Hybridization of atomic orbitals

In general VSEPR predicts the shape of molecules and ions accurately

CH_4 : tetrahedral

Four equal bonds with equal HCH angles

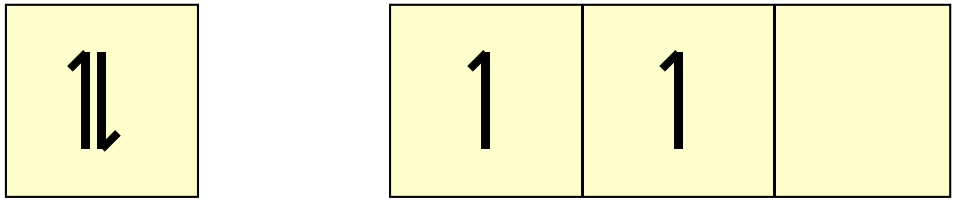
A covalent bond is formed by sharing two electrons by two atoms

Imagine an orbital (containing 1 electron) from one atom overlaps with an orbital from the other atom to form the bond

According to this view four orbitals are needed from the carbon atom to overlap with the four orbitals of the hydrogen atoms

The ground state of C: $1s^2\ 2s^2\ 2p^2$

Valence shell can be represents as:



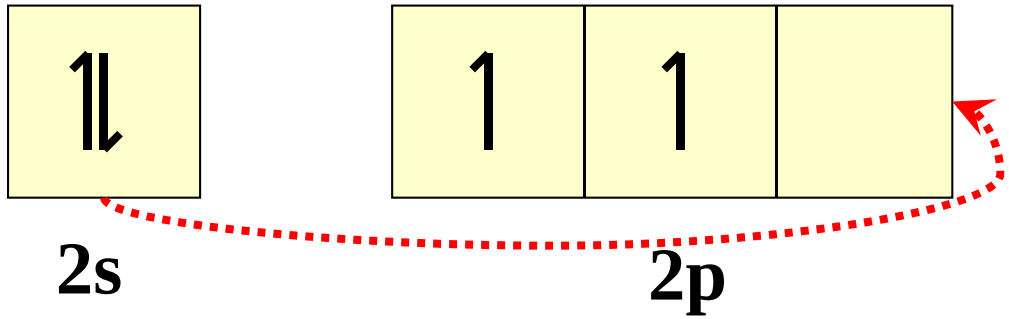
2s **2p**

there are only two orbitals with two single electrons!

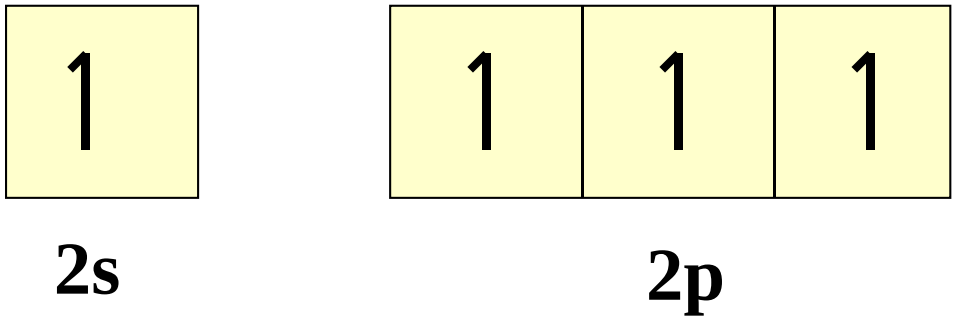
So, how the four bonds in CH_4 were formed?

This can be explained by the concept of hybridization

Ground state of C



Excited state of C



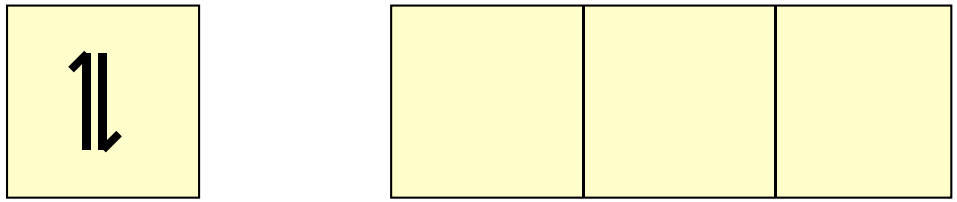
Now we have four orbitals with one electron in each orbital

