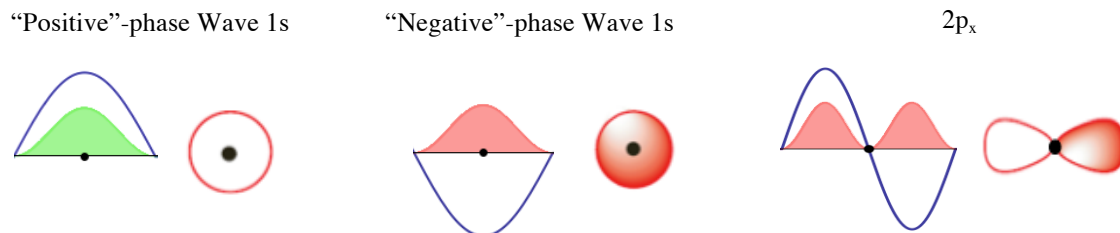


23. Bonding and Anti-Bonding Orbitals

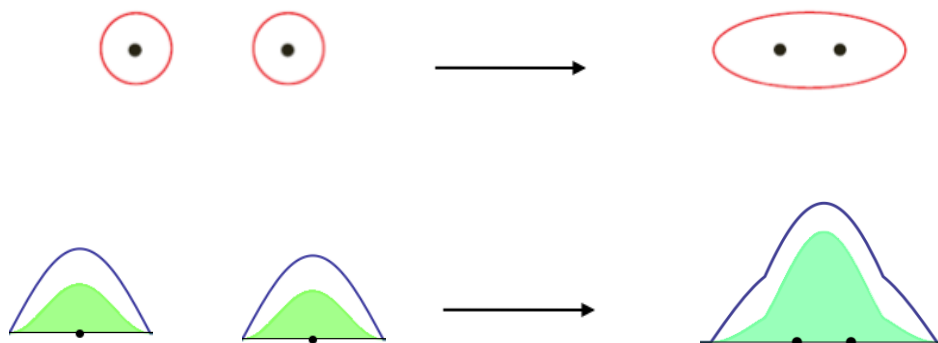
Electron orbitals of individual atoms interact with each other based on whether or not their corresponding electron waves are in phase or out of phase. During these interactions, constructive or destructive interference changes the electron density of the resulting molecular orbital. Now, let's take a look at what the resulting orbital looks like for each of these kinds of interactions. The images below show the 1D and 3D electron waves for 1s and 2p_x atomic orbitals. The negative-phase waves will be indicated by shaded orbitals



We will now use this notation to determine the resulting shapes of the electron orbitals for molecular orbitals. Below are a series of isolated atomic orbitals. Draw the resulting molecular orbitals based on how the electron waves interfere with each other. The results of the wave interference are either bonding σ orbitals (σ), or anti-bonding σ orbitals (σ^*). Use the two following applets to help you answer the questions below:

- (A) 1s orbitals <http://quantum.bu.edu/CDF/101/1sMolecularOrbitals.cdf>
 (B) 2p orbitals <http://quantum.bu.edu/CDF/101/2pMolecularOrbitals.cdf>

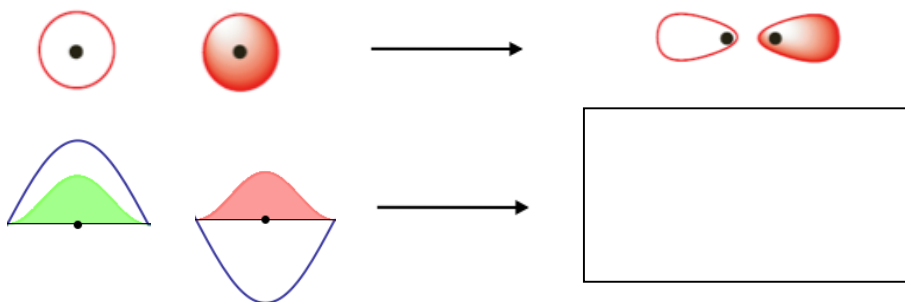
1) Use applet A to explore the overlap of two, 1s atomic orbitals that are in phase. Notice that *because of constructive interference between the two in phase electron waves, the electron density is the greatest in between the two nuclei.*



What is the name of the resulting orbital (on the right)?

