



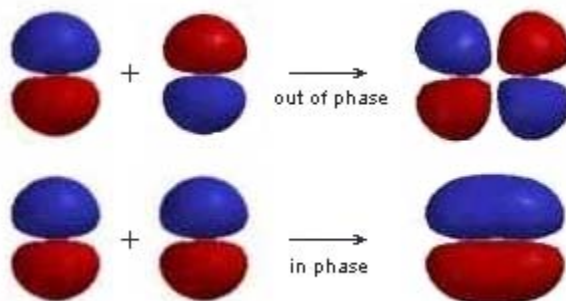
## Pi Molecular Orbitals of Ethene

- In chapter 1 we saw that the [molecular orbitals of H<sub>2</sub>](#) are created by the combination of 1s orbitals.
- The in-phase combination gave the bonding orbital.
- The out-of-phase combination the anti-bonding orbital.
- For ethene, the  $\sigma$  framework is created by the interaction of the  $sp^2$  hybrid orbitals of the C atoms and H 1s orbitals.
- Each C has a p orbital unused by the hybrids and it is these on the adjacent C atoms that interact to form the C-C pi bond.

The in-phase and out-of-phase combinations for the interaction of two p atomic orbitals in a  $\pi$  (*i.e.* side to side) fashion to give the two  $\pi$  molecular orbitals are shown below:

Here the different phases of the lobes in the p orbitals are represented by the two different colours.

Notice that *neither* of the molecular orbitals are symmetric with respect to the internuclear axis and that the out of phase combination has an extra vertical nodal plane between the nuclei.



**Question:** What type of molecular orbitals are symmetric with respect to the internuclear axis ? **ANSWER ?**

The diagram to the right shows the relative energies of the atomic p orbitals, the resulting  $\pi$  molecular orbitals and the electron configuration.

(The same rules for filling orbitals applies to molecular orbitals as is used for atomic orbitals: [review?](#))

The two electrons from the atomic p orbitals are now paired in the stabilised  $\pi$  bonding orbital. This is the highest occupied molecular orbital or **HOMO** in ethene (or any simple alkene).

In contrast, the  $\pi^*$  anti-bonding orbital contains no electrons. It is the lowest unoccupied orbital or **LUMO** in ethene (or any simple alkene).

