Localized Electron Model

Models for Chemical Bonding

Localized electron model

(Valence bond model)

Molecular orbital model

Localized Electron Model

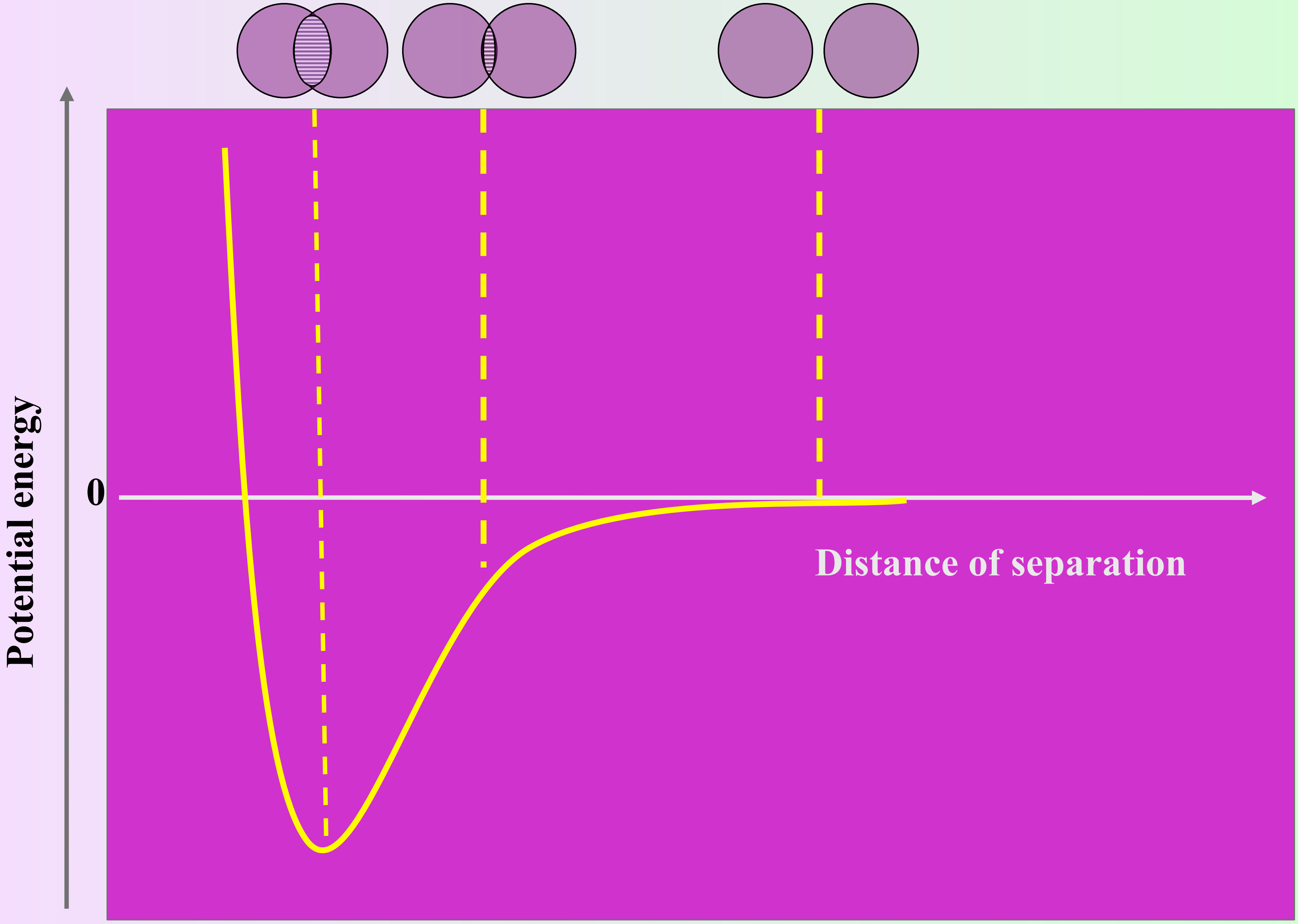
Useful for explaining the structure of molecules especially nonmetals bonded to nonmetals

Localized electron model

Electron pair can be shared when half-filled orbital of one atom overlaps with half-filled orbital of another.

δ Bond: orbitals overlap along the internuclear axis

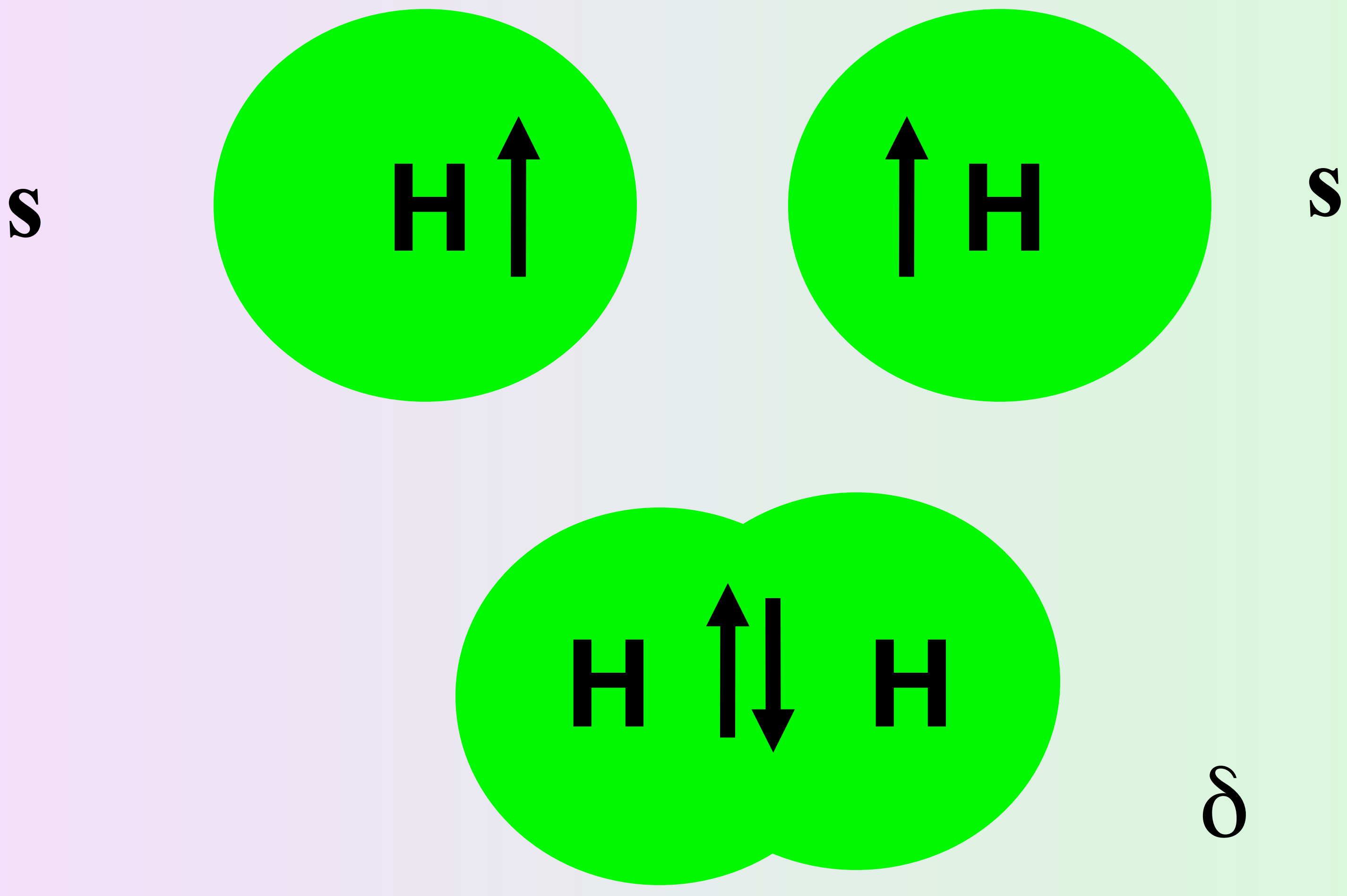
π Bond: side by side overlap of orbitals parallel to the internuclear axis



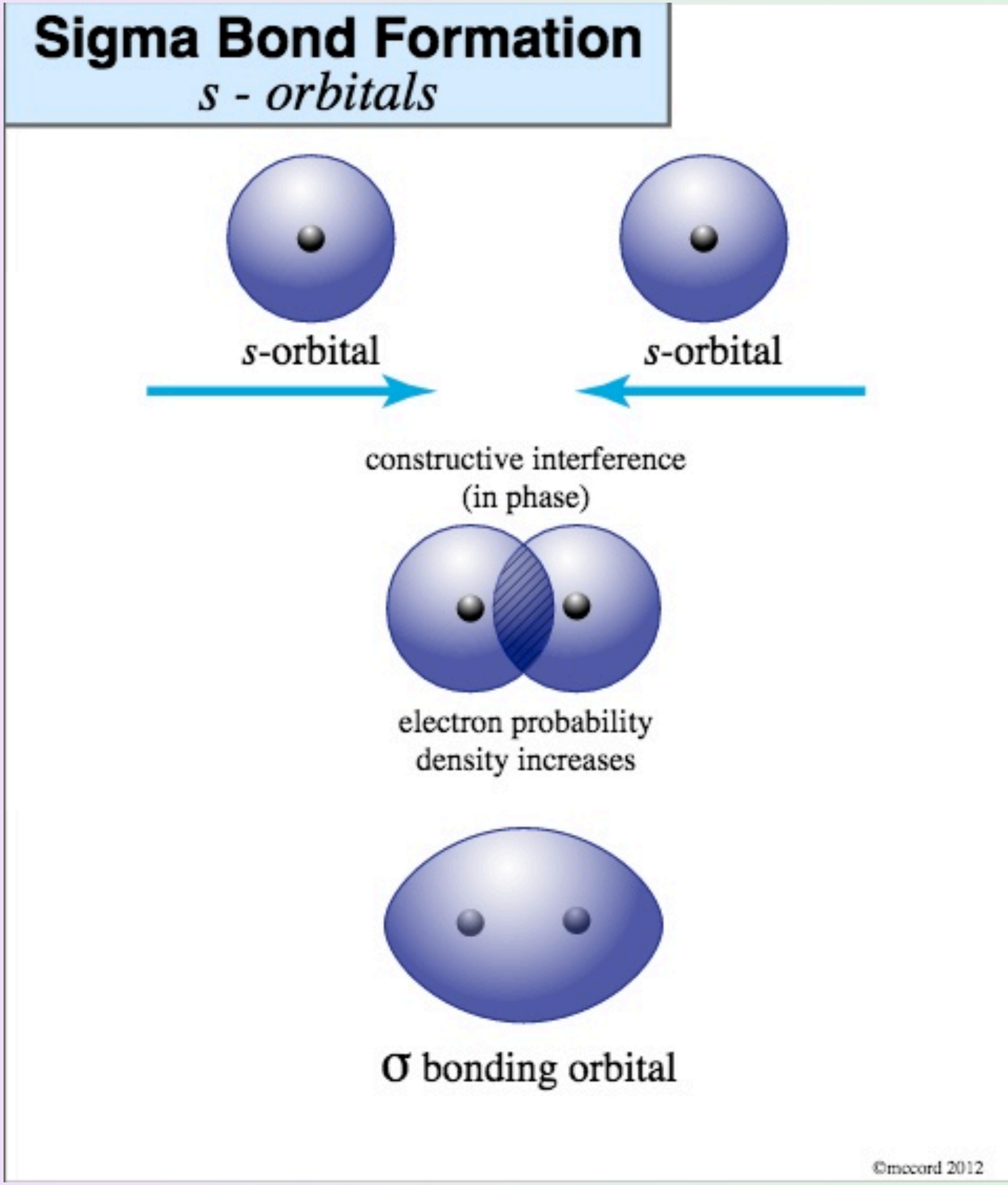
Potential energy
0
Distance of separation

As the atoms approach each other, each electron is attracted by the nucleus of the other atom; at the same time, the electrons repel each other, as do the nuclei

