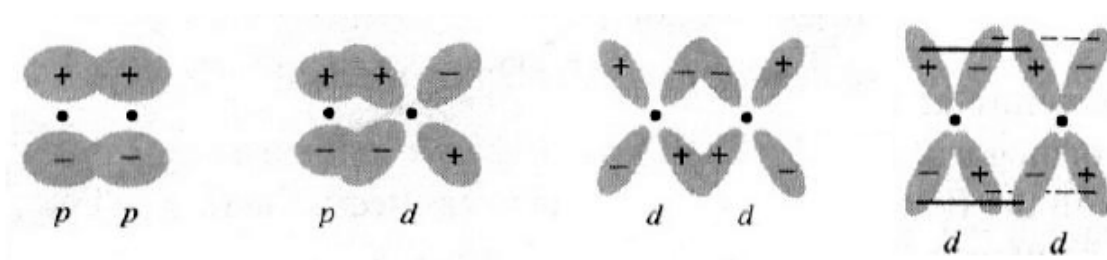


CH-107 Tutorial -4

1. What is a spin-orbital? 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 R_{ab}
6. Draw the contour plots of electron density for sigma bonding and antibonding of H_2^+ .
7. Qualitatively draw the bonding and antibonding MOs formed due to overlap of two $2s$ AOs.