Hybridization of Carbon

We can use hybridisation to explain the shape of organic molecules with respect to carbon.

Let's consider carbon in methane, CH_4.

Methane molecule has a tetrahedral shape according to Valence Shell Electron Pair Repulsion Theory (VSEPR).

the electronic configuration of carbon atom in the ground state is: $1s^2\ 2s^2\ 2p^2$..

Carbon has only 2 unpaired electrons in this case, so therefore it can only form 2 bonds in its ground state.

Of course we know that carbon always forms 4 bonds, so the concept of **excitation** comes in where an electron is promoted from the paired 2s orbital which is lower in energy to an empty 2p orbital which is higher in energy.

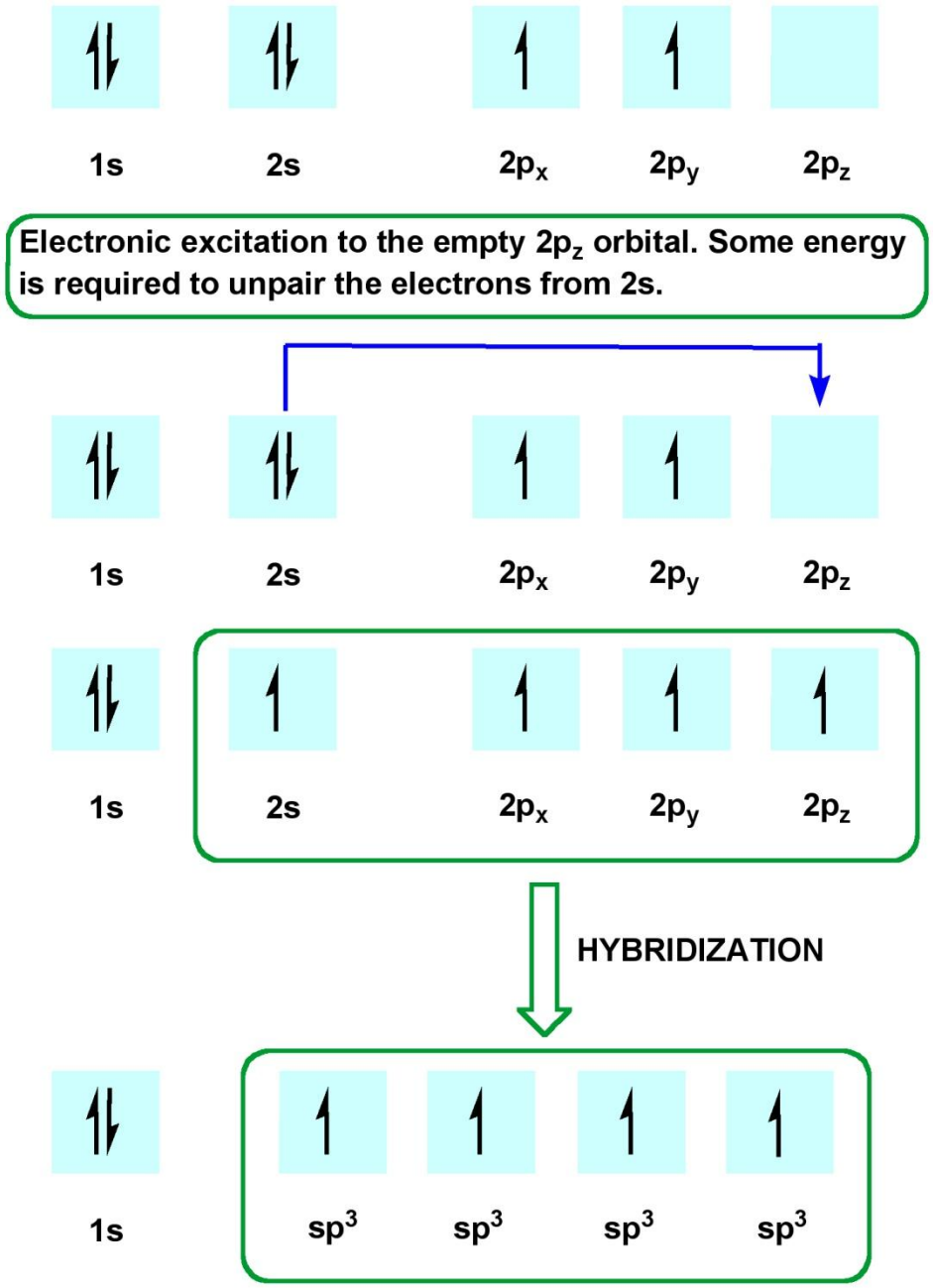
Carbon in its excited state now has 4 unpaired electrons so can form 4 bonds