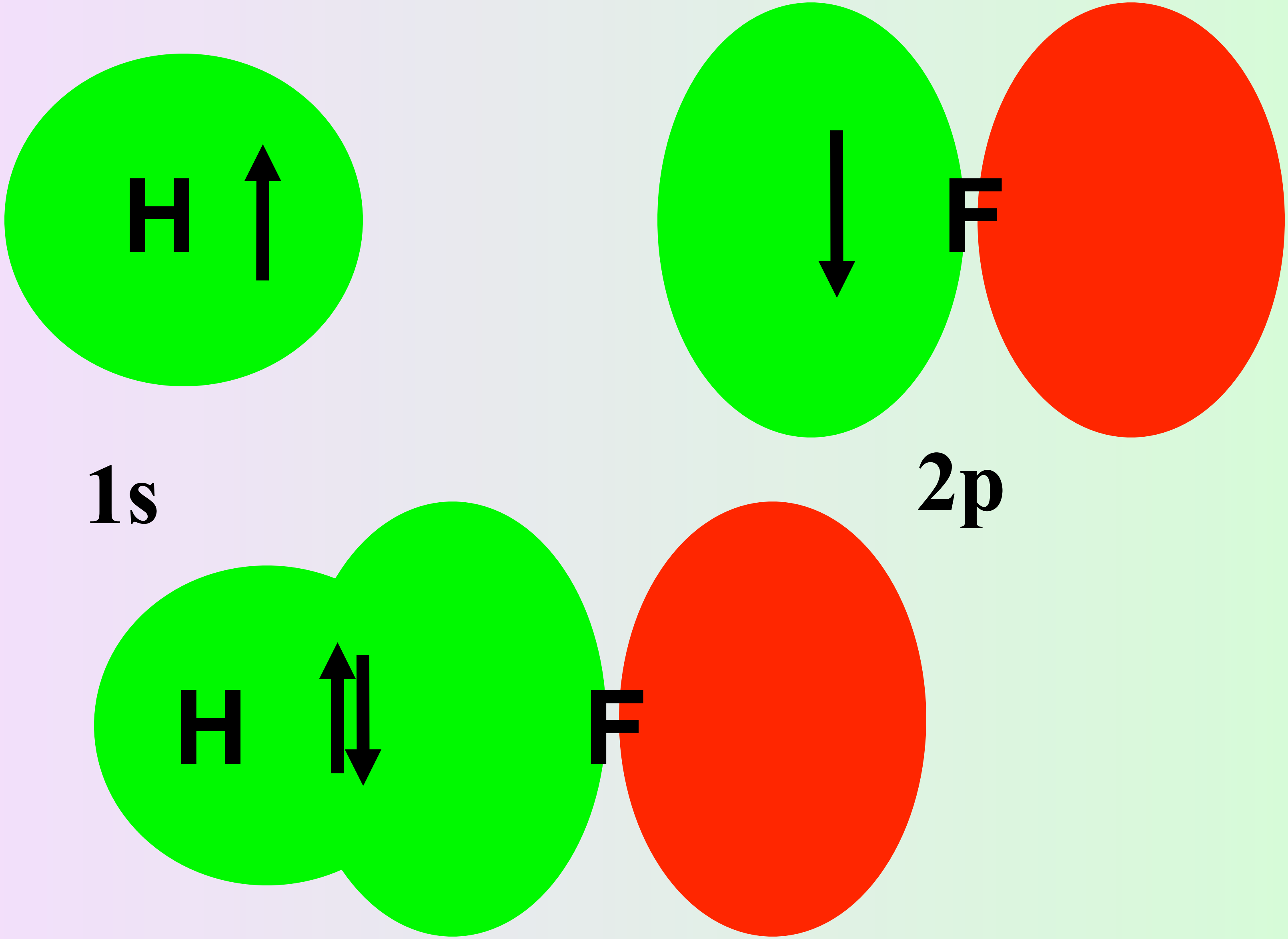
δ Bond in H_2



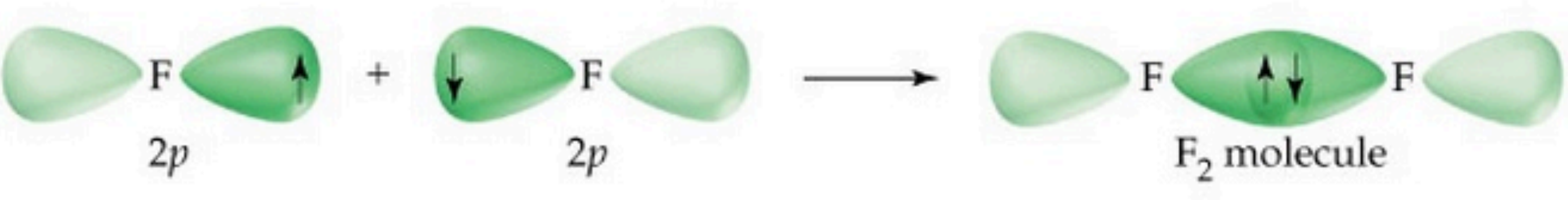
H_2


Sigma Bond Formation
s - orbitals
s-orbital
s-orbital
constructive interference
(in phase)
electron probability
density increases
σ bonding orbital
©mccord 2012

δ Bond in HF

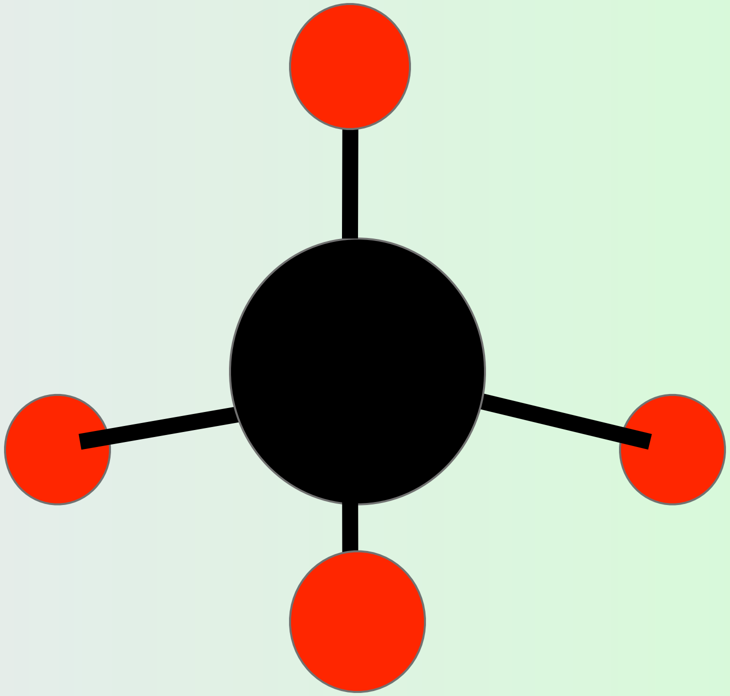


F_2



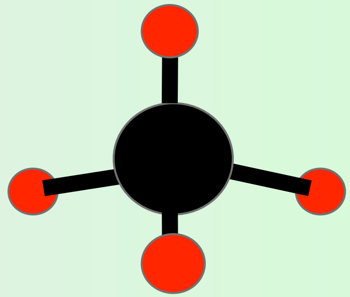
Structure of Methane (CH_4)

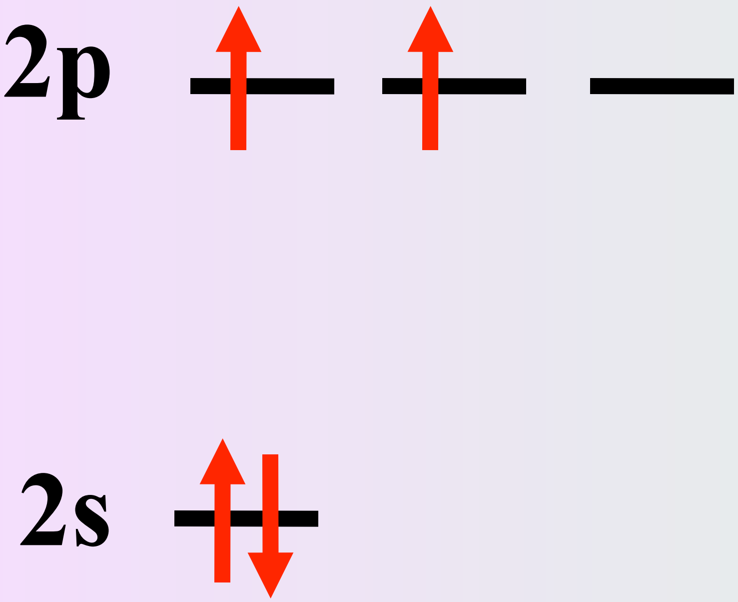
structure of methane seems inconsistent with electron configuration of carbon



carbon

only two unpaired electrons





Carbon Should form δ –bonds with only two Hydrogen atoms ?

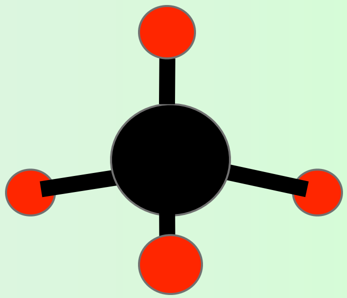
Hybridization of Atomic Orbitals

Hybrid orbitals

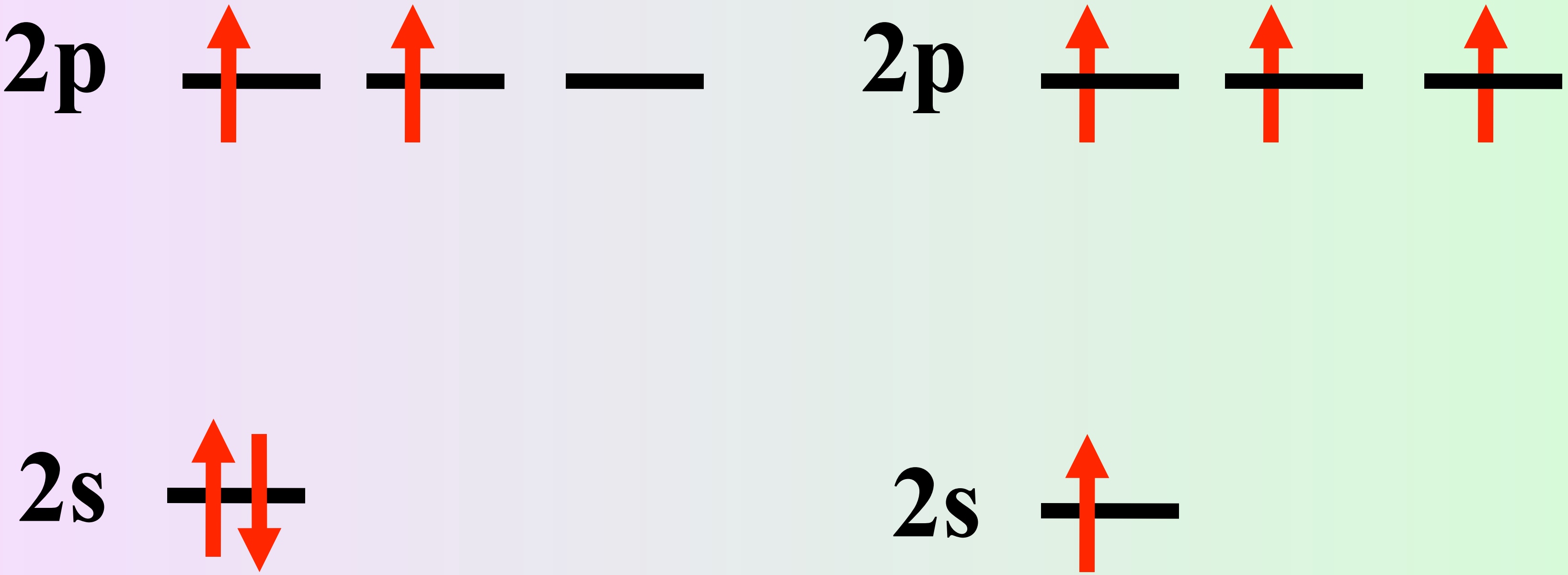
atomic orbitals obtained when two or nonequivalent orbitals of the same atom combine in preparation for covalent bond formation

sp^3 Hybridization

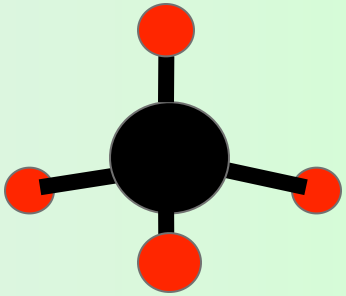
sp^3 Hybridization



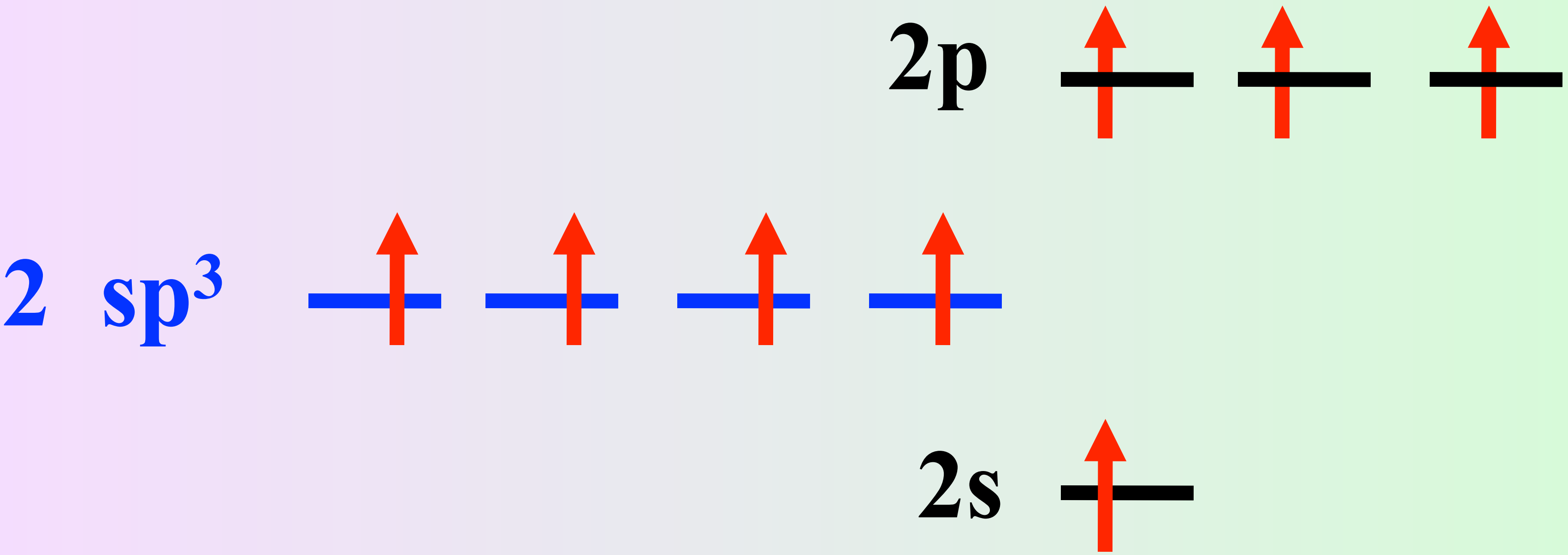
Promote an electron from the 2s to the 2p orbital



