

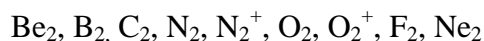
**Atoms, Molecules & Reactions, Spring 2006**

**Quantum Mechanics Homework –Week 6**

1. Determine that the following wavefunction is antisymmetric with respect to permutation. Show all work.

$$\psi = \frac{1}{\sqrt{2}} \frac{1}{2(S+1)} \{1s_A(1)1s_A(2) + 1s_A(1)1s_B(2) + 1s_B(1)1s_A(2) + 1s_B(1)1s_B(2)\} [\alpha(1)\beta(2) - \beta(1)\alpha(2)]$$

2. Draw molecular orbital diagram, fill in the appropriate number of electrons and determine the ground state term symbols for the following molecules and molecular ions. Use valence atomic orbitals only when constructing molecular orbitals. Make sure that all atomic and molecular orbitals are labeled with the appropriate symmetry.



Then determine the first excited state term symbol for each of the above molecules and molecular ions. For the purpose of this exercise, the first excited state is obtained by promoting an electron from the HOMO to the LUMO.