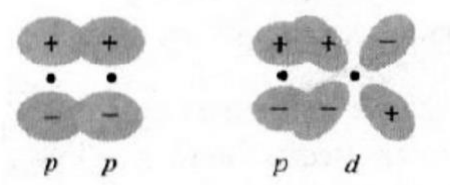
Problem Set 5

1. Construct a MO diagram for H_2^+ and make rough sketches of the form of the MO's. Explain how symmetry labels are assigned to the two MO's.

2. Use MO diagrams to rationalize why He_2 is an unknown species, but the ion He_2^+ has been observed. Make what predictions you can about the stability of the molecules He_2^{2+} and H_2^{2-} with respect to dissociation.

3. Draw qualitative MO pictures with proper signs (+ or -) and assign the symmetries (g/u) of MO's formed from the AO's as shown below.



4. In O_2, the lowest energy MOs (formed from the 1s AOs of O) are given the label σ_g and σ_u. Sketch the form of the MO's. Explain why it is that although both of these MO's are occupied, they make little contribution to the bonding in O_2.
Sketch the π^*_g and π_u MO's of O_2. How does the π^*_g and π_u MO's of O_2 occupied differently for the ground state (triplet state) and the first excited state (singlet state) of O_2.

5. What are the different spin states of O_2? Show the electron occupation in HOMO for the ground state, first excited state and second excited state of O2. Why did we see luminescence during the generation of singlet oxygen?

6. Write the balanced equation for the complete combustion of Methanol? If the ΔH of the reaction $H_2 + ½\ O_2 \rightarrow H_2O$ is 460 kJ/mol, what would be the predicted value of ΔH for the combustion of Methanol?