One (2s) orbital mixes with three (2p) orbitals to form Four orbitals of sp^3 type

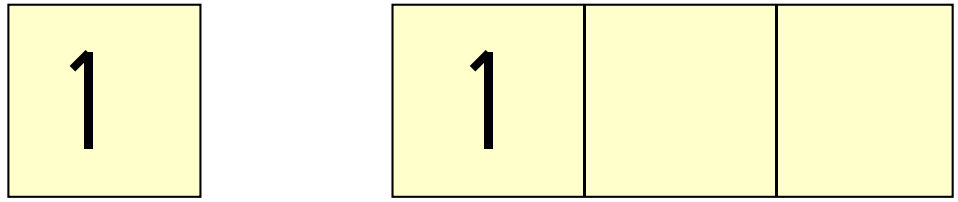
sp hybridization

$BeCl_2$ **Lewis structure: Cl—— Be —— Cl**

Ground state for B



Excited state for B

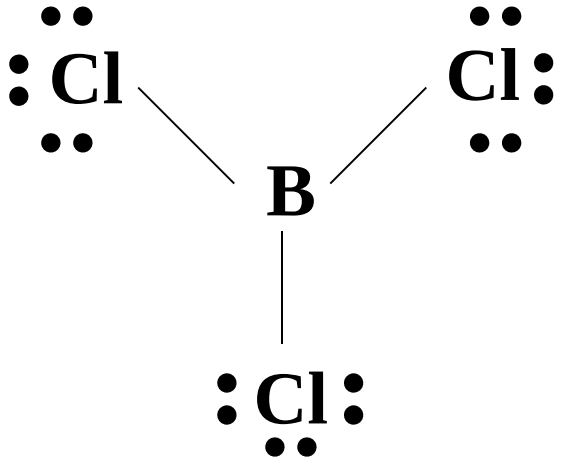


One (2s) orbital mixes with one (2p) orbital to form two orbitals of *sp* type

Molecules with sp hybridization are *linear*

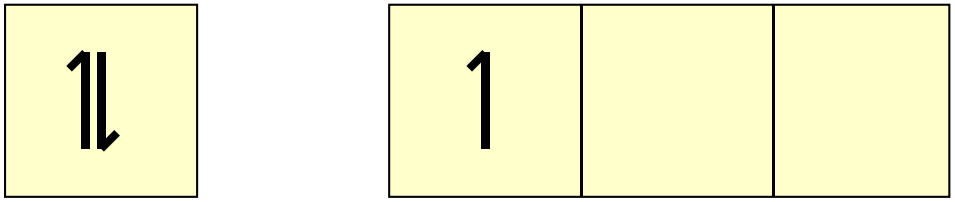
sp^2 hybridization

BCl_3 **Lewis structure:**

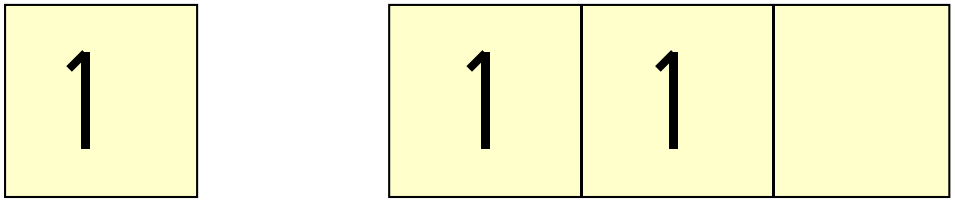


Shape: triangular & planar

Ground state for B



Excited state for B



One (2s) orbital mixes with two (2p) orbital to form three orbitals of *sp*^{2} type

