Quantum Mechanics and Spectroscopy
CHEM 3PA3
Assignment 20 **Name:** _____

1. (a) Write down the simple $1s$-orbital-bases "valence bond" wavefunction for the hydrogen molecule (H_2), including the ionic contribution.

   (b) Write down the simplee $1s$-orbital-based "molecular orbital" wavefunction for the hydrogen molecule including the configuration interaction with the state where both electrons are in the antibonding orbital.

   (c) Show that these two wavefunctions are equivalent; i.e., show that the coefficients of the bonding/antibonding configurations in molecular orbital theory can be derived in terms of the coefficients of the ionic/covalent contributions in valence bond theory.

2. In Lithium Hydride, LiH, in the molecular orbital approximation, the ground state is predicted to be a singlet state, and the occupied molecular orbitals are both sigma orbitals. The electron configuration can then be written as $1\sigma^2 2\sigma^2$. Let $\phi_{1\sigma}(\mathbf{r})$ and $\phi_{2\sigma}(\mathbf{r})$ denote these molecular orbitals.

   (a) Write the Slater determinant for the $1\sigma^2 2\sigma^2$ electron configuration of LiH. Write the determinant out in its entirety, showing all the occupied orbitals and the coordinates of all the electrons explicitly. Remember the normalization factor.

   (b) Write a reasonable expression for the highest (the 2σ) occupied molecular orbtial in LiH.

3. Draw the molecular orbital diagram for C_2, N_2, and F_2. For each of these molecules A_2, the cationic specie, A_2^2, and the anionic specie A_2^-:

   (a) Predict the ground state configuration.

   (b) Calculate the bond order.

   (c) Determine its multiplicity.

4. Draw the molecular orbital diagram for methane (CH_4).