Quiz 9.2 – Molecular Orbital Theory: Diatomic Molecules

Name: _____

Homonuclear Diatomics

O_2^{4+} and N_2^{2+} have the same number of electrons, so you might expect them to have identical electronic structure

○ Draw the molecular orbital energy level diagram for these two molecules, filled with the proper number of electrons

○ Give the bond order of both molecules

○ Describe how both molecules might interact with a strong magnetic field

Heteronuclear Diatomics

Consider the molecule HF. Because of the much higher nuclear charge on F, the H$1s$ orbital actually aligns best energetically with the F$2p_z$ orbital, so they are the two which combine to form a molecular orbital. $\alpha_{H1s} = -7.2eV$, $\alpha_{F2p} = -10.4eV$, and $\beta_{H1s-F2p} = -1.0eV$

○ Calculate the energies of the two molecular orbitals, and draw an energy-level diagram which includes both the energies of the atomic orbitals and molecular orbitals. Remember that for heteronuclear diatomics we usually assume that the overlap integral $S = 0$

○ Calculate the coefficients for both MOs and sketch how they might look considering the unequal contributions from both atoms