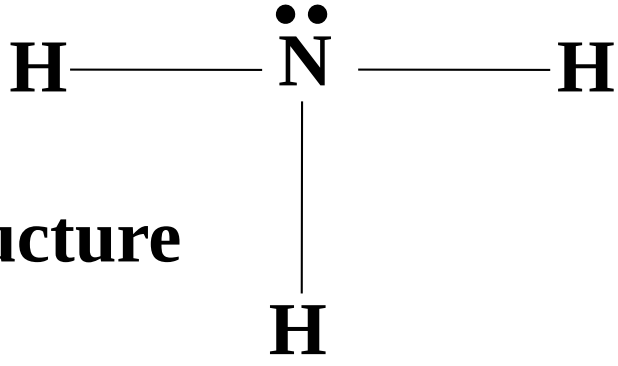
Molecules with sp^2 hybridization are *triangular and planar*

sp^3 hybridization

We saw the the tetrahedral CH_4 has a sp^3 hybridization

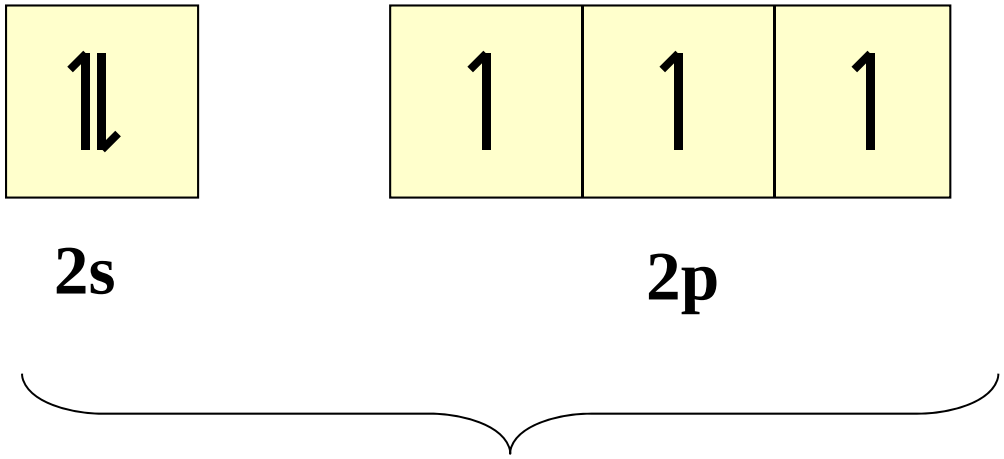
Consider NH_3

Lewis structure



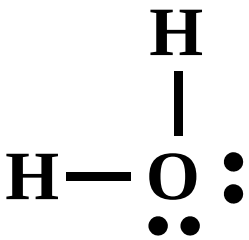
The valence shell of the central atom (N) in the molecule has four orbitals three bonding and one nonbonding

Ground state for N

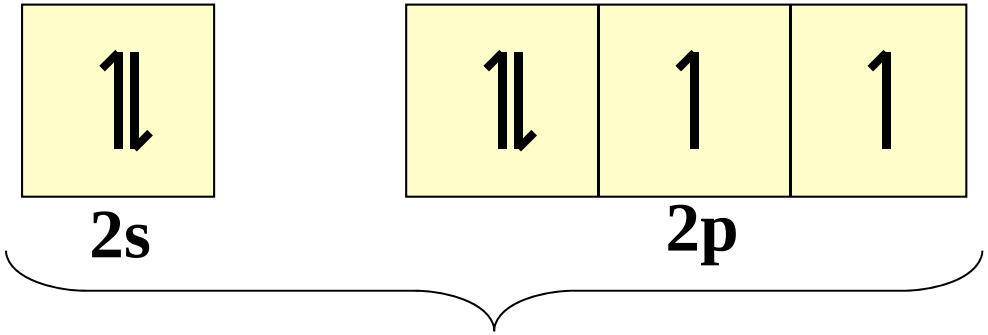


H_2O

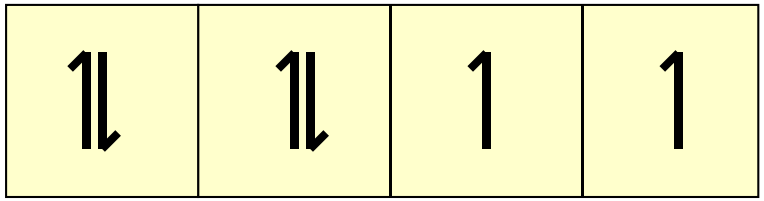
Lewis structure



Ground state for O:



