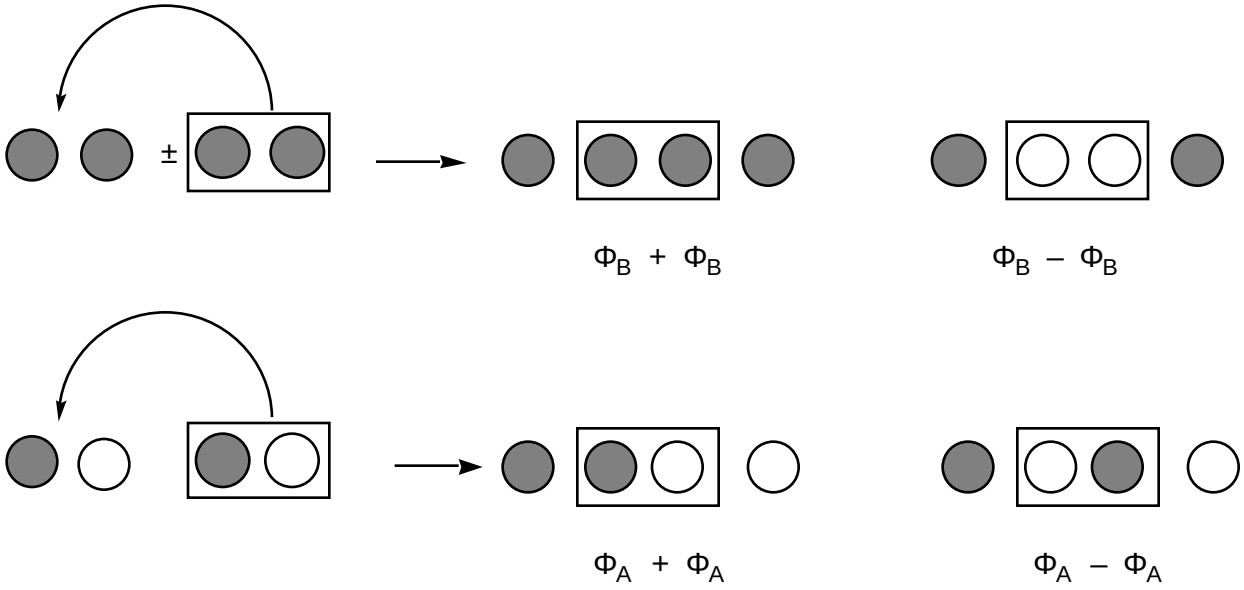
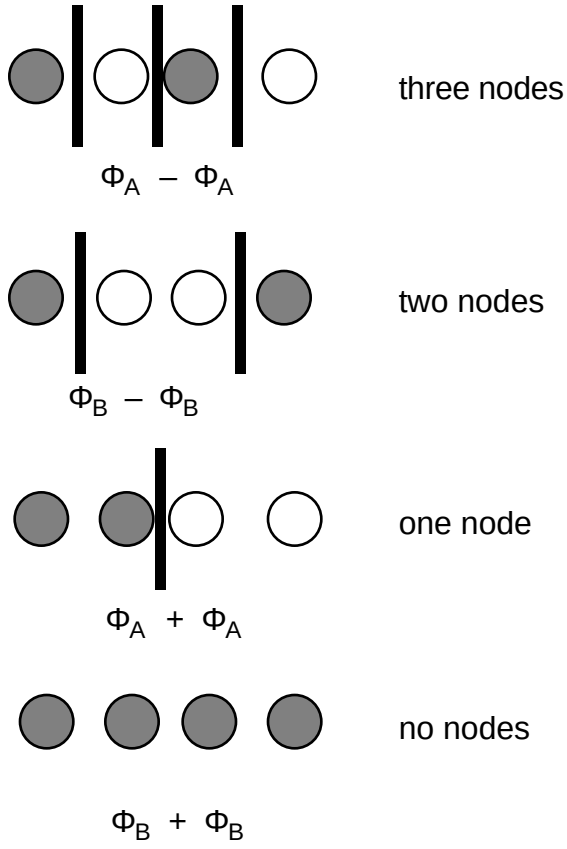
Answers to the ad hoc H_4 Problem Set

