1 Morning class week 5 day 5: The left-to-right H$_2$O MO diagram and photoelectron spectroscopy

The goal of today’s lecture is to generate the H$_2$O MO diagram and show its connection to photoelectron spectroscopy.

1. Constructing the H$_2$O MO diagram

(a) How many valence AOs are there in total for H$_2$O? How many MOs will there be in the H$_2$O MO diagram?
(b) The H 1s orbital has an energy of -13.6 eV. Oxygen 2s and 2p are at -14.8 and -32.3 eV. Start drawing the H$_2$O 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 area 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$_2$O 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$_2$O MO diagram with AOs placed on the side and the final MOs, filled or unfilled, placed in the center.
(j) What is the H$_2$O molecular bond order? How many lone pairs are there?
(k) Please draw the H$_2$O 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 molecule. Based on the H$_2$O 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$_2$O in gas and liquid forms