hybridize



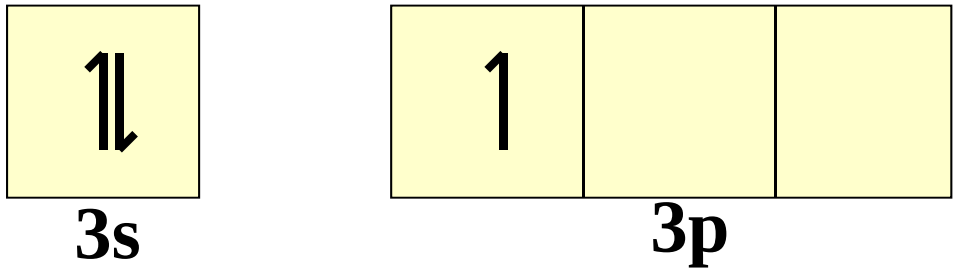
sp³

Example

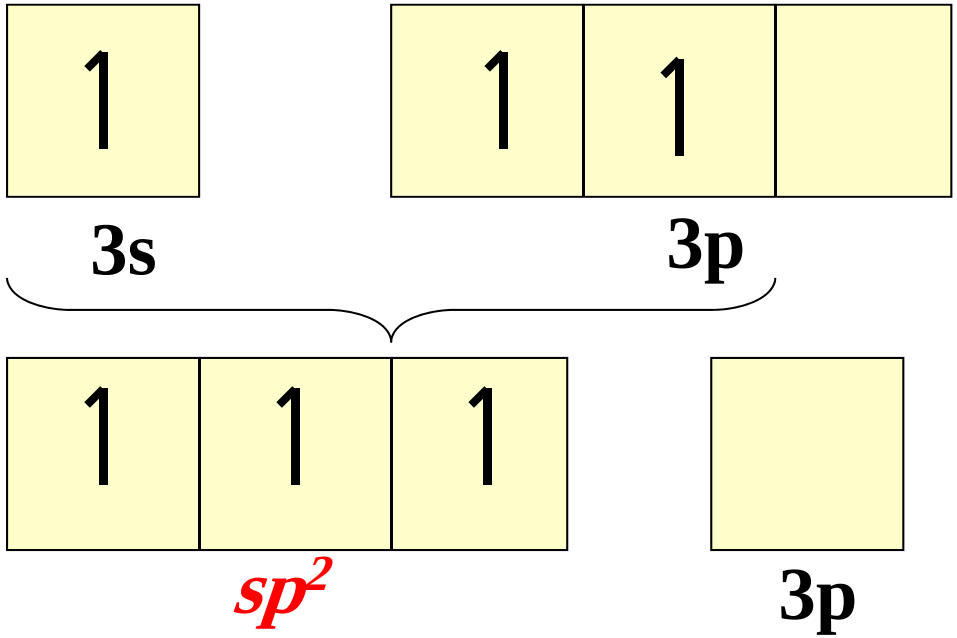
What type of hybrid orbital is employed by *Al* in AlI_3?