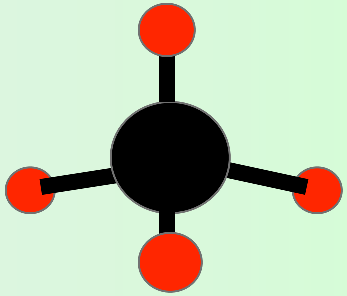
sp^3 Hybridization



Mix together (hybridize) the 2s orbital and the three 2p orbitals

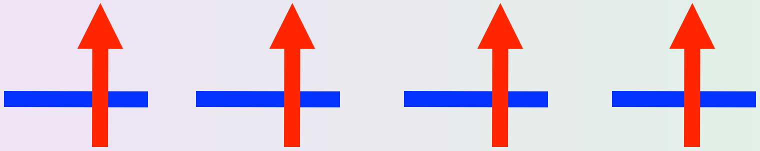


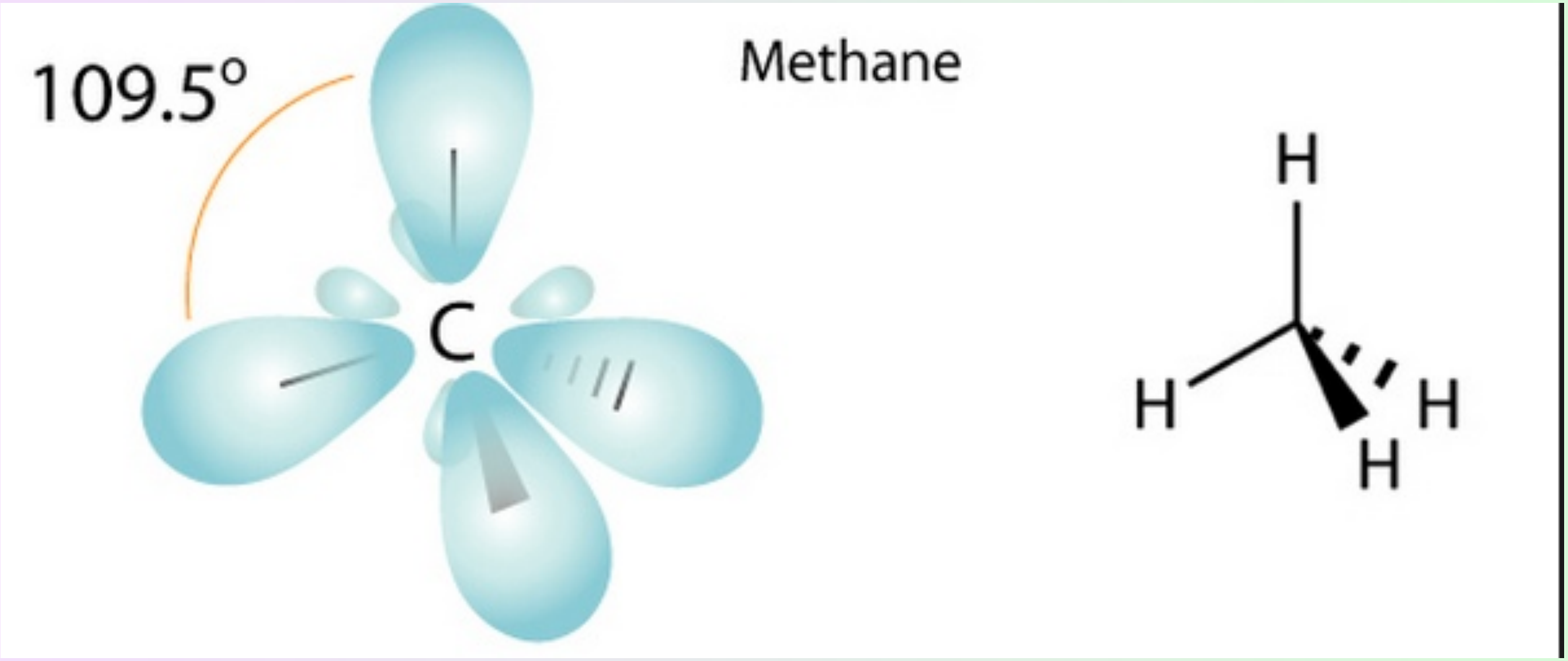
sp^3 Hybridization



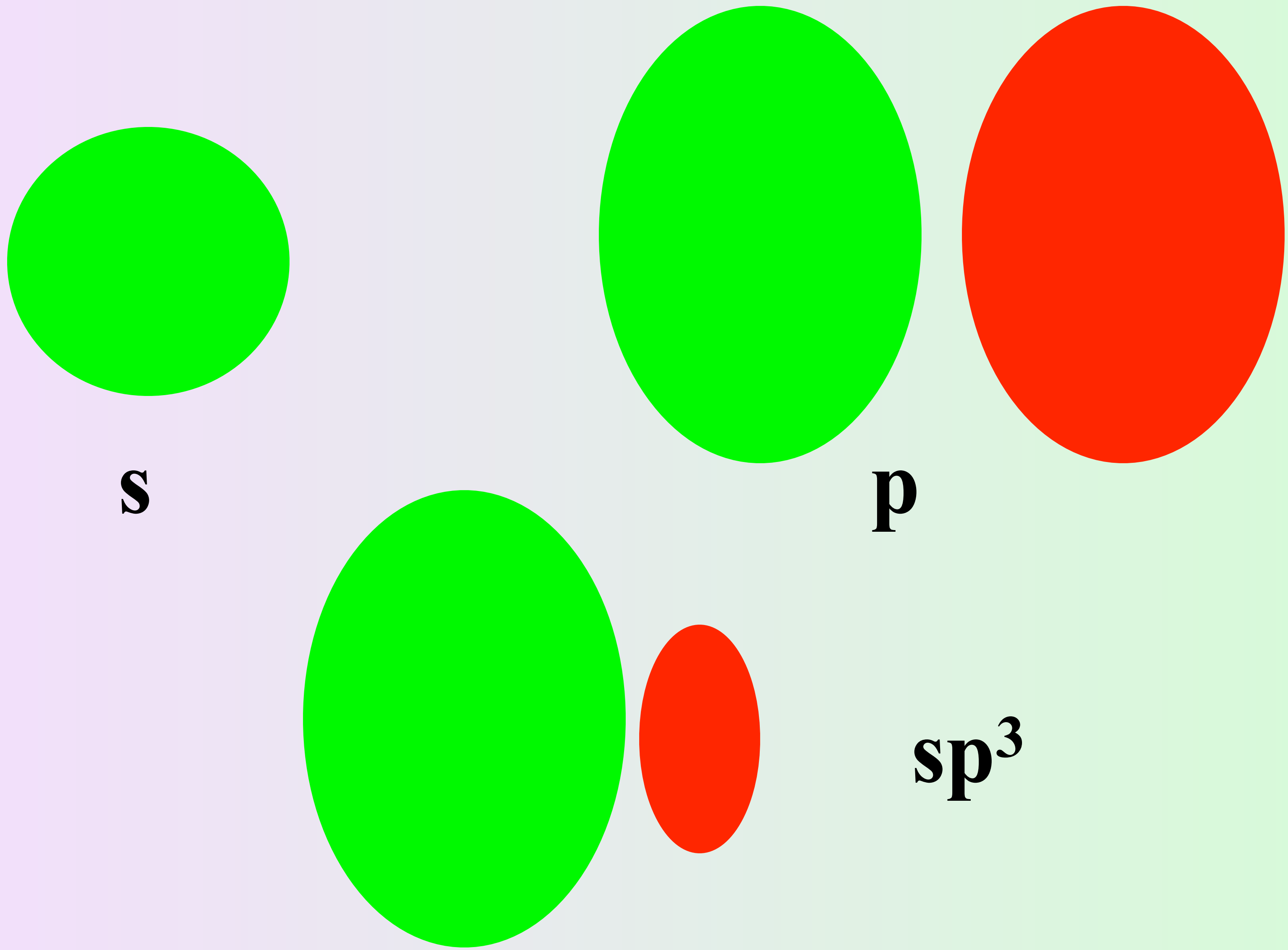
Mix together (hybridize) the 2s orbital and the three 2p orbitals

