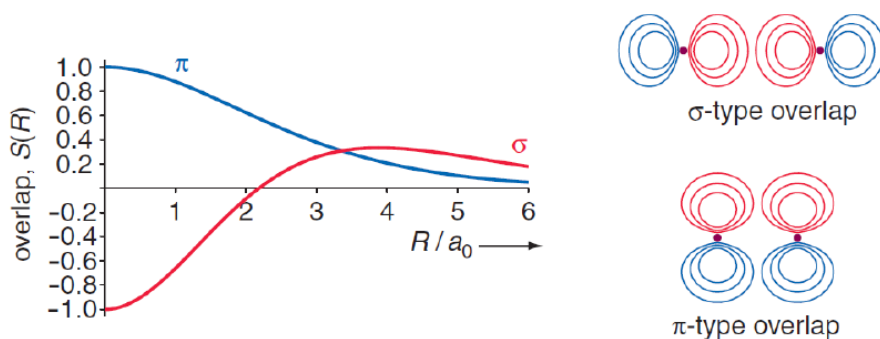
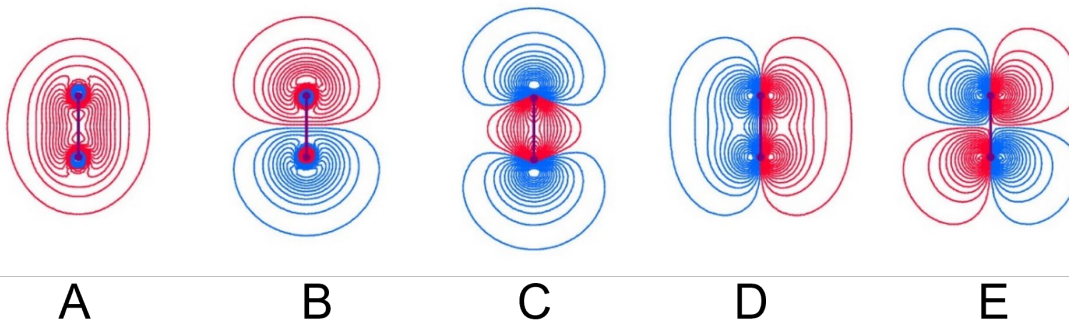


Problem set 2

1. Construct a MO diagram for H_2^+ , and make rough sketches of the form of the MO's. Explain how symmetry labels are assigned to the two MO's.
2. 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?
3. 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.



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



5. 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