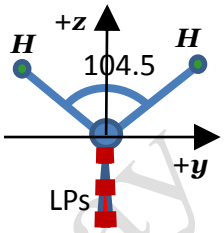
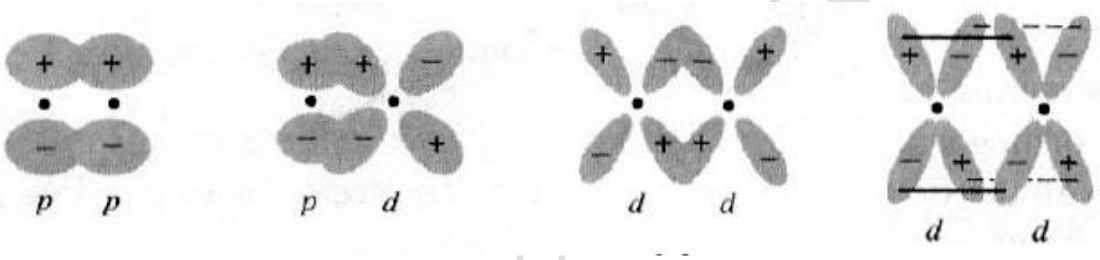
CH 107 Tutorial 6

Please solve these problems BEFORE the tutorial session

1. For water, it is experimentally determined that the H-O-H bond angle is 104.5°. Determine the coefficients of atomic orbitals of O that participate in hybridization (see schematic, lone pairs are in xz plane, not relevant).



2. a) Qualitatively plot the overlap integral, S_{AB}, as a function of inter-nuclear distance (R_{AB}) for the following LCAO-MOs (below).
   b) Write the MOs (LCAO expressions) for bonding and anti-bonding situations for each.
   c) Draw the MO pictures with appropriate signs and assign their symmetries (g/u).



3. Formulate the Hamiltonian for a triangular H_3^+ molecular ion (equal H – H bond lengths).
   b) Write the LCAO expression for the lowest energy MO using the AOs of H. Sketch the contour plot of this MO and show signs.
   a) What is the spin wavefunction of this molecule in the ground state?
   b) Express the ground state wavefunction of this molecule as a *single* Slater determinant

4. Qualitatively draw the bonding and antibonding MOs formed due to overlap of two 2s and 3p_z AOs. Assume the internuclear axis to be in z-direction. Show nodes and signs of MOs. *Hint: Draw the wavefunctions centered on the two nuclei along ±z to find nodes!*

5. Write the expressions for the delocalized *σ bonding* MOs of $\boldsymbol{BeH_2^+}$ as linear combinations of valence AOss of appropriate symmetry. *Do not invoke s-p mixing and consider +z to be the internuclear axis for this linear molecule.*

   a) Sketch the bonding MOs, show signs and nodes (if any), and assign symmetries (g/u).
   b) How many lines/bands are expected in the *entire* photoelectron (PE) spectrum?
   c) What are their relative intensities? (note that the molecule has +1 charge)