2 sp^3

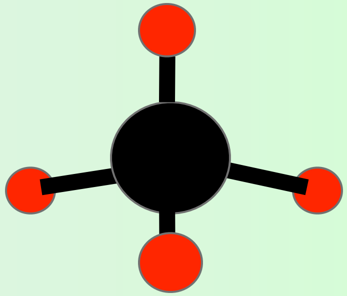


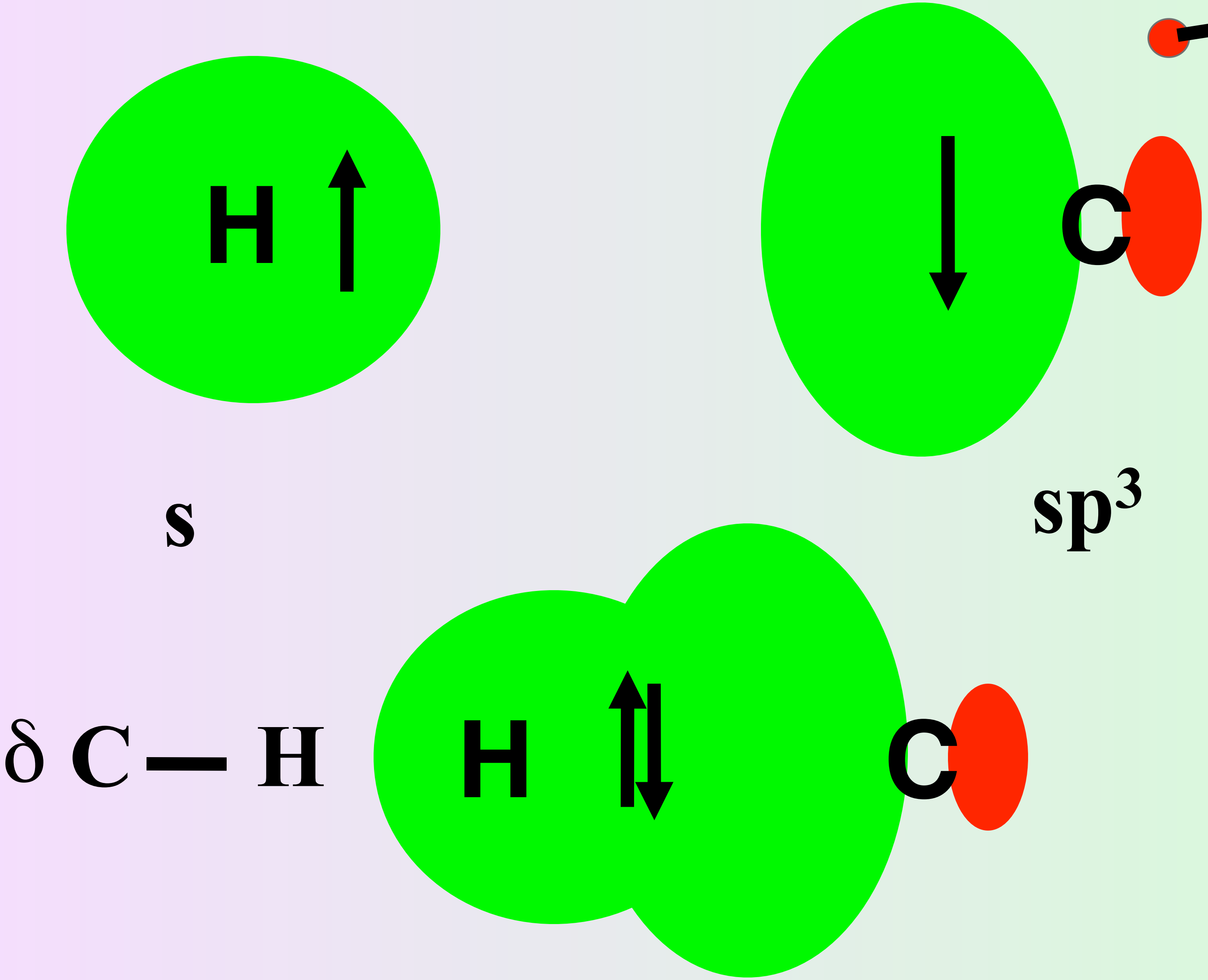

109.5°
Methane
C
H
H
H
H

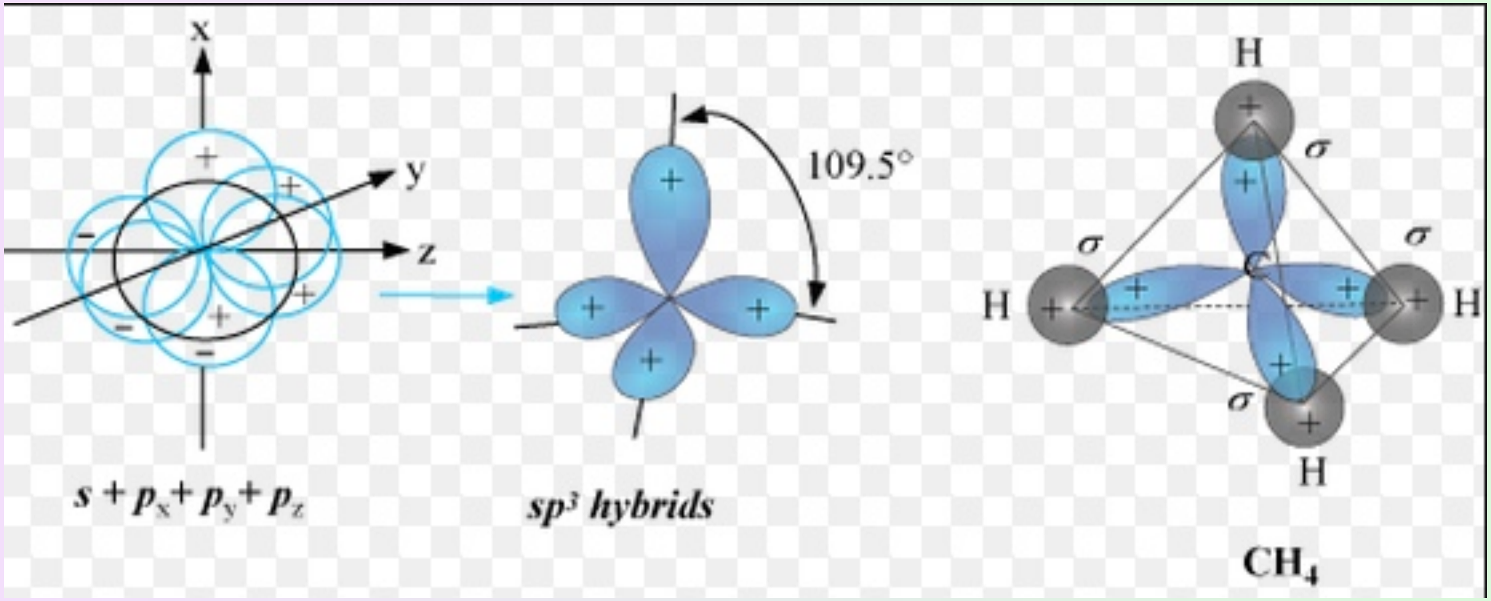
Shapes of orbitals



δ Bond in CH_4







x
y
z
109.5°
s + p_x + p_y + p_z
sp³ hybrids
H
σ
C
CH₄

Justification for Orbital Hybridization

The model is consistant with structure of methane

Allows for the formation of more bonds (4 rather than 2)

Bonds involving sp^3 orbitals are stronger than s-s overlap or p-p overlap

Remember

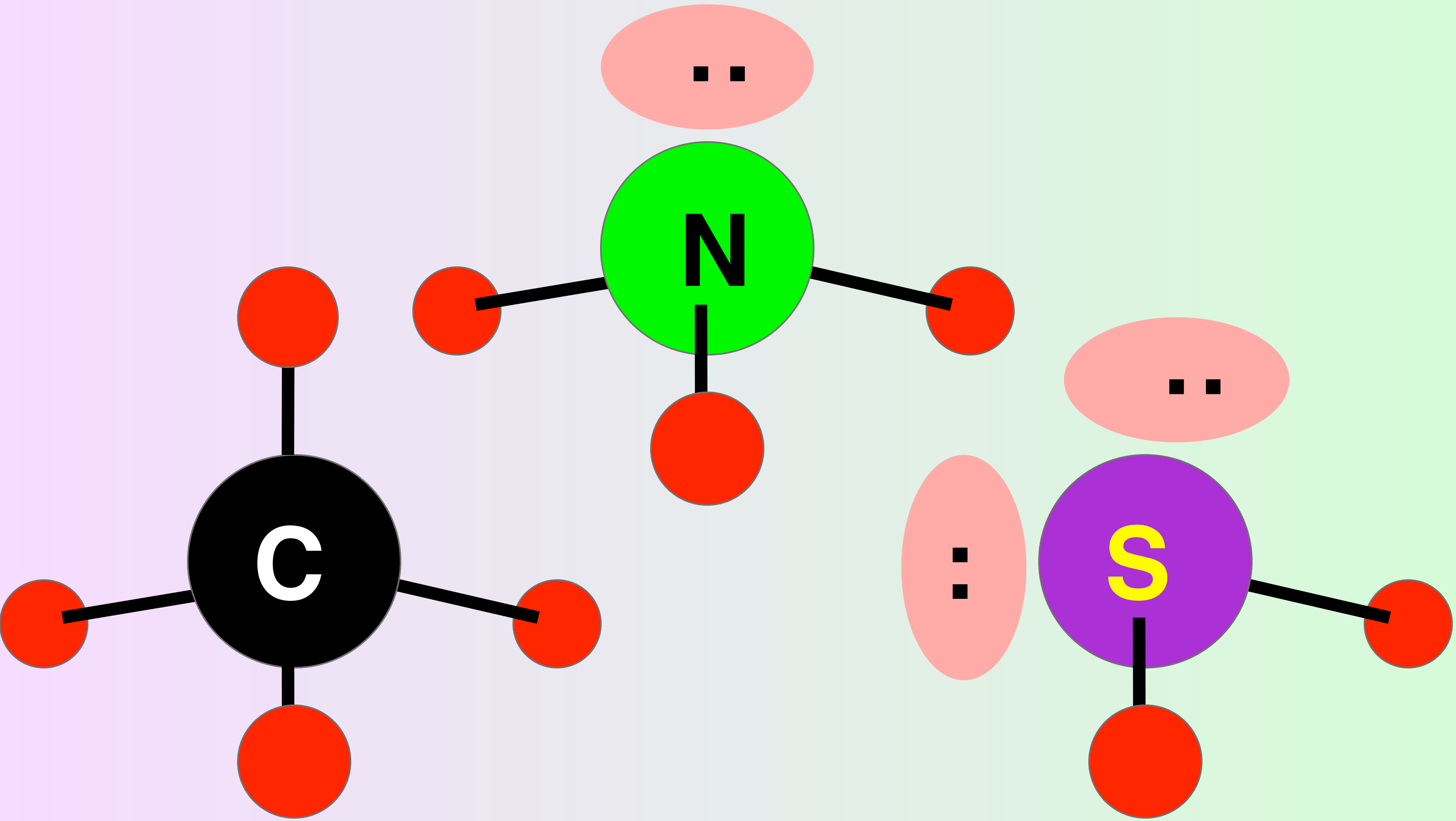
Four electron pairs

= tetrahedral arangement of those electron pairs

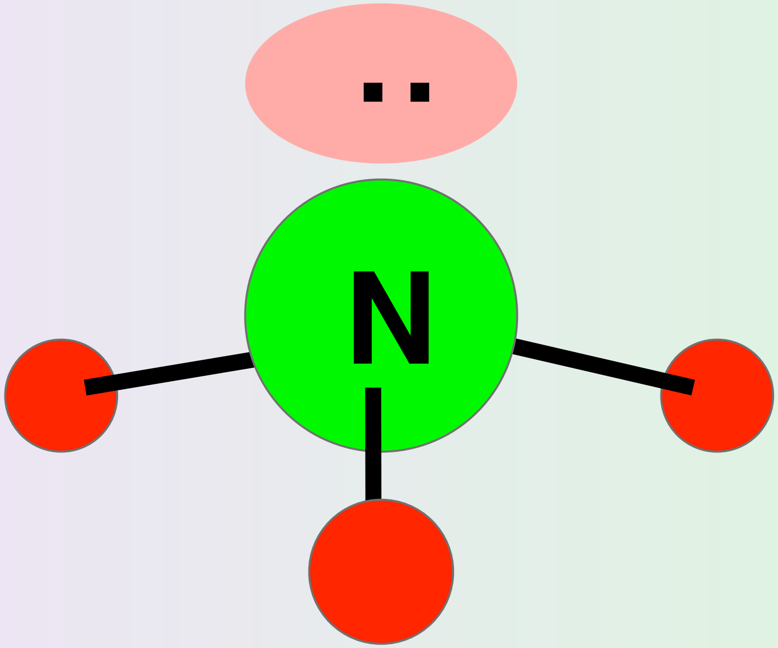
= sp^3 hybridization

Four electron pairs

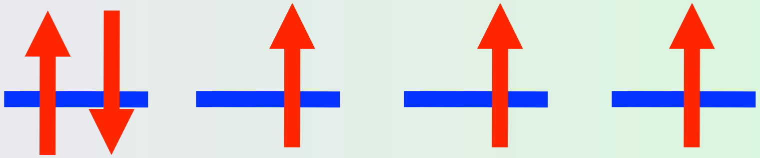
tetrahedral arrangement of electron pairs



NH_3



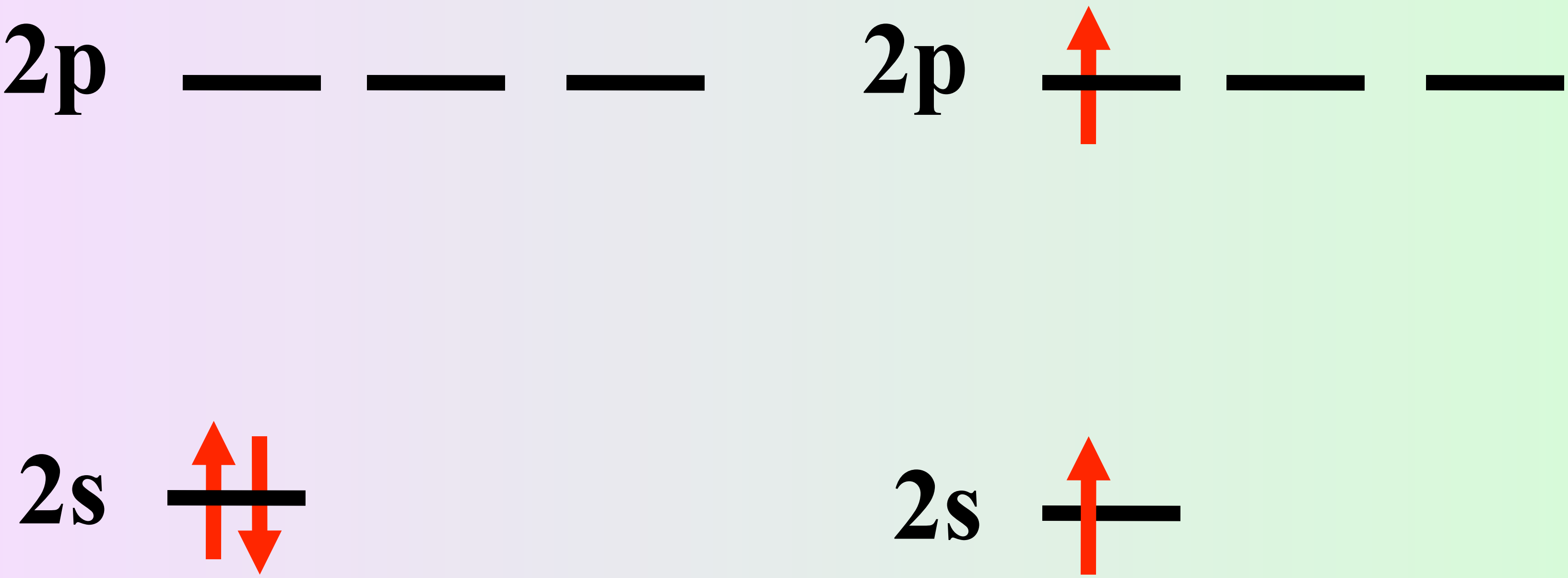
$2\ sp^3$



sp Hybridization

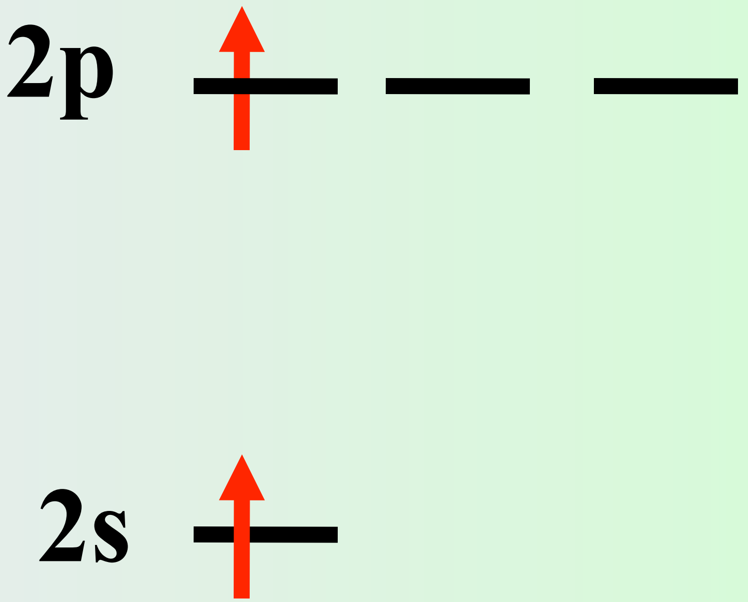
Beryllium chloride ($BeCl_2$)