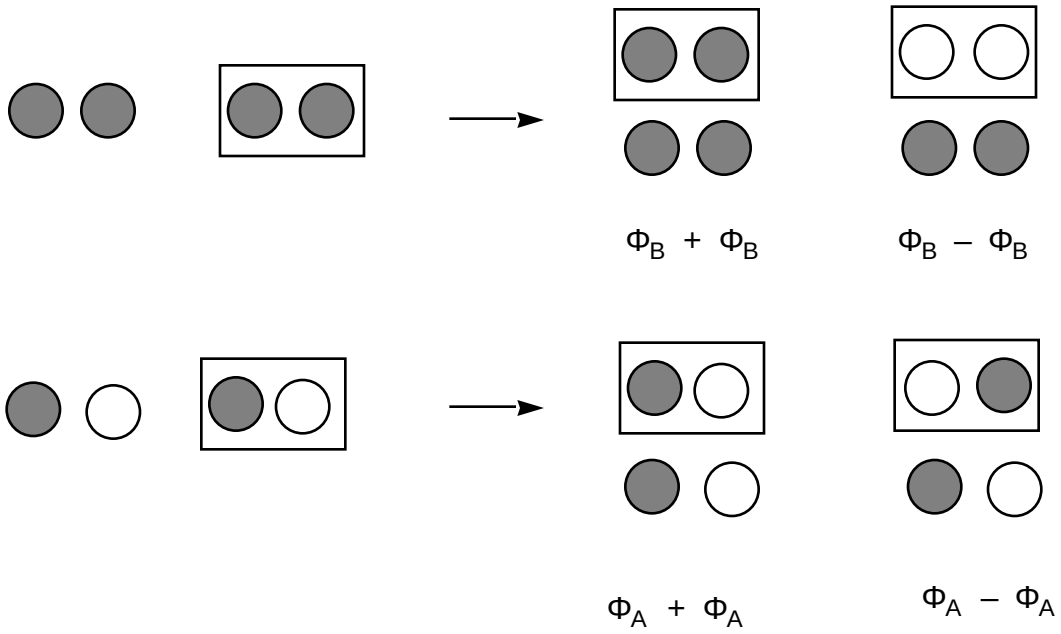
1. Once again we take combinations: $\Phi_B \pm \Phi_B$ and $\Phi_A \pm \Phi_A$:



