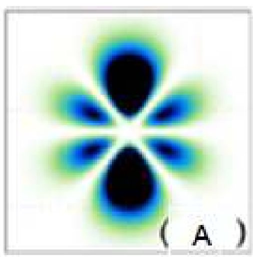
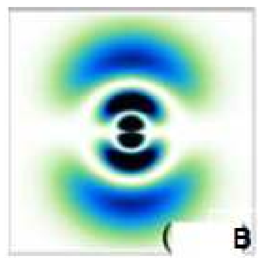
CH-103 Tutorial-3

1. **Sketch the polar plot of dz2 orbital. Pictorially (using lines/planes etc), depict all the nodal planes present in the $3d_z2$ orbital of hydrogen atom. [$3d_{z^2} = N_1(r/a_0)^2(3\cos^2\theta - 1)e^{-r/3a_0}$]. How many nodal planes are present?**

2. **Where is the probability of finding an electron in 1s and 2pz orbital greatest?**

3. **From the projections of the hydrogenic orbitals shown below, guess the quantum numbers n and l. Assign the signs (+/-) to each lobe and show the angular nodes for each orbital. (Vertical direction is z-axis)**





4. **In a single graph with proper axes labels, draw the Radial Distribution Functions for 1s, 2s, 2p and 3d orbitals for a H-like atom, clearly indicating the nodes and relative position of the maxima.**

5. **Write general Hamiltonians for a many electron atom and expand it for Li and N atoms?**

6. **Why is the function 1s (1) + 1s (2) not a wavefunction for the helium atom?**

7. **Write the total wave function (space and spin) of the He atom in the ground and first excited states.**

8. **The spectral line corresponding to the transition 2p → 2s in lithium has been observed at λ = 671 nm. Calculate the shielding constant due to two 1s electrons for a 2p electron (I.E. of Li = 0.52 10^6 J/mol).**

9. **The ionization energy of Li, Be^+, B^{+2} and C^{+3} is 0.52, 1.756, 3.658, 6.221 10^6 J/mol respectively. Plot a graph of square root of the ionization energy versus the nuclear charge for the above elements. Explain the observed relationship with the help of Bohr's expression for the binding energy of an electron in a one electron atom.**

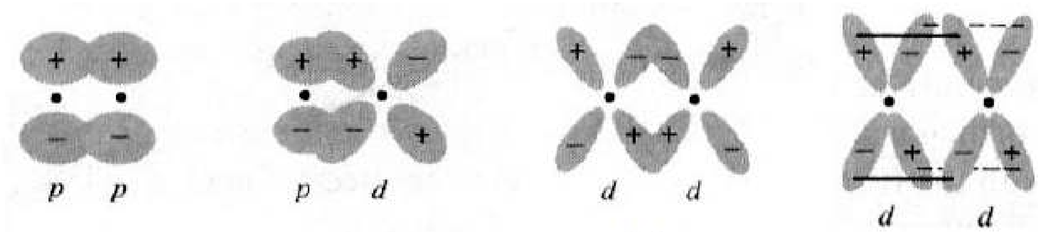
10. **Find the position of the radial node (in Å) for 2s orbital of Li if the radial part of the wavefunction can be expressed in the form $\Psi_{2s}^{200} = N''(2-\rho)e^{-\rho/2}$ where $\rho = Zeff \cdot r/a_0$ Given, first ionization energy of Li is 5.4 eV and that of H is 13.6 eV.**

CH-103 Tutorial -4

1. **The binding energy of N_2^+ is less than that of N_2 whereas the binding energy of O_2^+ is greater than that of O_2. Explain on the basis of M.O. configurations.**

2. **The bond dissociation energy of N_2 is 1837 kJ/mol and that of CO is 2081 kJ/mol. On the basis of M.O. theory, account for the difference in bond energy.**

3. **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 (lateral overlaps).**



4. **Write down the Hamiltonian for a linear H_3^+ molecular ion (*hypothetical*), where the two H – H bond lengths are equal. Draw a qualitative sketch of a bonding and an antibonding MO for this ion, using the 1s orbitals of the three hydrogen atoms.**

5. **Molecular nitrogen and acetylene (C_2H_2) are isoelectronic (14 electrons in each) and both have a triple bond. Using the structure of N_2 an analogue, predict the geometry of acetylene. What hybrid orbitals are used by the carbon atoms?**

6. **What are the coefficients of the AOs in the hybrid orbitals sp, sp^2 and sp^3. Rationalize the values of the coefficients of the above hybrid orbitals. Using the coefficients, compute the angles between the hybrid orbitals.**