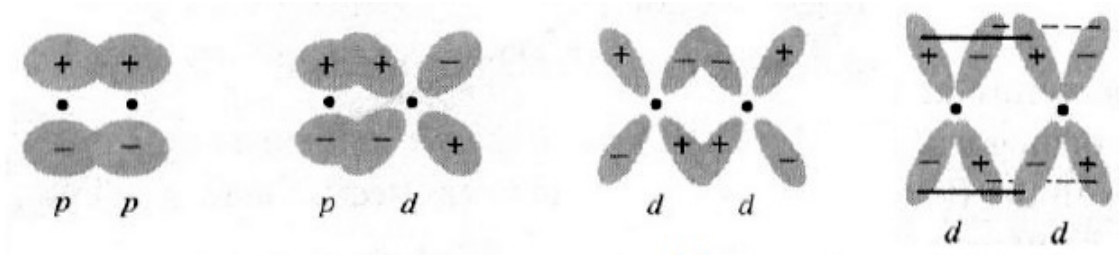
CH-107 Tutorial -4

1. **What is a spin-oribital? Why are $\alpha(1)\beta(2)$ or $\beta(1)\alpha(2)$ not acceptable two electron spin-functions?**

2. **Write the total wavefunctions (space and spin) of the He atom in the ground and first excited states. Now write the total wavefunctions in the form of Slater determinants.**

3. **Show that for Li, it is impossible to have the third electron occupy the 1s orbital (when the other two electrons already reside in 1s).**

4. **In four separate graphs, qualitatively plot the value of the overlap integral (S_{ab} in y-axis) as a function of the inter-nuclear distance (R_{ab} in x-axis) between the two nuclei for the following bonding situations. Write the MO functions for both bonding and antibonding orbitals. Draw qualitative MO pictures with proper signs (+ or –) and assign the symmetries (g/u).**



5. **Derive the expression for E+ and E- in terms of energy of H-atom and Coulomb and Exchange integrals. Draw E+ and E- as a function of Rab**

6. **Draw the contour plots of electron density for sigma bonding and antibonding of H2+.**

7. **Qualitatively draw the bonding and antibonding MOs formed due to overlap of two 2s AOs.**