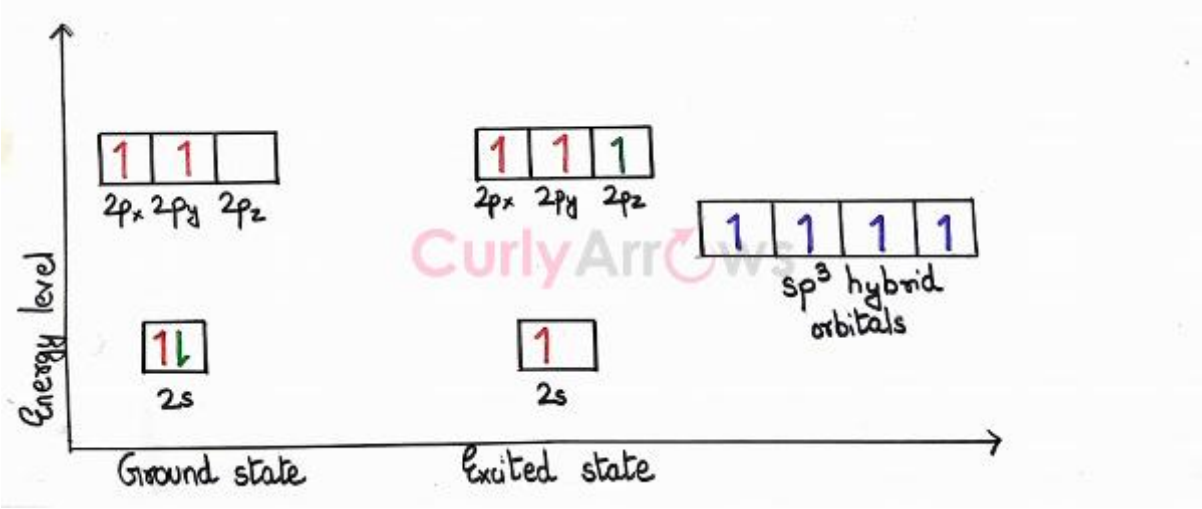
However, if carbon just uses these 2s and 2p orbitals for bond formation, the shape with respect to carbon will not be tetrahedral.

since 2s orbital is more stable and closer to the nucleus so bond formed will be shorter, while 2p orbital is less stable and further away from the nucleus so bond formed will be longer.

This mean that we will have one shorter C-H bond (from 2s orbital) and 3 longer C-H bonds (from the 2p orbitals), which not give the tetrahedral shape of methane.

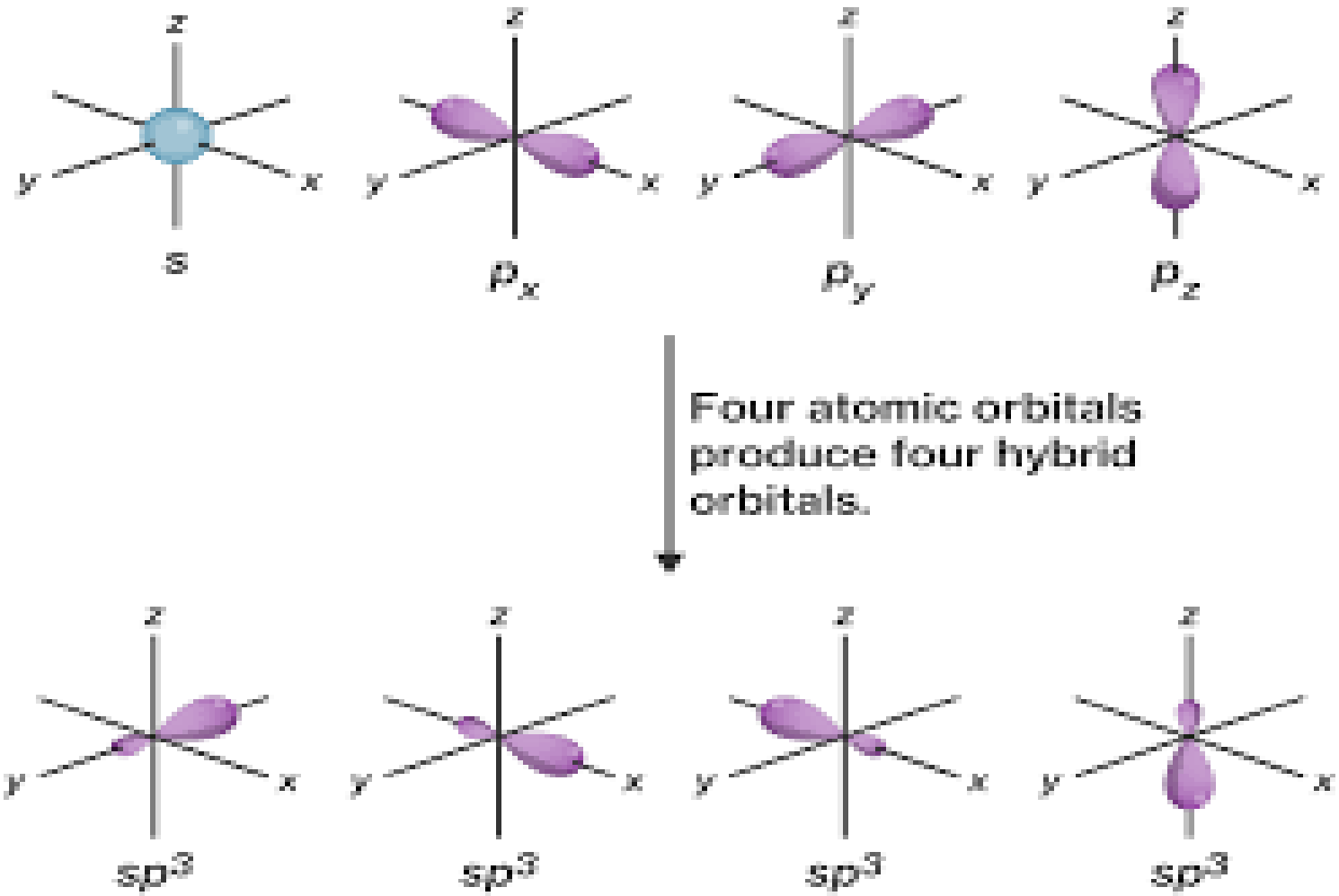
Therefore we need another concept to connect between excitation and the final shape of methane - hybridisation.


