Worksheet VII

1. Draw the potential energy curve for a diatomic molecule. Clearly label the bond dissociation energy and equilibrium bond length on your drawing.

2. Two 3*d* orbitals can overlap in either a σ fashion or in a π fashion.
   (a) Show how two 3*d* orbitals can have cr overlap. Draw the resulting molecular orbitals.

   (b) Show how two 3*d* orbitals can have π overlap. Draw the resulting molecular orbitals.

3. For a diatomic molecule of oxygen (O_2), we define the bond as lying along the *z* axis.
   (a) Draw the valence MO diagram for O_2. Include labels for the molecular orbitals.

   (b) Which valence atomic orbitals combine to form σ MOs in O_2? *Be specific.*

   (c) Which valence atomic orbitals combine to form π MOs in O_2? *Be specific.*

   (d) Write the valence orbital occupancy for O_2.
   (e) Is O_2 diamagnetic or paramagnetic?
   (f) What is the net σ bond order for this molecule?
   (g) What is the net π bond order for this molecule?
   (h) What is the overall bond order for this molecule?
   (i) How many electrons must be added to O_2 to reduce the bond order to zero? If this number of electrons is added, what product(s) will be formed?

For questions 4 and 5, you will want to sketch the MO diagram for N_2 in order to work out the orbital occupancies. There is no need to draw out the same diagram twice (once for each question).
Remember that N_2^+ has one less electron than N_2 and N_2^- has one more electron than N_2.

4. The bond dissociation enthalpies for N_2 and N_2^- are 945 kJ/mol and 765 kJ/mol respectively. *(There is only a small difference between enthalpies and energies.)* Using an argument based on MO theory, explain why N_2^- has a smaller bond dissociation energy than N_2.

5.
   (a) Draw Lewis diagrams for N_2^+ and N_2^-. What bond orders would you predict from the Lewis diagrams?
   (b) Determine the bond orders for these two ions using MO theory. Do they agree with the values obtained for your Lewis diagrams?

6. When we draw Lewis diagrams, we ignore the core electrons and focus only on the valence electrons. Discuss how MO theory provides support for this practice.

7. Use an MO diagram to show that Be_2 should not exist.

8. In the gas phase, it is possible to make exotic diatomic molecules like LiF (which normally exists in a lattice rather than as a diatomic molecule).

Atomic Orbital Energies

Li	
1*s*	-4.77 Ry
2*s*	-0.40 Ry

F	
1*s*	-51.2 Ry
2*s*	-2.95 Ry
2*p*	-1.37 Ry

$$*1 \text{ Ry} = R_H = 2.179\times10^{-18} \text{ J}$$

   (a) The above energies were determined experimentally. Name and briefly describe the technique used to make these measurements.
   (b) Develop the MO diagram for LiF. Clearly indicate which atomic orbitals mix to make which molecular orbitals. Show the orbital occupancy in LiF and estimate the bond order.
   (c) We would expect LiF to have substantial ionic character. Does your MO work agree with this expectation? Explain.

   (d) Does your MO work agree with a Lewis diagram for LiF?