Problem Set 4

1.. Explain what is meant by the overlap integral between two AO's, and also explain why this quantity goes to zero for large distances between the two AO's. How would you expect the plot of $S(R)$ to compare between two 1s AO's and two 2s AO's?

2. Shown below is a plot of the overlap integral between two 2p orbitals. The blue line is for the sideways –on overlap to give π MO's, whereas the red line is for the head-on overlap to give σ MO's. Explain the form of these two curves.
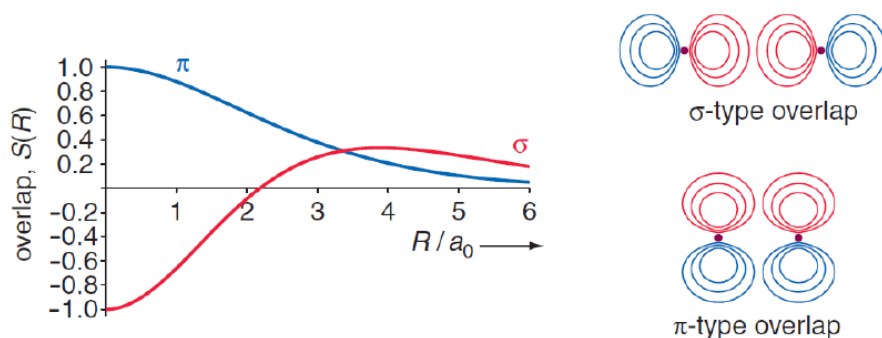
3. Suppose there is overlap between the 2p AO's from two atoms of **A**, where z is the internuclear axis. Sketch the form of the MO diagram, and the form of the bonding and antibonding MO's.

4. Label the following molecular orbitals with the appropriate symmetry labels σ, π, g and u (such as σ_u)

A   B   C   D   E
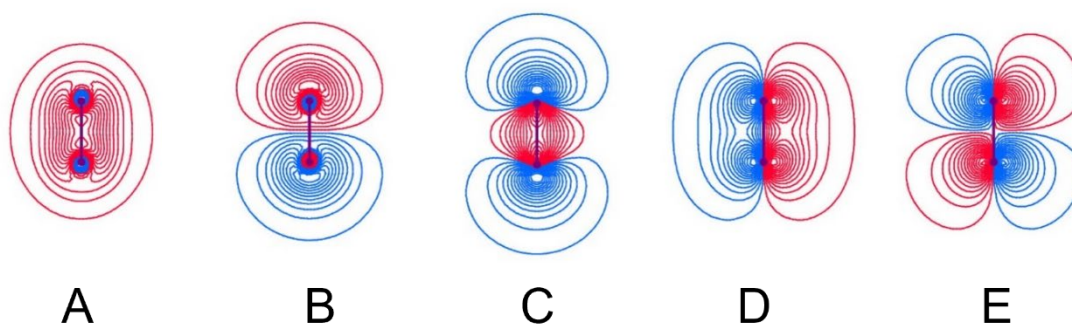
5. For a molecule A_2, one of the MO's can be formed using $2p_z$ orbital. If the internuclear axis lies along the z direction, please write the appropriate wavefunctions for the bonding MO and the ani-bonding MO using linear combination of the $2p_z$ orbital. Sketch the molecular orbitals formed.

6. For a molecule A_2, which of the following linear combination of AOs would give a zero overlap-integral ($S = 0$). Consider the internuclear axis to lie along the x-axis.
(i) s and p_z, (ii) s and p_x, (iii) p_z and p_z, (iv) p_x and p_z, and (v) p_x and p_x