Promote an electron from the 2s to the 2p orbital



Beryllium chloride ($BeCl_2$)

Mix together (hybridize) the 2s orbital and one 2p orbitals



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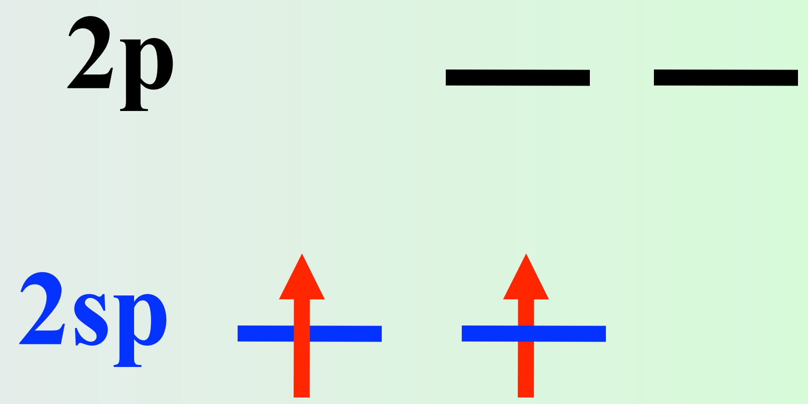
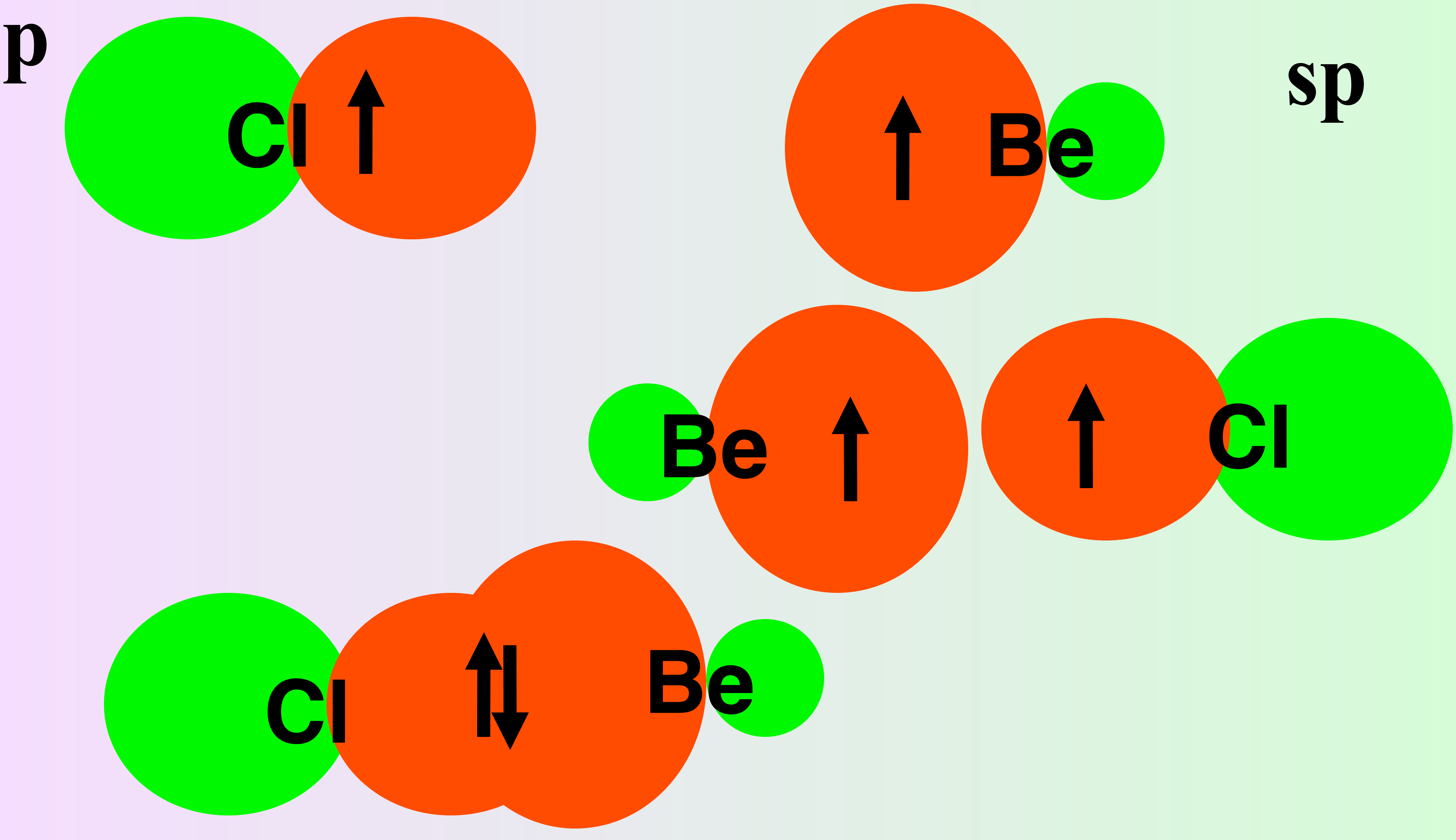
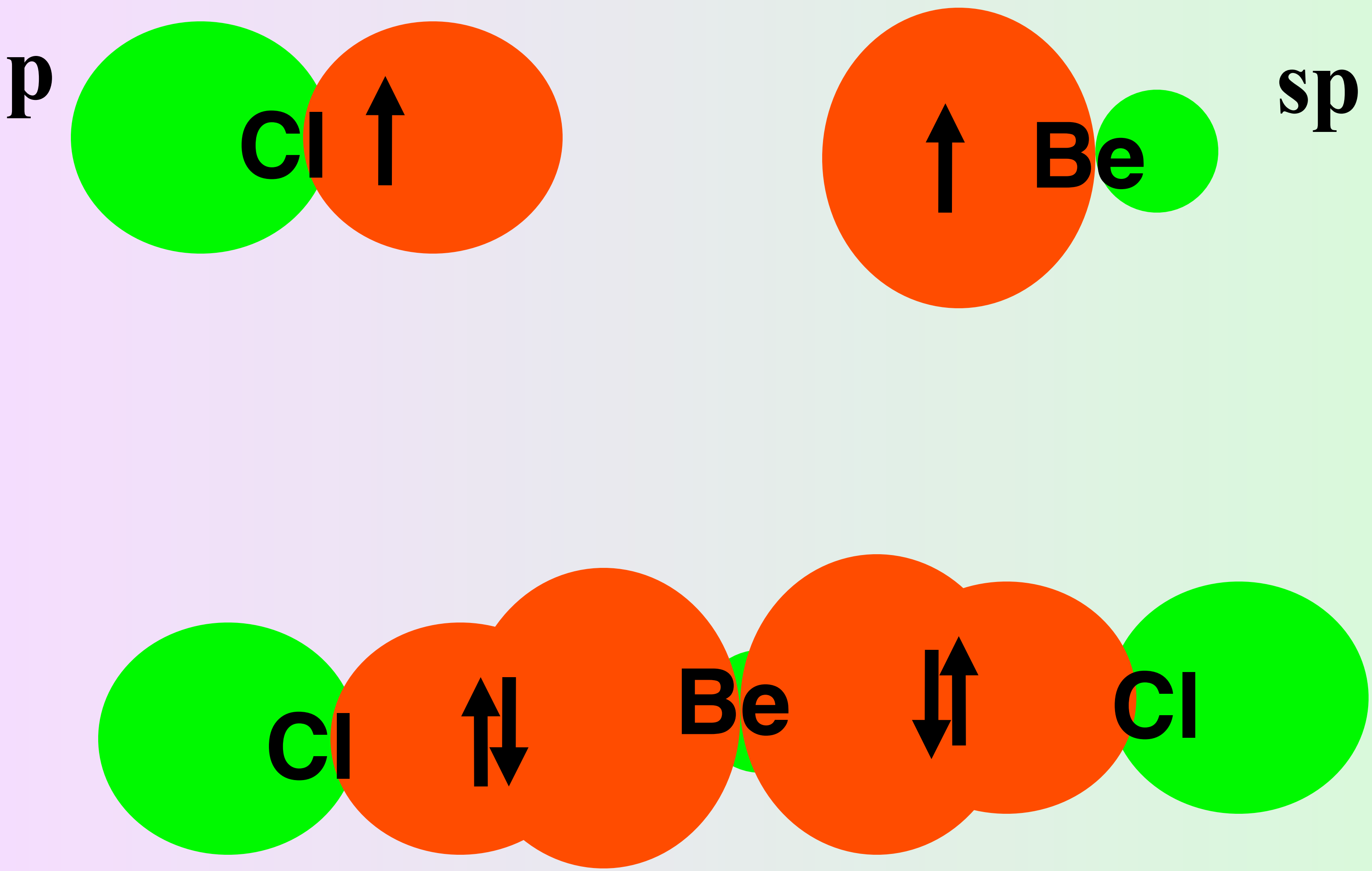


