbitals*. *SIMPLIFICATION: DO NOT COMBINE* $2s$ *ORBITALS WITH* $2p$ *ORBITALS.*

(g) Calculate the bond orders for each of the above molecules.

(h) Please draw the Lewis structures for each of the above molecules.

Table 1: Energies of hydrogen, second row main group and bismuth valence AOs

Element	Valence s energy	Valence p 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
Bi	-15.2 eV	-7.8 eV