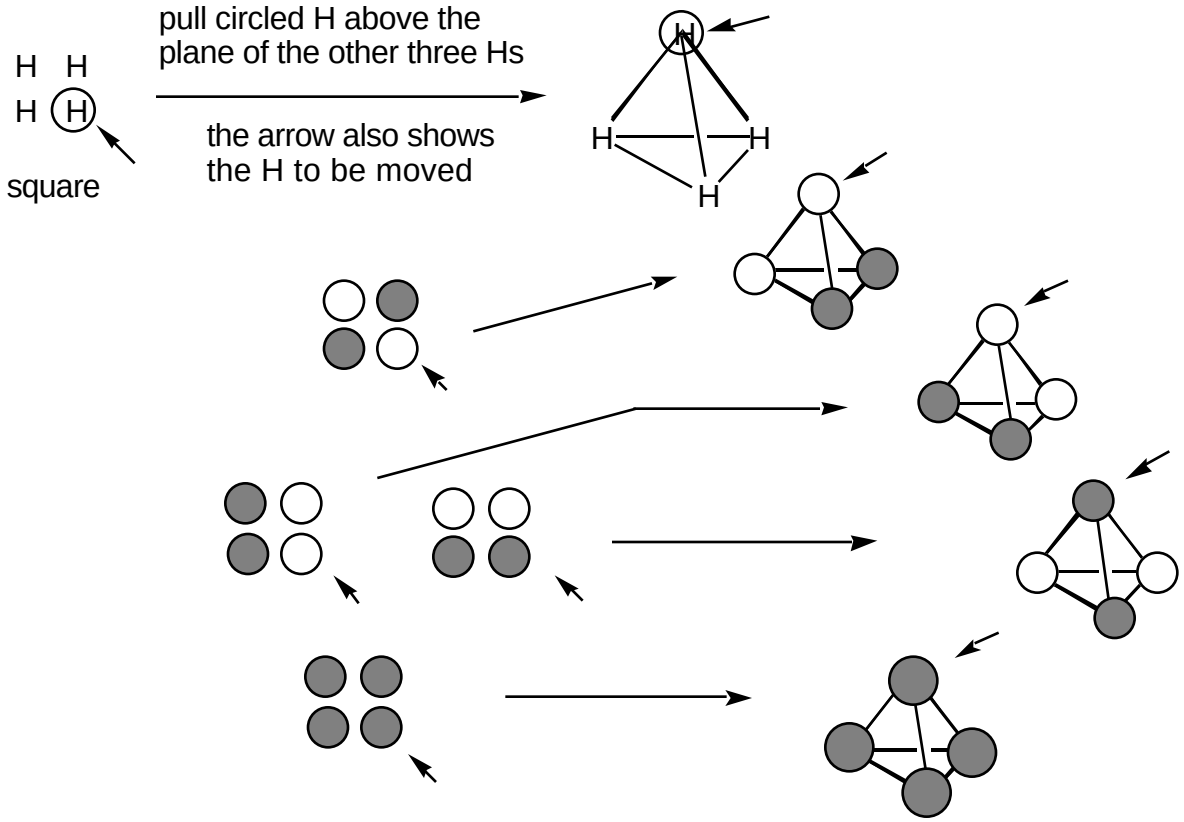
Order in energy by counting nodes.



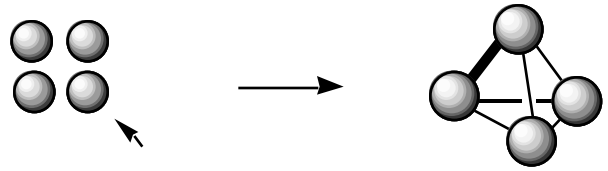
2.



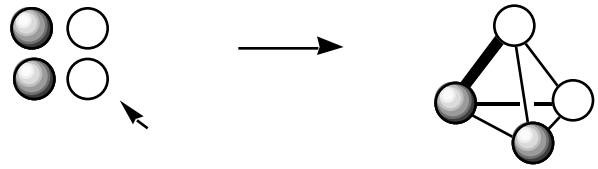
3. Here are the new MOs - just pop that one lobe up as instructed:



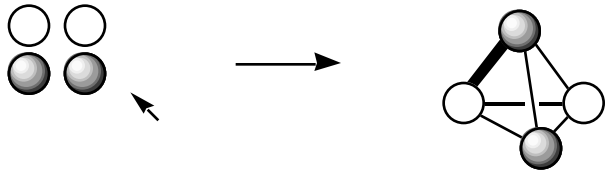
Here is how the old orbitals change in energy as the new ones are formed. The boldface line shows the new interaction.



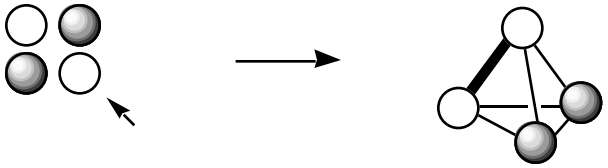
Two new 1,2 bonding interactions. Energy does down



Two new 1,2-antibonds
Energy goes up



Two new 1,2-antibonds
Energy goes up



Two new 1,2-bonding interactions. Energy does down

Here's a diagram showing all the orbitals. The critical (and not so easy) thing to see is that three of the new MOs are equivalent - they have exactly the same form, and hence the same number of new nodes (one), and will be at exactly the same energy.