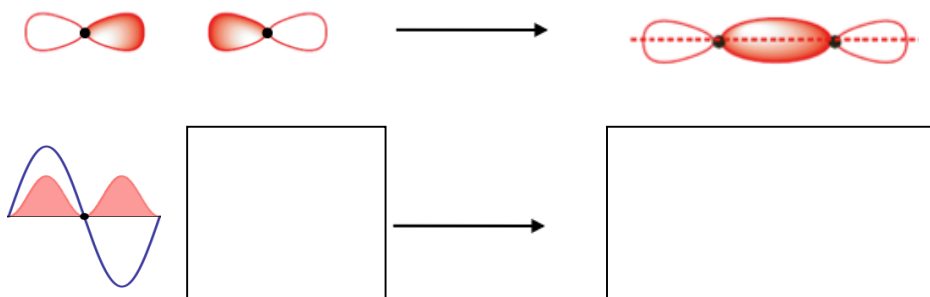
2) Two, $1s$ atomic orbitals that are out of phase: *Because of destructive interference between the two out of phase electron waves, a nodal plane is created in between the two nuclei where the electron density is zero. The electron density for the molecular orbitals is greatest on the outside of the two nuclei.*

In the box, draw the graph for the resulting molecular orbital. What is the name of this molecular orbital?

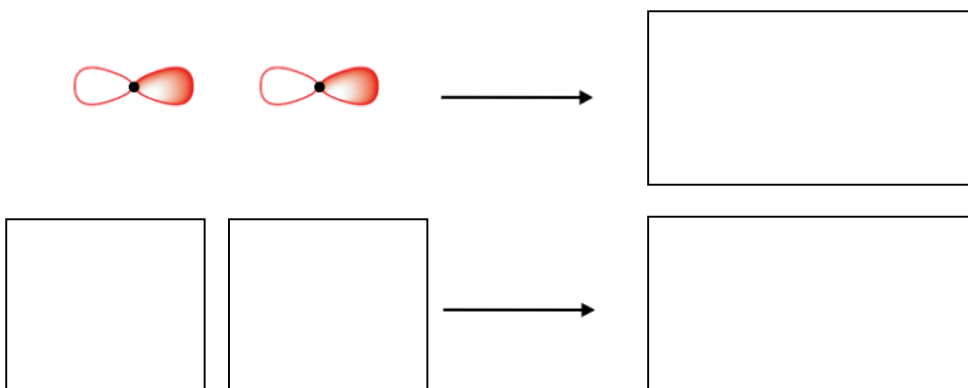


3) Two, $2p_x$ atomic orbitals overlapping in phase: *The center two loops of the $2p_x$ atomic orbitals create one large loop in the center of the molecular orbital because of constructive interference of the electron waves between the nuclei)*

In the boxes, draw the graphs for the missing atomic orbitals and the resulting molecular orbital.



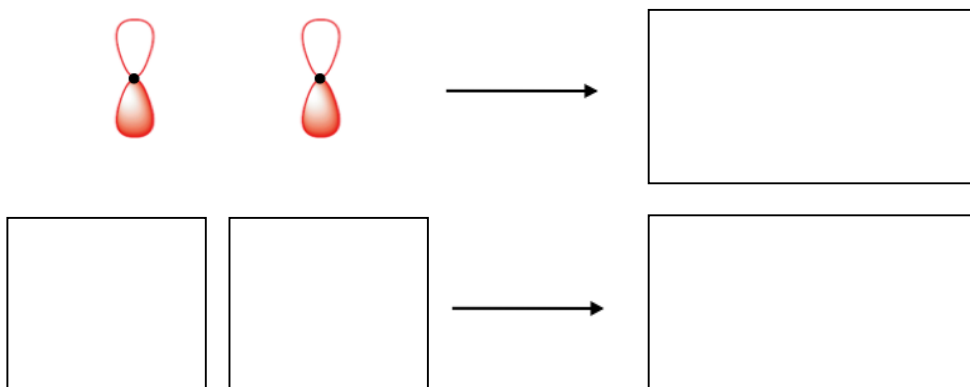
3) Two, $2p_x$ atomic orbitals that overlap out of phase: Draw the resulting molecular orbital and the graphs showing this type of interference.



When the orbitals are not aligned on the same axis as the interference, a different type of interference occurs. For example, when two $2p_y$ orbitals combine along the x-axis (drawn below), the interference occurs both above and below the nuclei. The results of this interference are either bonding π orbitals (π), or anti-bonding π orbitals (π^*).

In the two examples given below, draw the resulting molecular orbitals and determine whether they are bonding or anti-bonding orbitals.

4) Two, $2p_y$ atomic orbitals that are in phase



5) Two, $2p_y$ atomic orbitals that are out of phase