Electronic configuration of *Al*: [Ne] $3s^2\ 3p^1$

Ground state



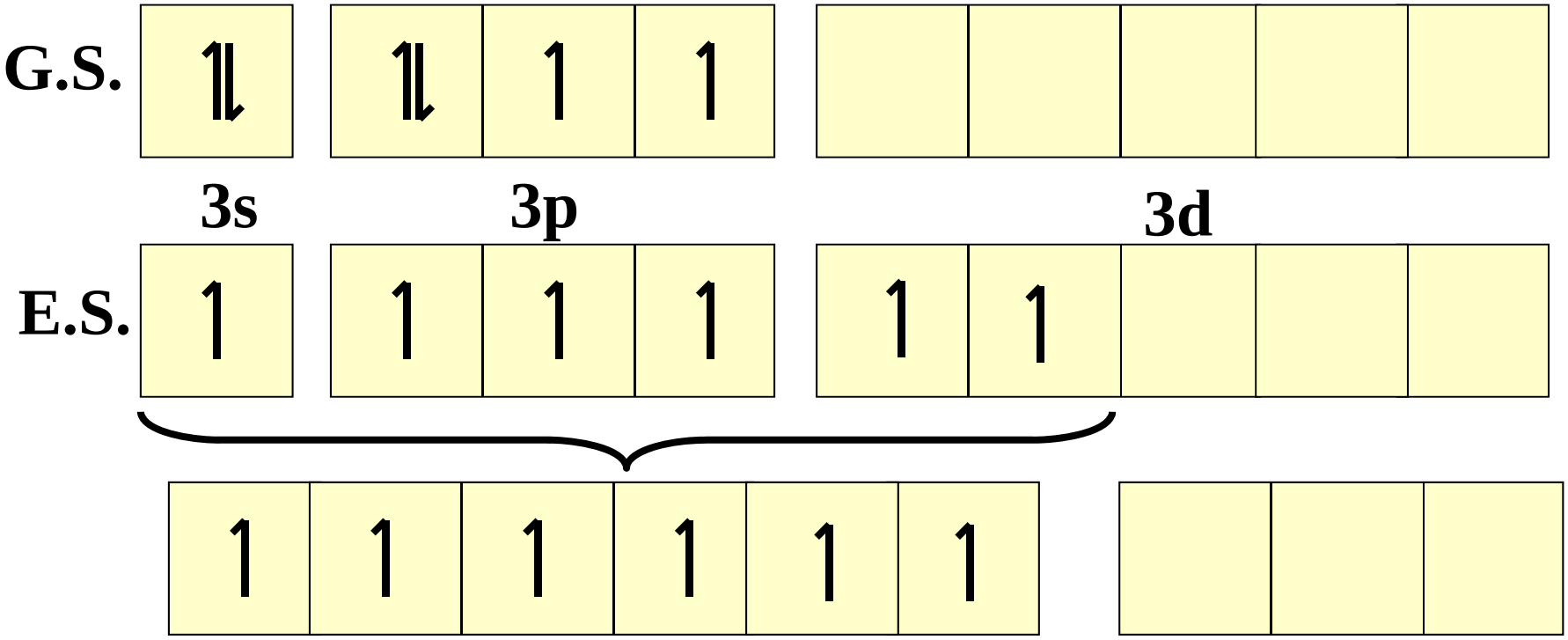
Excited state



s, p, and d hybridization

SF_6 : 6 covalent bonds, Octahedral

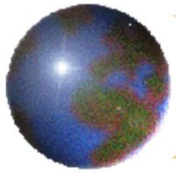
S: [Ne] $3s^2$ $3p^4$



sp^3d^2

Empty 3d orbitals