The Be — Cl δ **Bond in BeCl**



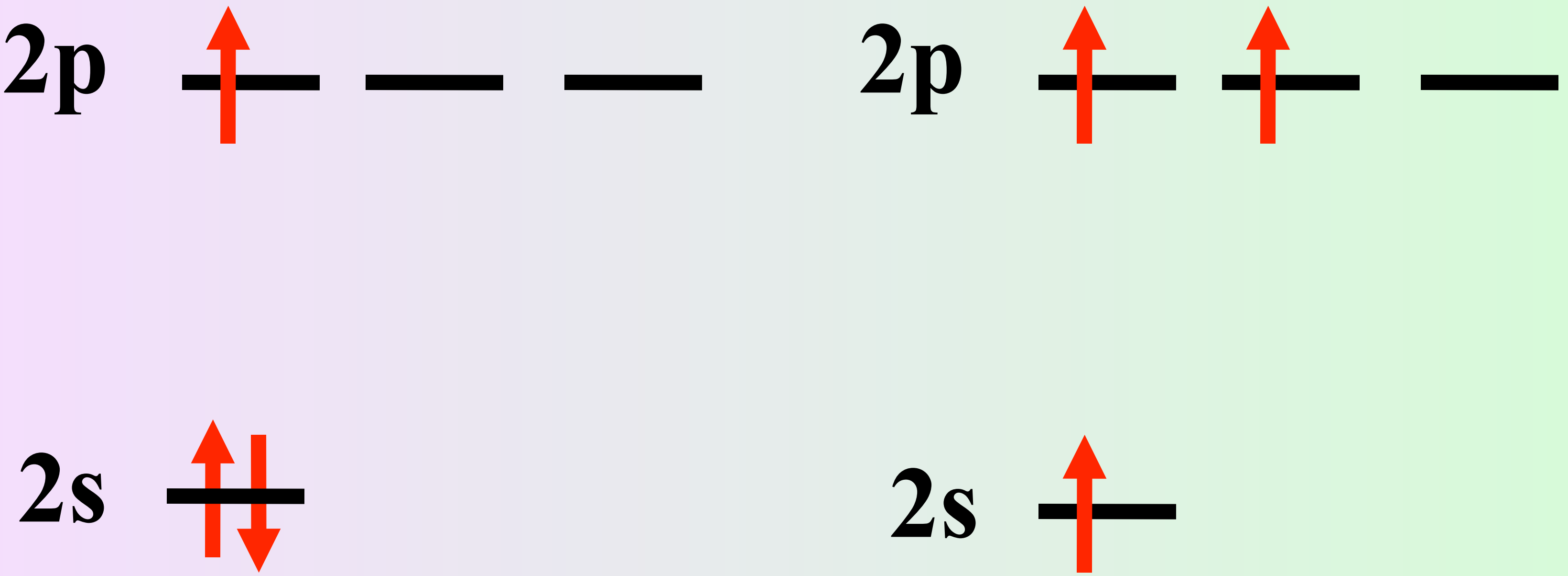
The Be — Cl δ **Bond in BeCl**



sp^2 Hybridization

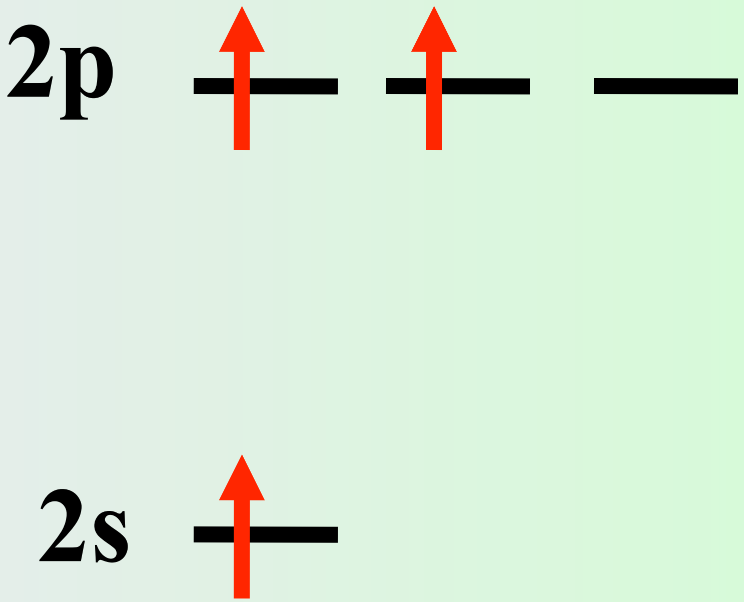
Boron trifloride

Promote an electron from the 2s to the 2p orbital



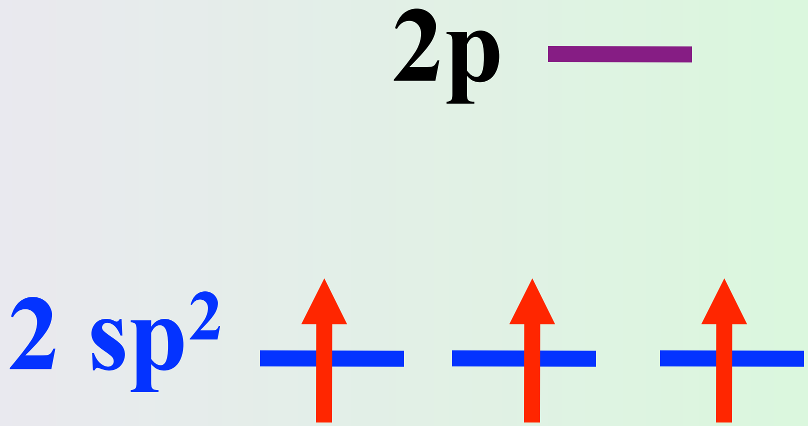
Boron trifloride

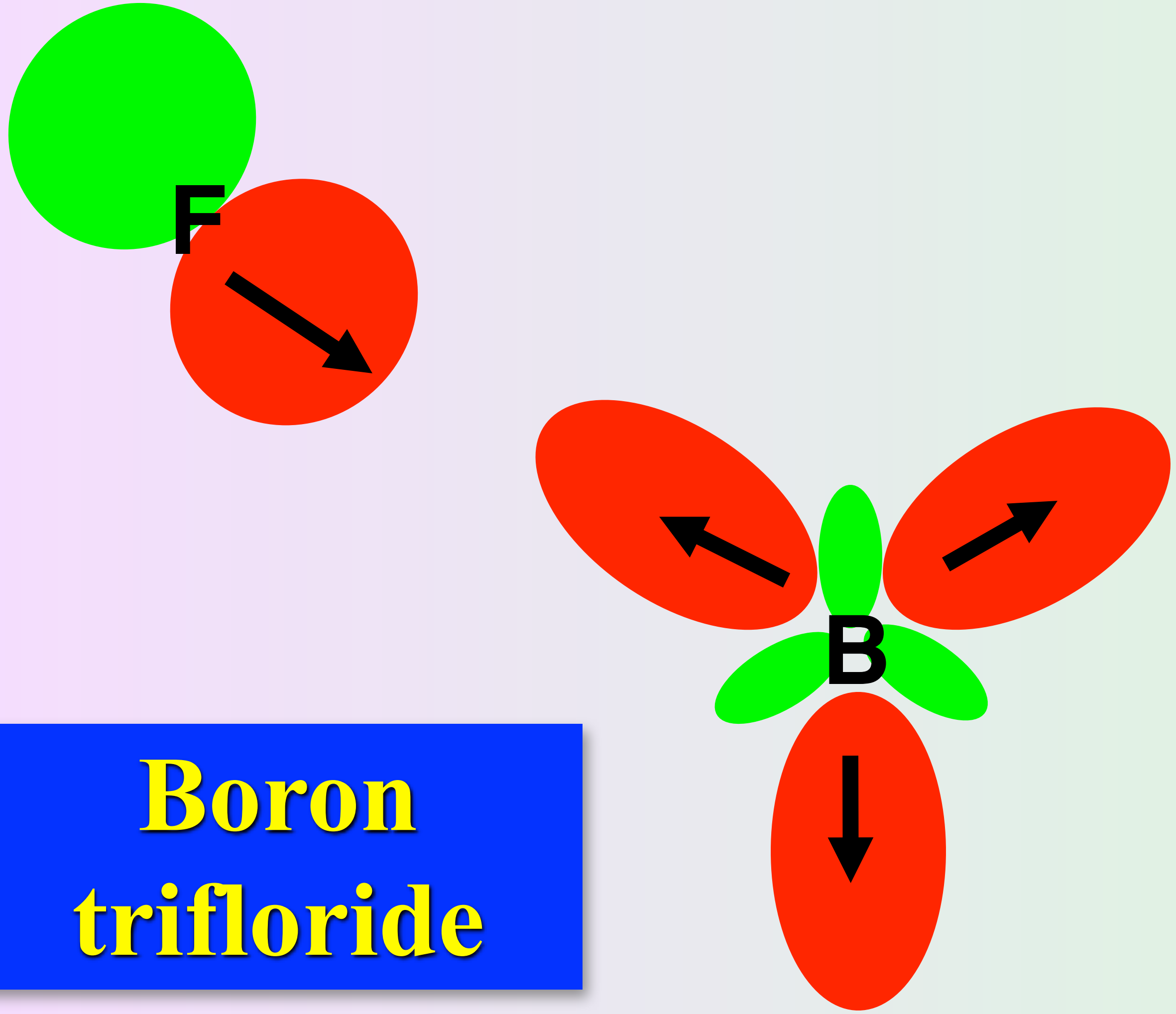
Mix together (hybridize) the 2s orbital and two 2p orbitals



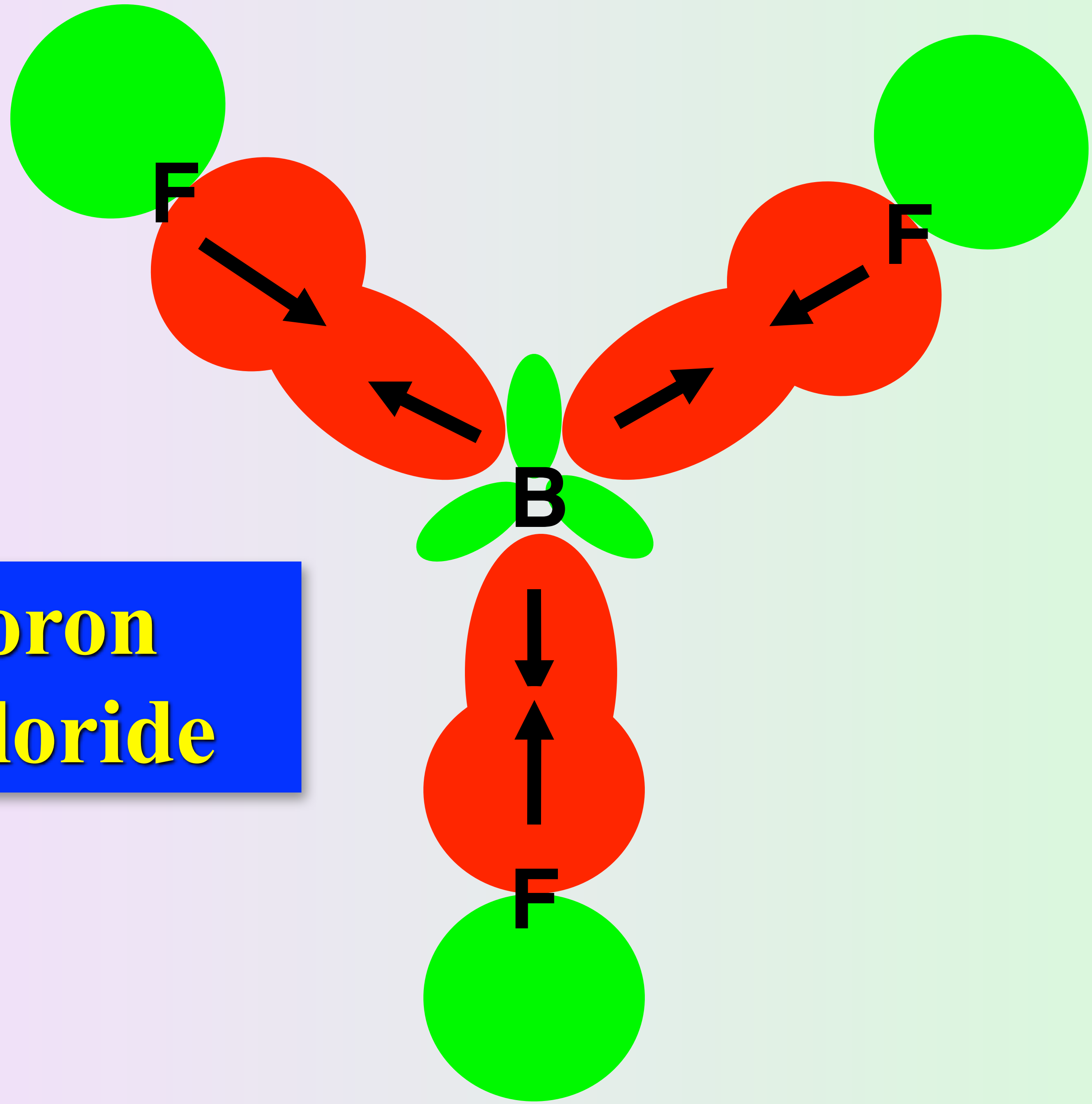
Boron trifloride

Mix together (hybridize) the 2s orbital and two 2p orbitals





Boron trifloride



Boron trifloride

Hybridizing Atomic Orbitals

hybrid orbitals are used only for atoms in a molecule, not for isolated atoms

hybrid orbitals are different in shape from the atomic orbitals from which we derive them

number of hybrid orbitals equals number of atomic orbitals from which they were generated

hybridization permits more bonds and stronger bonds

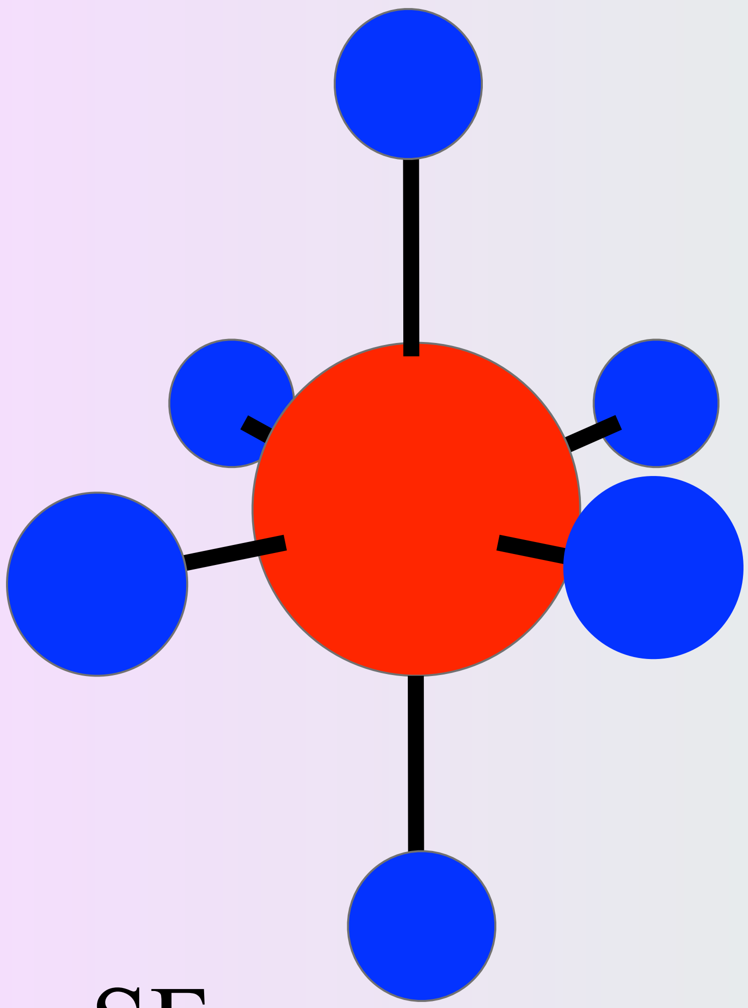
covalent bond results from overlap of half-filled orbitals

