1 Morning class week 5 day 5: The left-to-right H_2O MO diagram and photoelectron spectroscopy

The goal of today's lecture is to generate the H_2O MO diagram and show its connection to photoelectron spectroscopy.

1. **Constructing the H_2O MO diagram**

   (a) How many valence AOs are there in total for H_2O? How many MOs will there be in the H_2O MO diagram?

   (b) The H 1*s* orbital has an energy of -13.6 eV. Oxygen 2*s* and 2*p* are at -14.8 and -32.3 eV. Start drawing the H_2O MO diagram by placing the AOs at the correct relative height to one another.

   (c) Rather than draw these AOs on the two borders of the MO diagram, we will draw them on a single side, the left side.

   (d) Draw on another area of the paper the lowest possible MO which you can imagine.

   (e) Draw on another are of the paper the highest possible MO which you can imagine.

   (f) Which orbitals will you have to mix in order to make these two orbitals? We will have to do this mixing in three distinct steps, as will be shown in class. Note that at each step, we retain six orbitals in each and every column of orbitals.

   (g) At this point we will have made the lowest and highest possible energy orbitals which we can imagine. Among the remaining orbitals, which orbitals will we have to mix to make the next lowest and highest energy possible orbitals? This step will lead to six MOs, the final six MOs of the H_2O MO diagram.

   (h) Please follow the Aufbau principle and fill these orbitals with the correct number of valence electrons.

   (i) Based on the above results please draw a conventional H_2O MO diagram with AOs placed on the side and the final MOs, filled or unfilled, placed in the center.

   (j) What is the H_2O molecular bond order? How many lone pairs are there?

   (k) Please draw the H_2O Lewis structure.

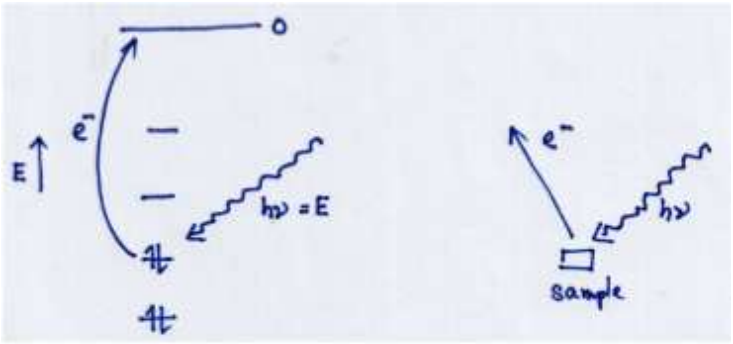
   (l) Please review what you have learned.

2. **Photoelectron spectra of molecules**

   (a) Please recall the set-up of the photoelectric effect, shown on the next page. It is also the basis of photoelectric spectroscopy, PES.

   (b) The middle panel of the second figure on the next page is the PES of an individual water molelcule. Based on the H_2O MO diagram, draw next to each peak the MO responsible for the peak. Low energy MOs are shown to the *left* of the horizontal axis.

   (c) The third picture on the next page is the PES of N_2 gas. Based on the N_2 MO diagram, draw next to each peak the MO responsible for the peak. Low energy MOs are shown to the *right* of the horizontal axis.



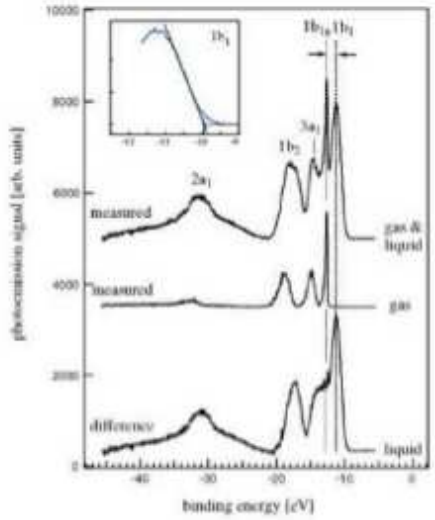


Figure 1: PES of H_2O in gas and liquid forms