1s
2s
2p$_x$
2p$_y$
2p$_z$
Electronic excitation to the empty 2p$_z$ orbital. Some energy is required to unpair the electrons from 2s.
1s
2s
2p$_x$
2p$_y$
2p$_z$
1s
2s
2p$_x$
2p$_y$
2p$_z$
HYBRIDIZATION
1s
sp^3
sp^3
sp^3
sp^3

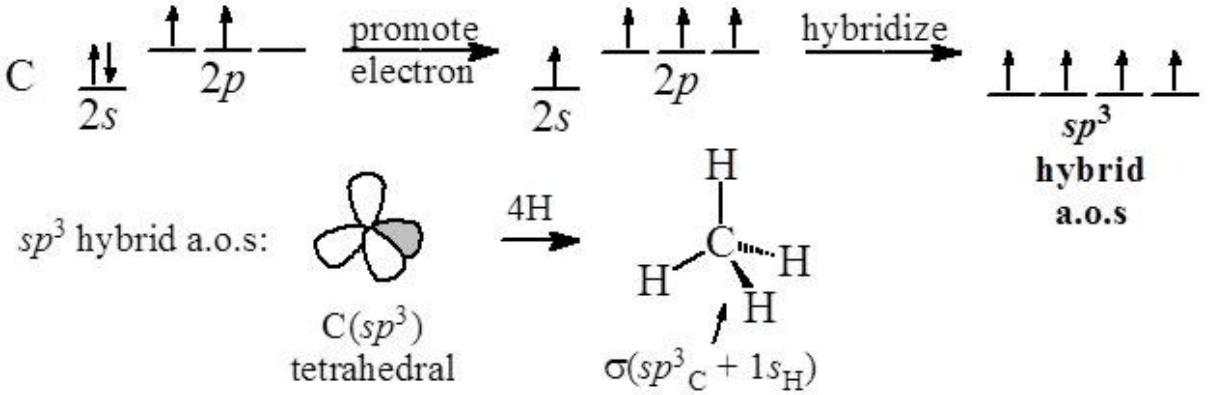

Energy level
1 1
2px 2py 2pz
1↓
2s
Ground state
1 1 1
2px 2py 2pz
1
2s
Excited state
1 1 1 1
sp3 hybrid orbitals

Hybridisation is the mixing of valence orbitals to form sigma bonds.

Since carbon in methane forms 4 sigma bonds, it will mix 4 of its valence orbitals (2s, $2p_x$, $2p_y$, $2p_z$) to form 4 identical orbitals with equal shape and energy.


z
y
x
s
p_x
p_y
p_z
Four atomic orbitals produce four hybrid orbitals.
sp^3
sp^3
sp^3
sp^3

The name of the hybridised orbitals will be sp^3 hybridised orbitals and since they have the same shape and energy, they repel each other equally and give sp^3 hybridised carbon in CH_4 its highly symmetrical tetrahedral shape.



sp^3 Hybridization

When the carbon atom is bonded to four other atoms the hybridization is said to be sp^3 type. Here 1s orbital and 3p orbitals in the same shell of an atom combine to form four new equivalent orbitals. The arrangement is tetrahedral with a bond angle of 109.5^o.