Procedure For Hybridizing Atomic Orbitals

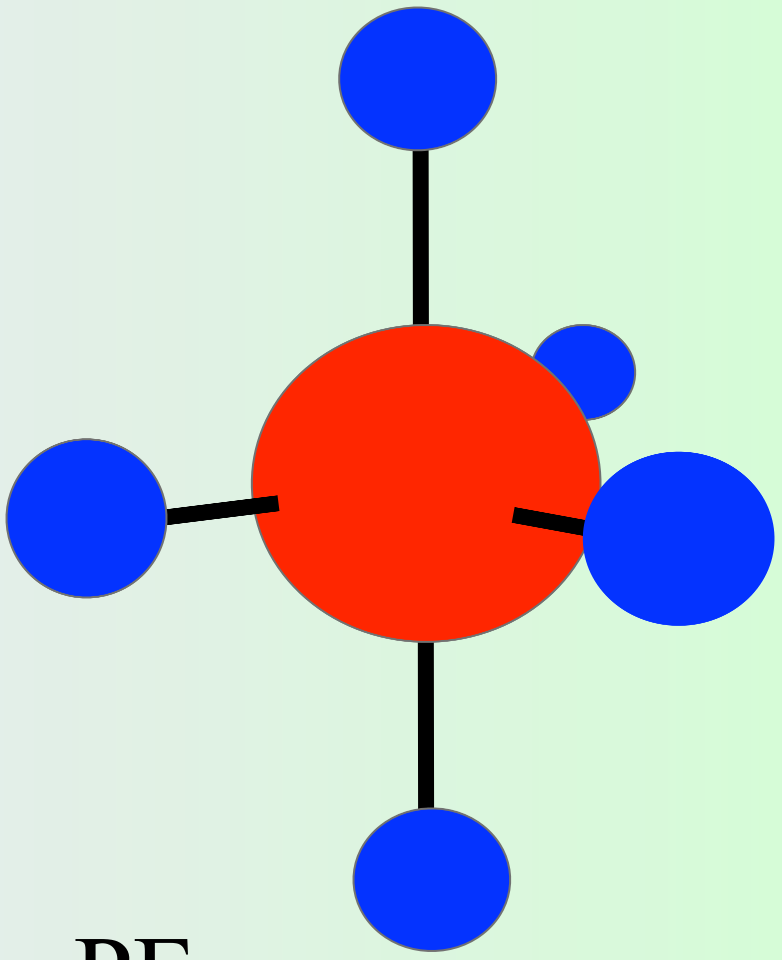
draw the Lewis structure of the molecule

predict the overall arrangement of the electron pairs using the VSEPR model

deduce the hybridization of the central atom



SF_6



PF_5

Hybridization of s, p, and d Orbitals

Beginning with the third period of the periodic table

1 3s orbital + 3 3p orbital + 1 3d orbital

gives sp^3d

Permits five electron pairs (trigonal bipyramidal)

1 3s orbital + 3 3p orbital + 2 3d orbital

gives sp^3d^2

Permits six electron pairs (octahedral)

π -Bonds

Review :Valence bond model

Electron pair can be shared when the half-filled orbital of one atom overlaps with half-filled orbital of another.

