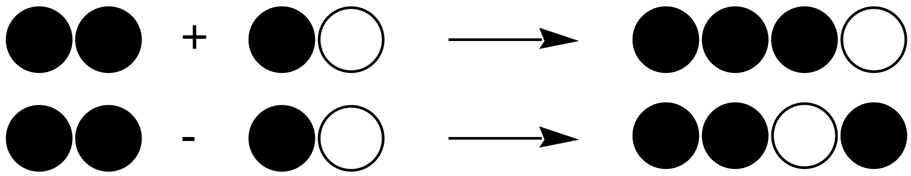
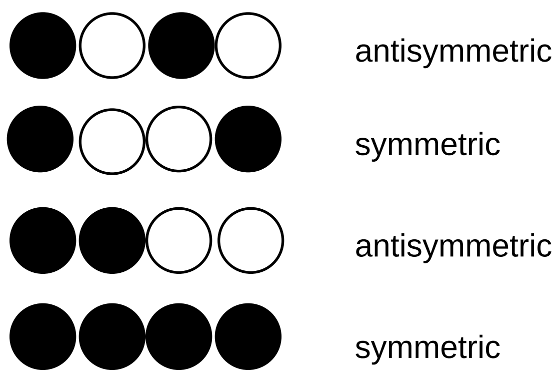
Question: When we constructed the MO's for linear H_4, why didn't we try combining the bonding MO (ψ_b) of the left-hand H_2 molecule with the antibonding MO (ψ_a) of the right-hand H_2 molecule, as shown below?



Answer: In principle, we could have also tried these combinations. However, not all combinations are legal, and it turns out that the two MO's for H_4 shown above are struck down by the dreaded purple X of impossibility. The reason has to do with *symmetry*.

Note that linear H_4 is a symmetric molecule. The left-hand side of the molecule is identical to the right-hand side, since the individual H atoms are indistinguishable except for their relative positions. It turns out that, in general, any legal MO must obey the symmetry of the molecule. (This isn't quite true, but is close enough for the present purposes). Thus in the case of linear H_4, the left-hand and right-hand halves of each MO must either be identical, or identical except for a change of sign. In the former case, the MO would be called *symmetric*, and in the latter case, *antisymmetric*. All the legal MO's for H_4 can readily be categorized as either symmetric or antisymmetric:



Now you can see the problem with the other two MO's proposed at the beginning of the question: they are neither symmetric nor antisymmetric. That is, they do not obey the symmetry of the molecule.

There are other principles as well, which we have not discussed, governing which combinations of atomic orbitals (AO's) constitute legal MO's. However, for small molecules, one can often derive the correct set of MO's just by using symmetry together with the fact that the number of MO's you get out has to equal the number of MO's or AO's with which you began.