1 Morning class week 4 day 3: Molecular orbital diagrams

1. An understanding of molecular orbitals, like atomic orbitals starts with sand patterns on drums.

   (a) **The atomic orbital drum analog:** Draw a shelf (energy) diagram which goes with the picture below. Draw contour maps and balloon diagrams for each wavefunction.

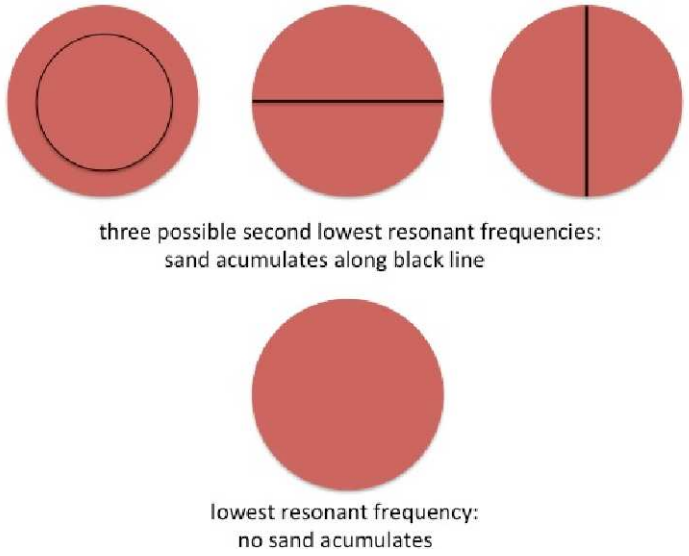

Figure 1: The lowest energy portion of the atomic orbital diagram.

   (b) **The H_2 molecular orbital drum analog:** Draw a shelf (energy) diagram which goes with the picture below. Draw contour maps and balloon diagrams for each wavefunction.

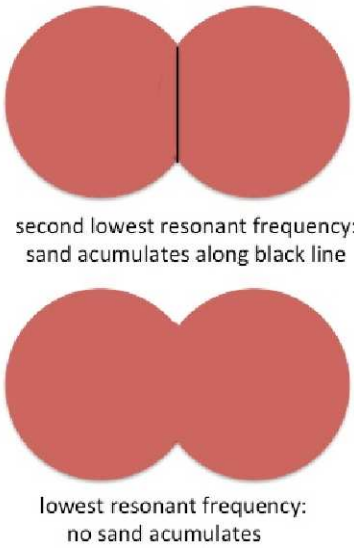

Figure 2: H_2 molecular orbital diagram.

   (c) **The H_3^+ molecular orbital drum analog:** H_3^+ is an interstellar ion in which the three hydrogen atoms form a perfect equilateral triangle. Draw a shelf (energy) diagram which goes with the picture below. Draw contour maps and balloon diagrams for each wavefunction.

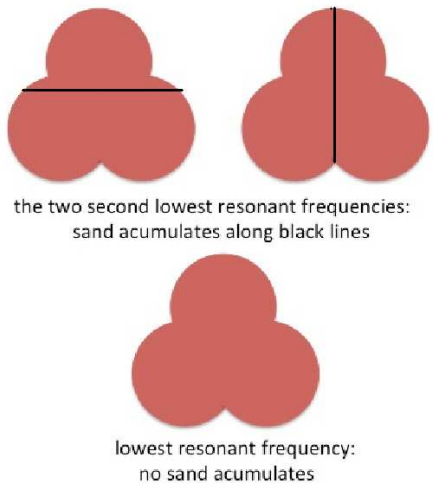

Figure 3: The H_3^+ molecular orbital diagram.

2 Making MO diagrams

Making 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.

2. **The flow chart:** Please carry out the steps below to generate the MO diagram for H_2:

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

   (b) Place the correct electron fillings for the two AO diagrams, in this case one electron for each AO.

   (c) Mix the AOs as we did yesterday to derive the two MOs. One of the AOs is bonding, the other antibonding. They are indicated by horizontal lines in an orbital energy diagram at the middle of the page.

   (d) Draw the MOs which correspond with the new horizontal lines.

   (e) Follow the Aufbau principle and fill the middle horizontal lines with the correct number of electrons.

3. **The rules** There are 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.

4. Please examine the H_2 MO diagram you have just made with the H_2 drum analog which you previously analyzed. Are the two diagrams in agreement with one another? If so, how so? If not, why not?