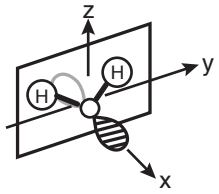
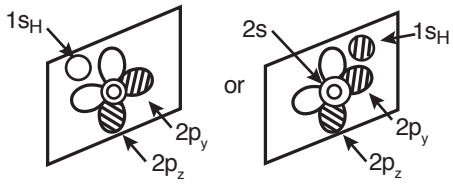
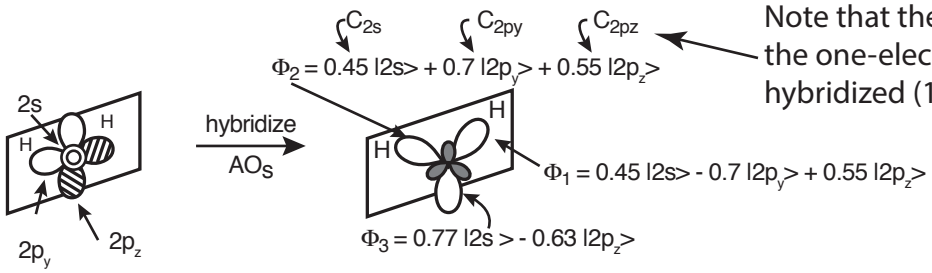
Structure and orbital energies of water with VB orbital basis set:



No net bonding or antibonding overlap of hydrogen 1s with oxygen $2p_x$: $\langle 1s|\hat{h}_1|2p_x\rangle = 0$

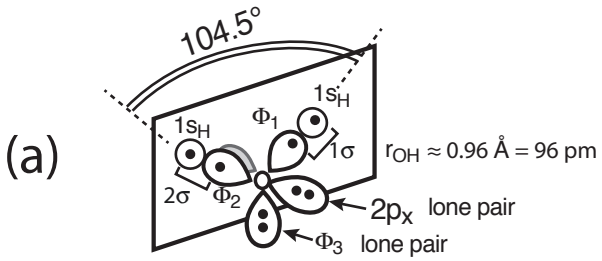


Bonding or antibonding overlap of each hydrogen 1s with oxygen 2s, $2p_y$, and $2p_z$ is possible

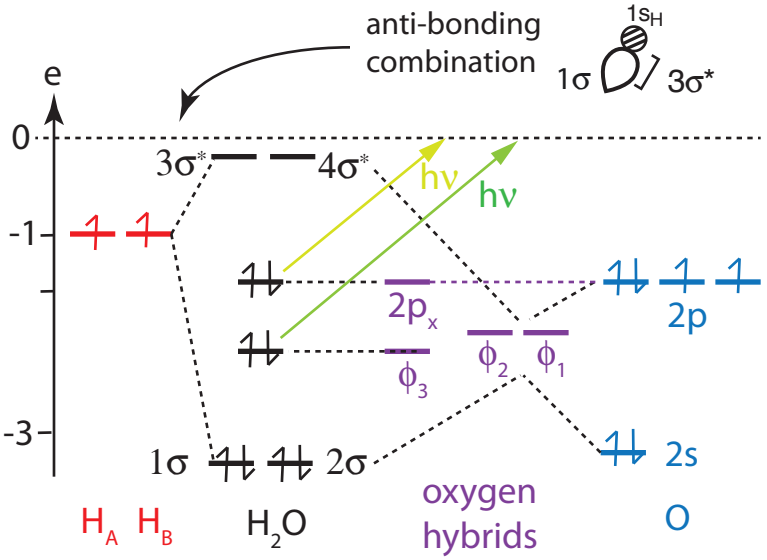


Note that the optimized coefficients c_i of the one-electron orbitals are not quite sp^2 hybridized (120°), but rather 104.5°.

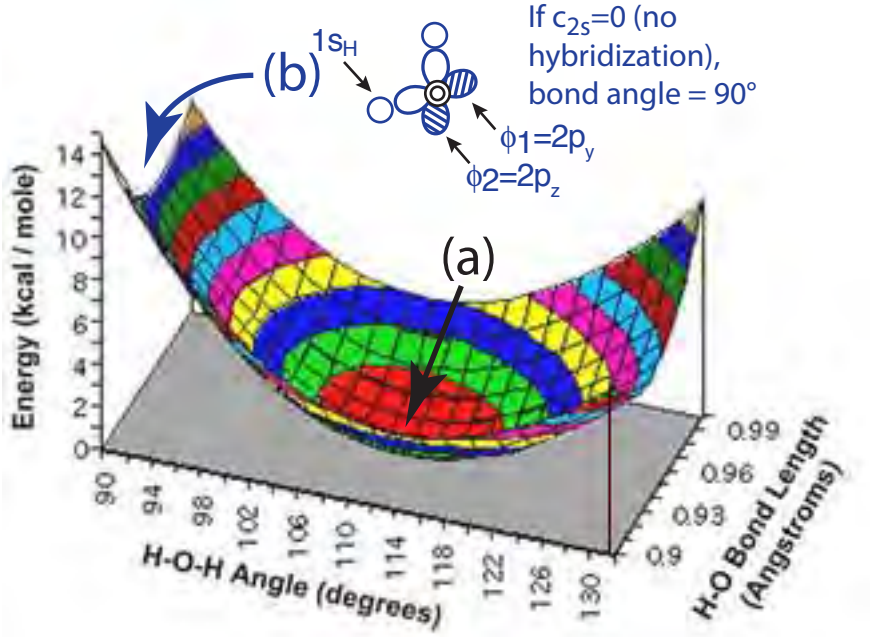
VB bonding in H_2O



Note: lone pairs are in different shape and energy orbitals, but the e- density fills out space below O symmetrically and in a plane perpendicular to the two bonds.



Potential surface of water (only 2 coordinates shown)



The photoelectron spectrum of H_2O has 2 peaks in the energy range of the non-bonding (lone pair) orbitals.