PBr_5 : sp^3d hybridization for the P atom

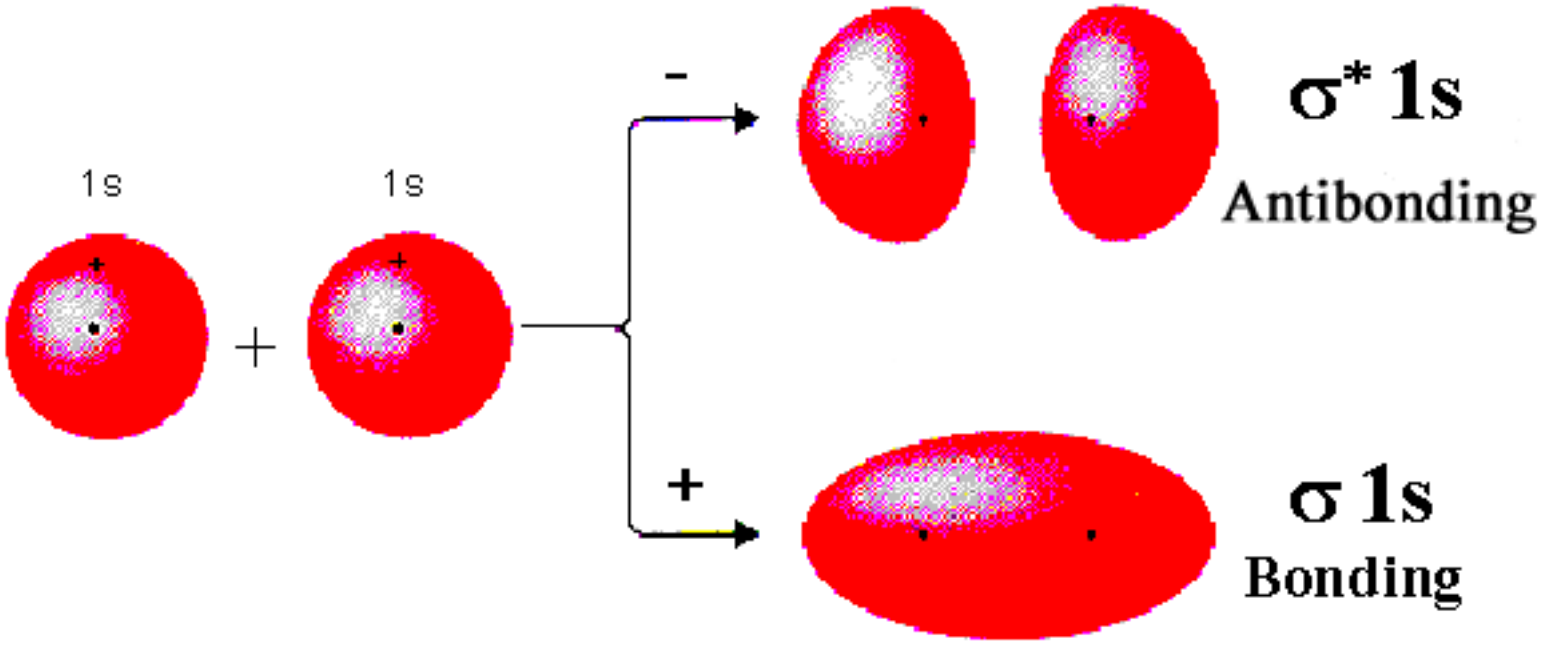


Molecular orbitals

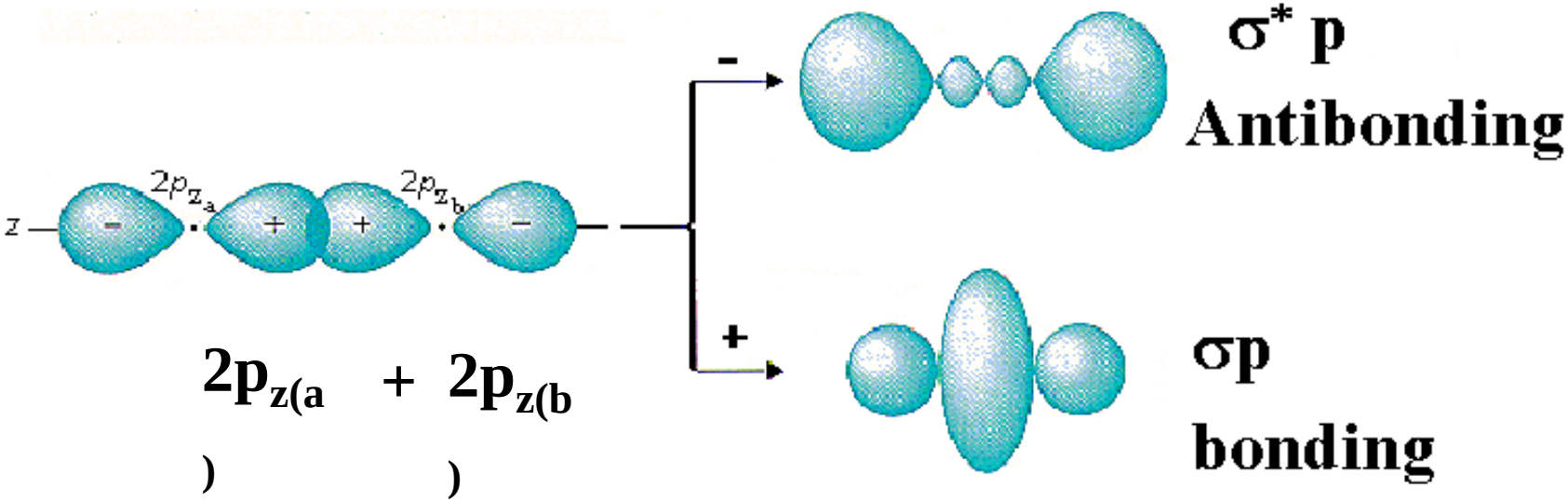
All bonding methods discussed so far are in terms of atomic orbital

Molecular orbital theory discusses bonding in terms of orbital associated with the molecule s a whole

