Atomic and Molecular Physics

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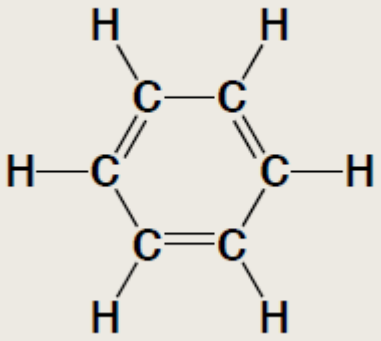
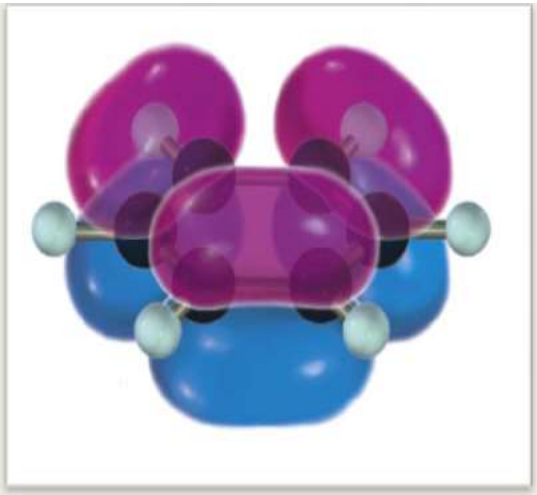
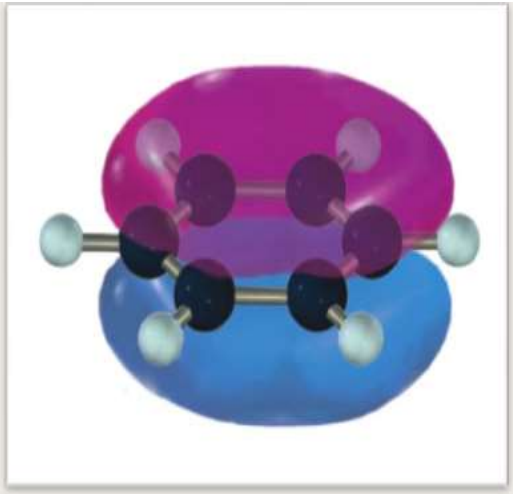
Molecular Orbital Theory

A more accurate theory than valence bond theory is molecular orbital (MO)theory. In molecular orbital theory, we imagine that electronic orbitals cover the whole molecule and are not localised on one atom. These diagrams show the difference between valence bond theory and molecular orbital theory when considering the orbitals of benzene.





Valence bond theory: three sets of **localised** π-bonds (the σ-bonds are shown as sticks).

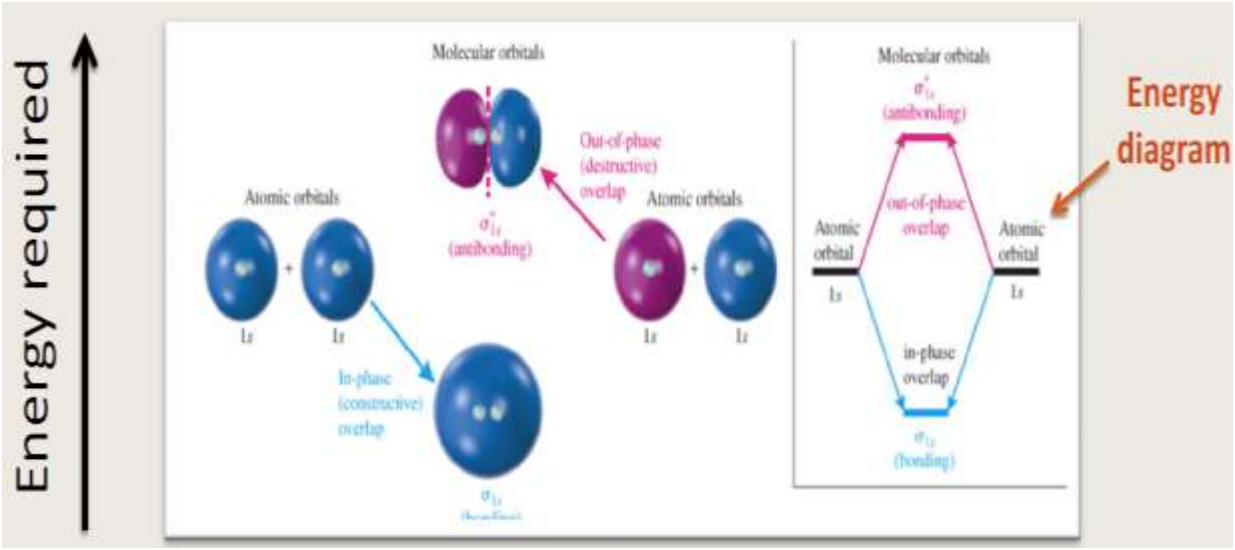


Molecular orbital theory: orbitals are spread over whole molecule.

Energy Diagrams

Now let's look at the simplest molecule, dihydrogen (H_2).

A H_2 molecule is made by superimposing (overlapping) the 1s orbitals of two H atoms. If the orbitals have the same phase, they will interfere construcDvely and form a molecular orbital with greater electron density between the posiDvely charged nuclei. It will require less energy to hold the atoms together if there are electrons in this orbital and the orbital is called a bonding orbital.



- **Atomic orbitals mix together and make:**
  - **Bonding Orbitals**
    Electrons in these orbitals help hold atoms near each other
  - **Antibonding Orbitals**
    Electrons in these orbitals push atoms apart from each other
  - **Nonbonding Orbitals**
    Electrons in these orbitals have no effect on bonding