HW # 9. Due Nov. 19.

1. Using the HF method and the 6-31G(d) basis set calculate the bond energy for H_2, N_2, O_2, F_2. You can use experimental bond lengths in calculated the bond energies. How do your results compare with experiment? Do they improve significantly when using DFT (e.g., B3LYP) or MP2. Note that if you do an MP2 calculation, you automatically get the HF results, so these don't have to be run as separate calculations.

2. Calculate the energy (HF/6-31G*(d)) of H_3 in linear and equilateral geometries, with a bond length of 0.8 A. Which structure is more stable? Make a correlation diagram showing how the valence orbitals of the triangular structure correlate with those of the linear structure.

3. Consider insertion of Be into H_2 to give linear BeH_2. Is the reaction exothermic? Make a correlation diagram correlating the orbitals of the reactants with the product assuming the reaction occurs in C_{2v} symmetry. The reaction pathway has a high barrier. Why is this?