



- **CONDITIONS FOR COMBINATION OF ATOMIC ORBITALS**

- For atomic orbitals to combine, resulting in the formation of molecular orbitals, the main conditions are :
- The combining atomic orbitals should have almost the same energies. For example, in the case of diatomic molecules,  $1s$ -orbital of one atom can combine with  $1s$ -orbital of the other atom, but  $1s$ -orbital of one atom cannot combine with  $2s$ -orbital of the other atom.
- The extent of overlap between the atomic orbitals of the two atoms should be large.
- The combining atomic orbitals should have the same symmetry about the molecular axis. For example,  $2p_x$  orbital of one atom can combine with  $2p_x$  orbital of the other atom but not with  $2p_z$  orbital .
- *Note*: It may be noted that  $Z$ -axis is taken as the inter-nuclear axis according to modern conventions.

Atomic orbitals



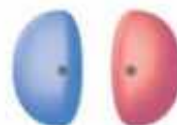
Combine  
atomic orbitals



Subtract

Add

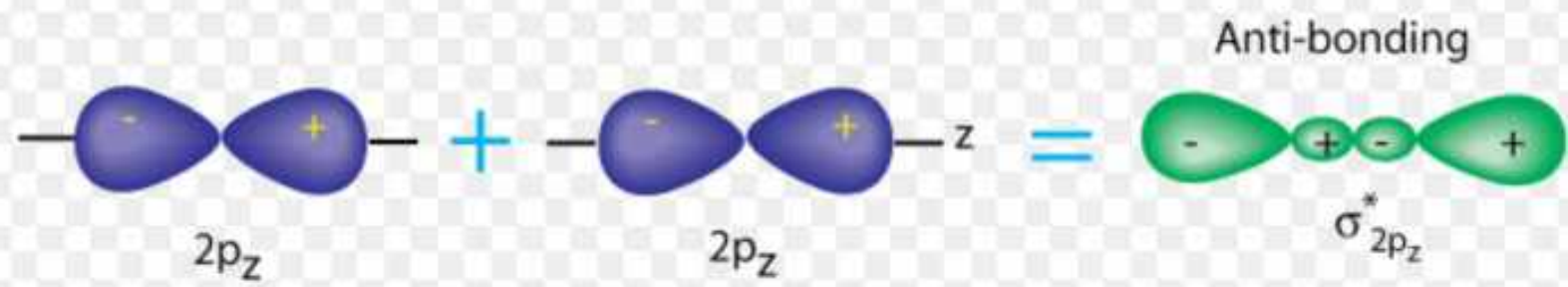
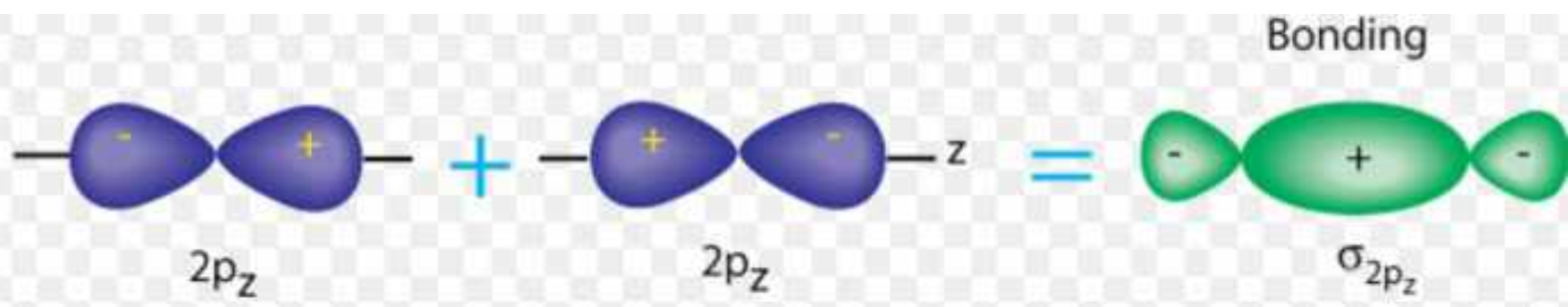
Molecular orbitals



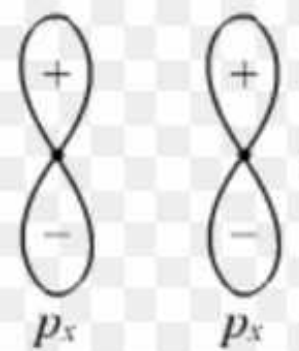
Antibonding  
orbital,  $\sigma_s^*$



Bonding  
orbital,  $\sigma_s$



Atomic orbitals



Molecular orbitals