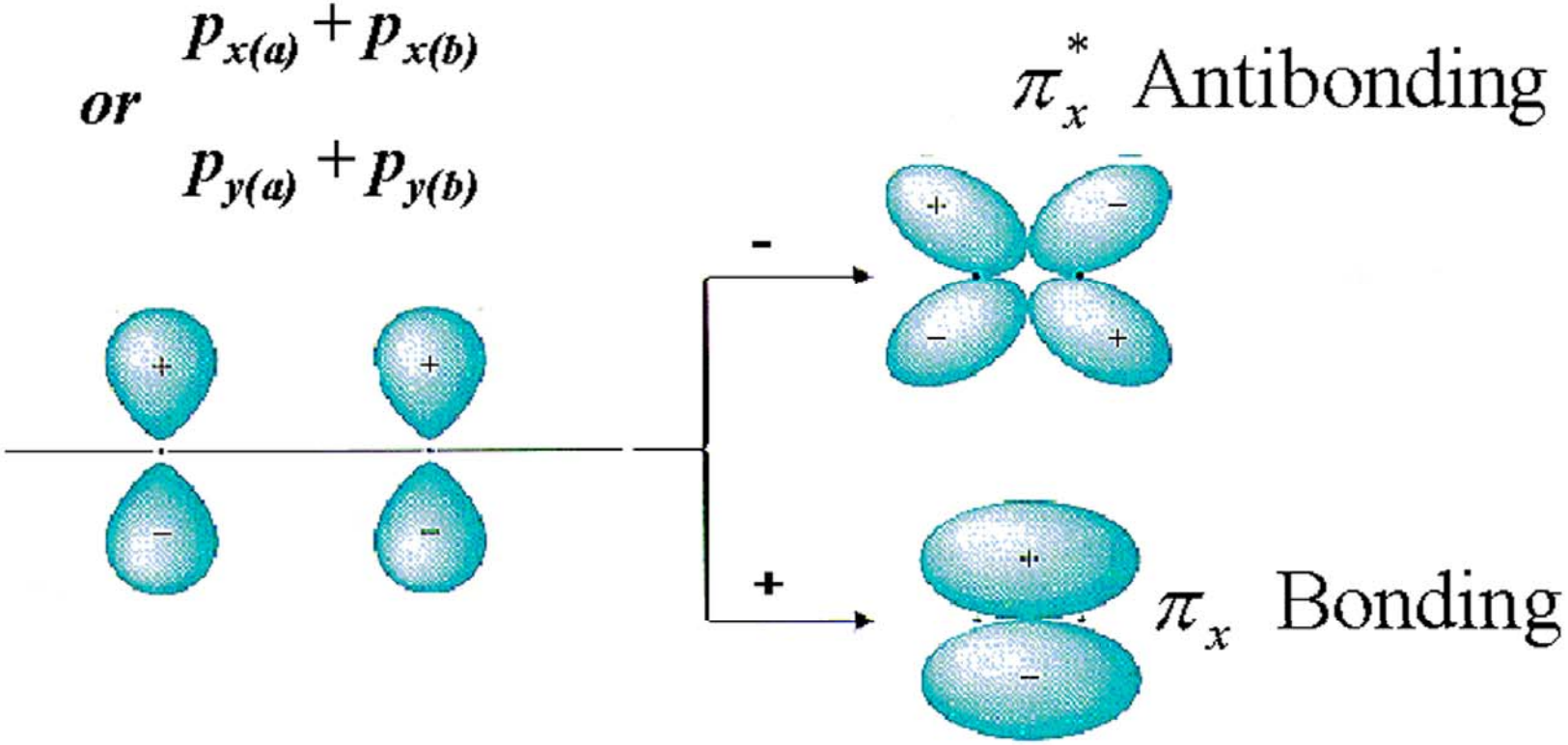
- **Atomic orbitals overlap to give equal number of molecular orbitals**
- **Molecular orbitals are arranged according to increase in energy**



Atomic orbitals **Molecular orbitals**



$2p_{z(a)} + 2p_{z(b)}$


$p_{x(a)} + p_{x(b)}$
or
$p_{y(a)} + p_{y(b)}$
π_x^* Antibonding
-
+
π_x Bonding