# CH 107 Tutorial 6

**Please solve these problems BEFORE the tutorial session**

1. Photoelectron spectrum of a second-row homonuclear-diatomic molecule was recorded using 21.21 eV photons. It is observed that $KE_{Max}$ of ejected electrons from the top three HOMOs were 10.01, 8.23 and 5.22 eV, having intensity ratios of 1:2:1. Sketch the MO energy level diagram and hence identify the molecule. Could be both O2 and N2

2. Qualitatively draw the bonding and antibonding MOs formed due to overlap of (*i*) two 2s and (*ii*) two $3p_Z$ AOs. Assume the internuclear axis to be in z-direction. Show nodes and signs of MOs. *Hint: Draw the wavefunctions centered on the two nuclei along ±z to find nodes!*

3. Write the expressions for the delocalized *σ bonding* MOs of $\boldsymbol{BeH_2^+}$ as linear combinations of valence AOs of appropriate symmetry. *Do not invoke s-p mixing and consider +z to be the internuclear axis for this linear molecule.*

   a) Sketch the bonding MOs, show signs and nodes (if any), and assign symmetries ($g/u$).

   b) How many lines/bands are expected in the *entire* photoelectron (PE) spectrum?

   c) What are their relative intensities? (note that the molecule has *+1* charge)

4. Draw a qualitative contour sketch of a 2s-2p hybridized orbital oriented along −y direction carefully showing the position of the nucleus, and the nodal plane/surface.

5. For water, it is experimentally determined that the H-O-H bond angle is 104.5°. Determine the coefficients of atomic orbitals of O that participate in hybridization (see schematic, lone pairs are in *xz* plane, not relevant).