δ Bond: orbitals overlap along the internuclear axis

π Bond: side by side overlap of orbitals

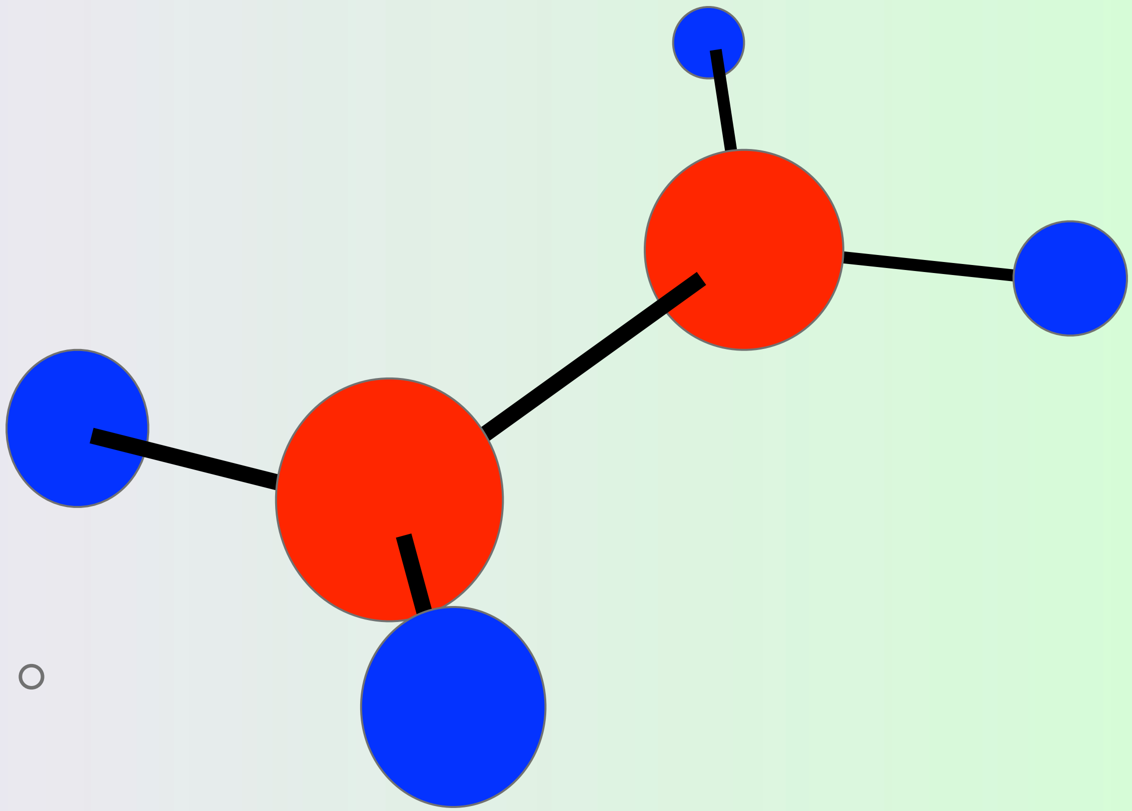
Structure of Ethylene

C_2H_4

$CH_2 = CH_2$

planar

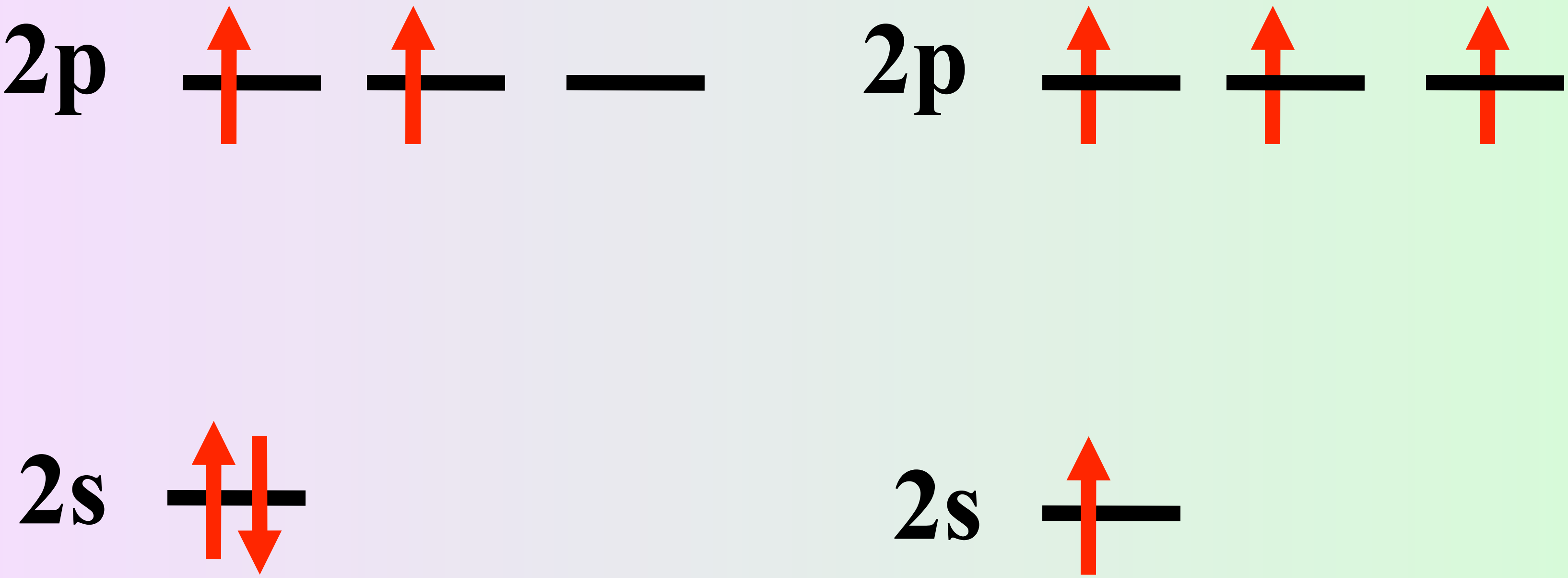
Bond angle 120 °



Requires hybridization different from sp^3

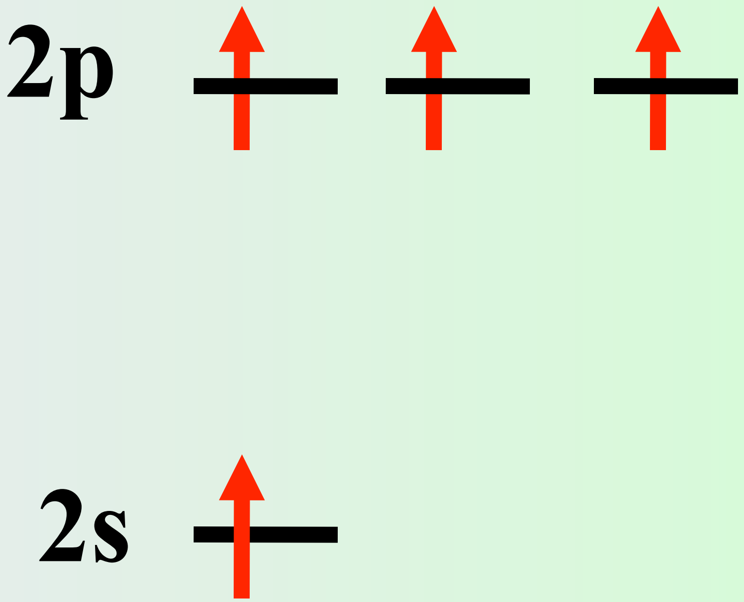
Orbital Hybridization

Promote an electron from the 2s to the 2p orbital



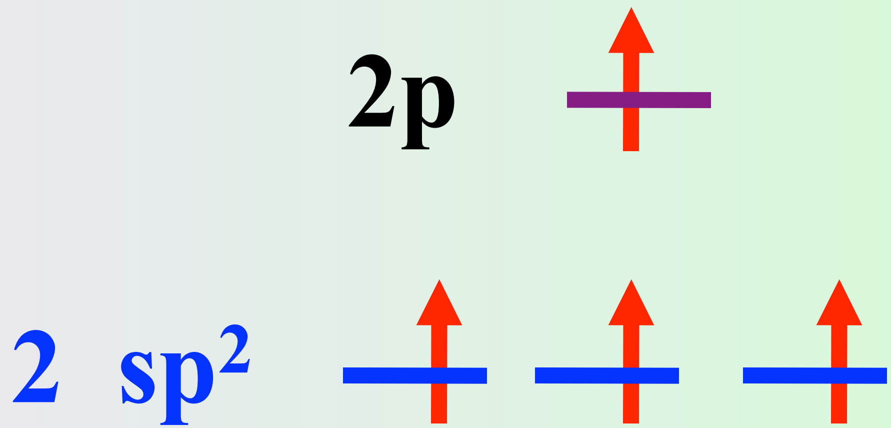
Orbital Hybridization

Mix together (hybridize) the 2s orbital and the two 2p orbitals

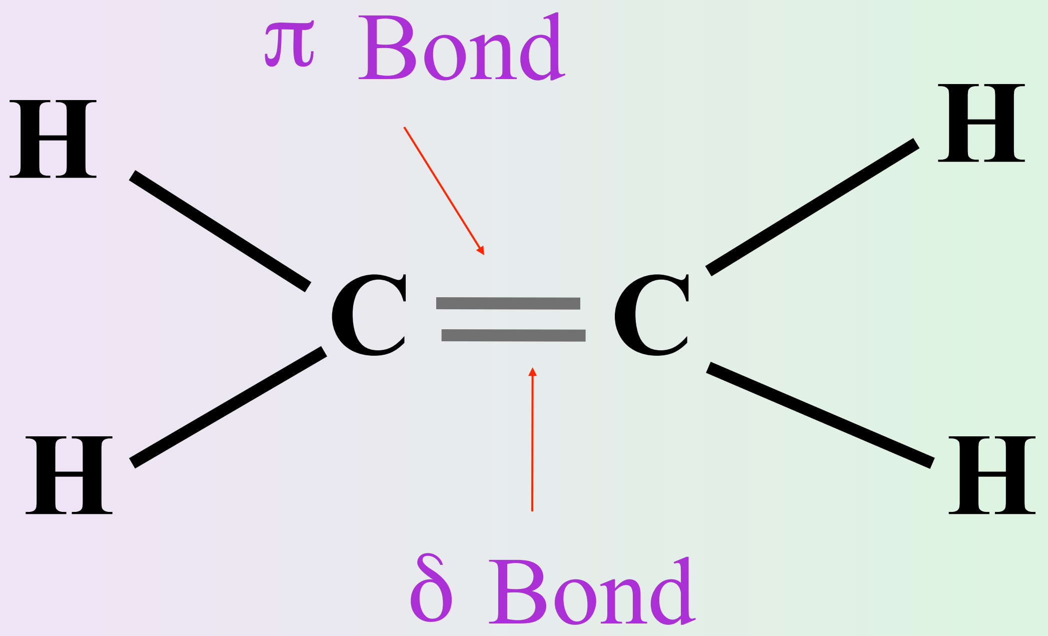


Orbital Hybridization

Mix together (hybridize) the 2s orbital and the two 2p orbitals

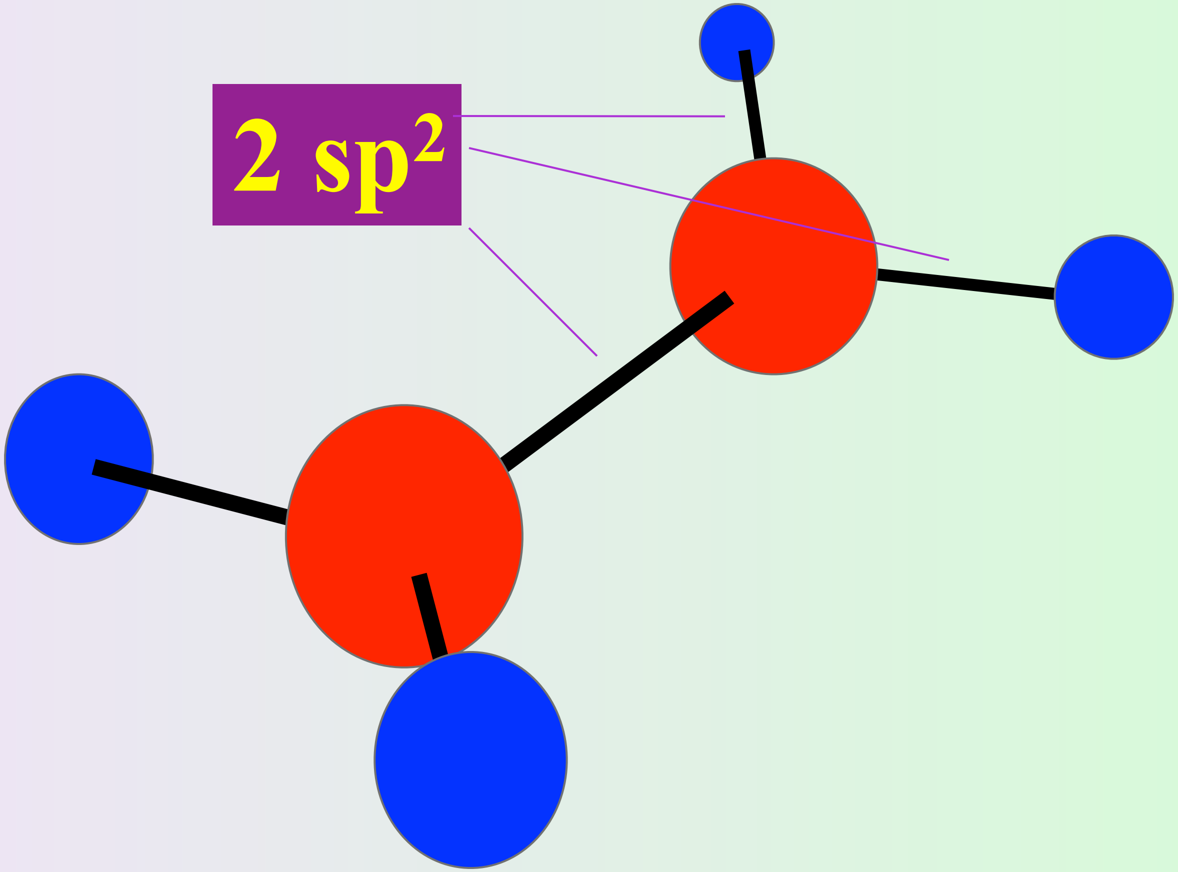


Lewis model : Ethylene

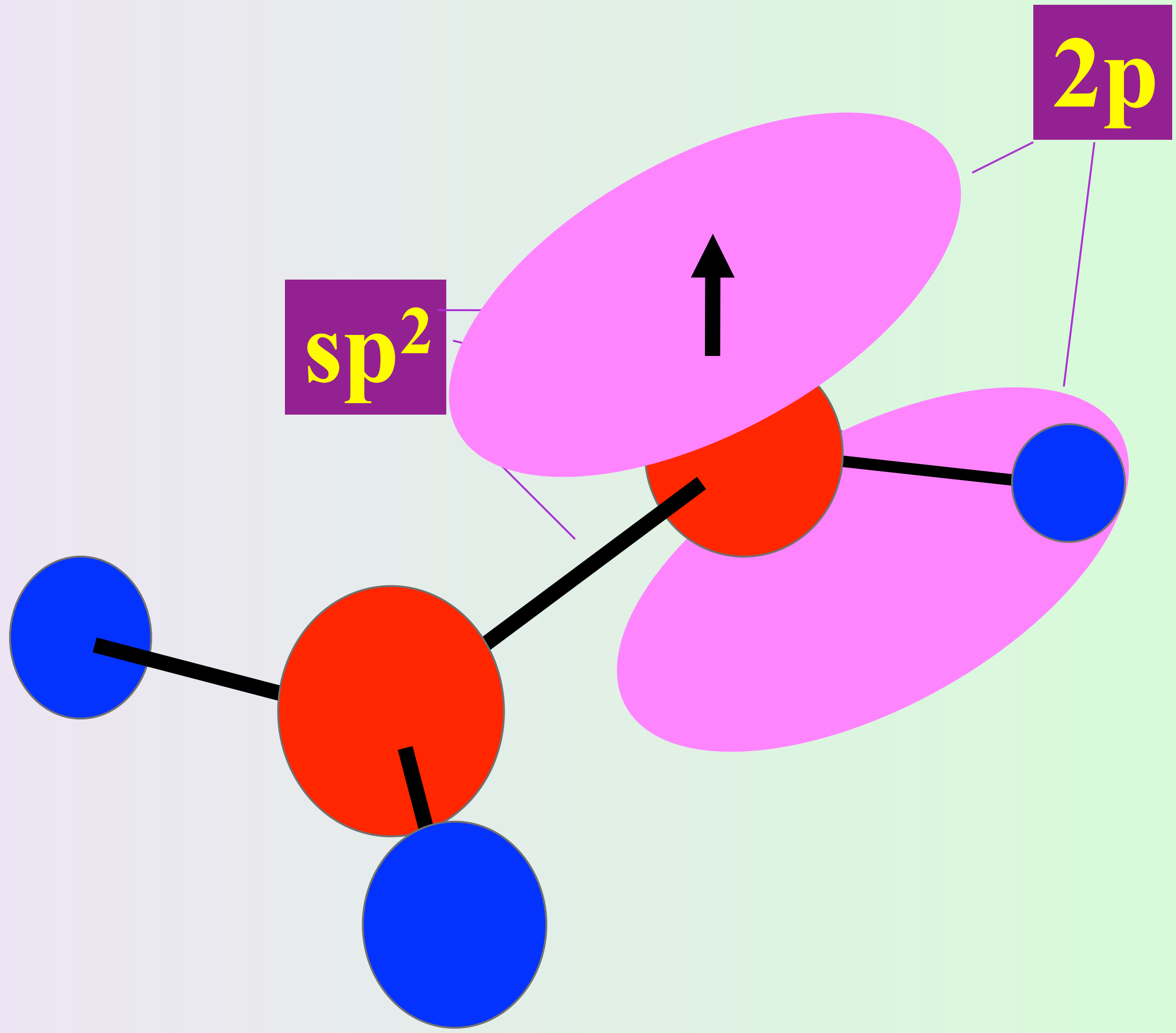


The carbon-carbon double bond of ethylene is a combination of an δ Bond **and** πBond

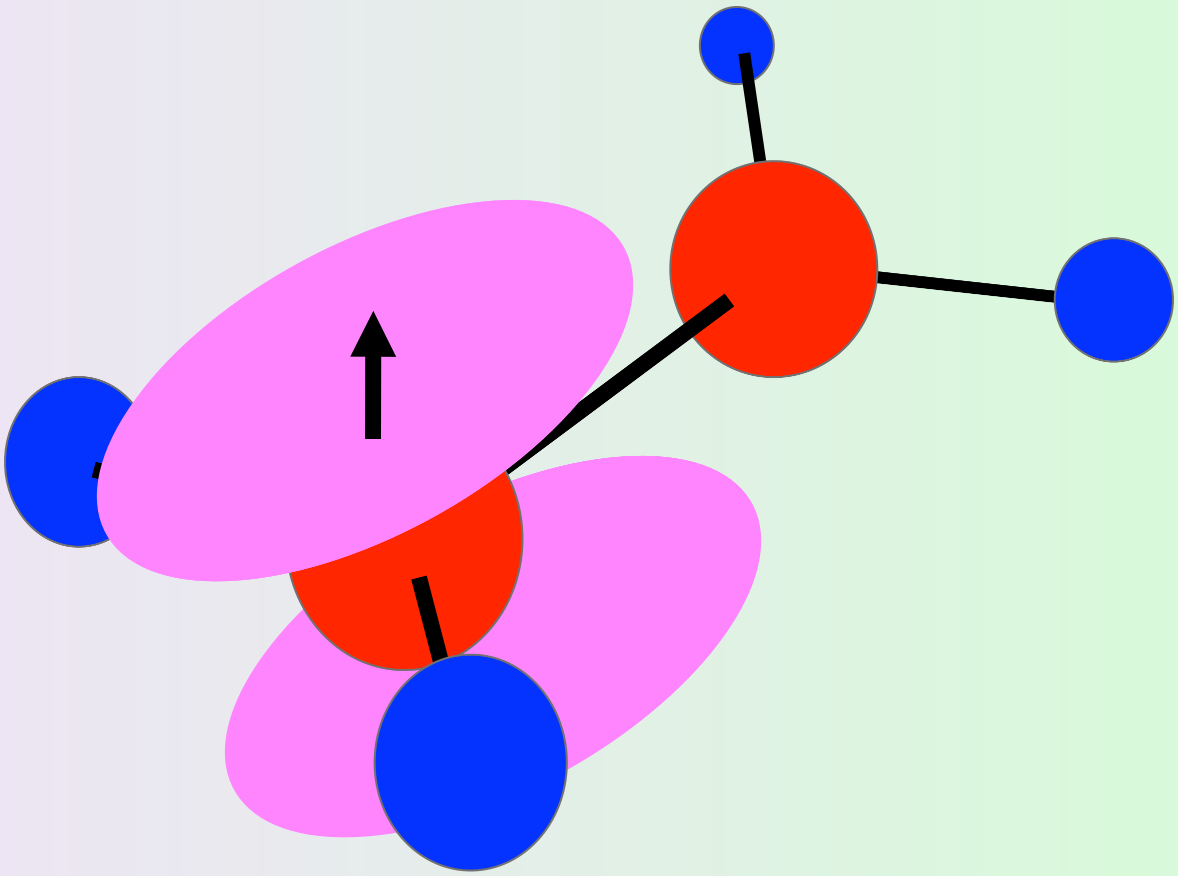
π –Bonding in Ethylene



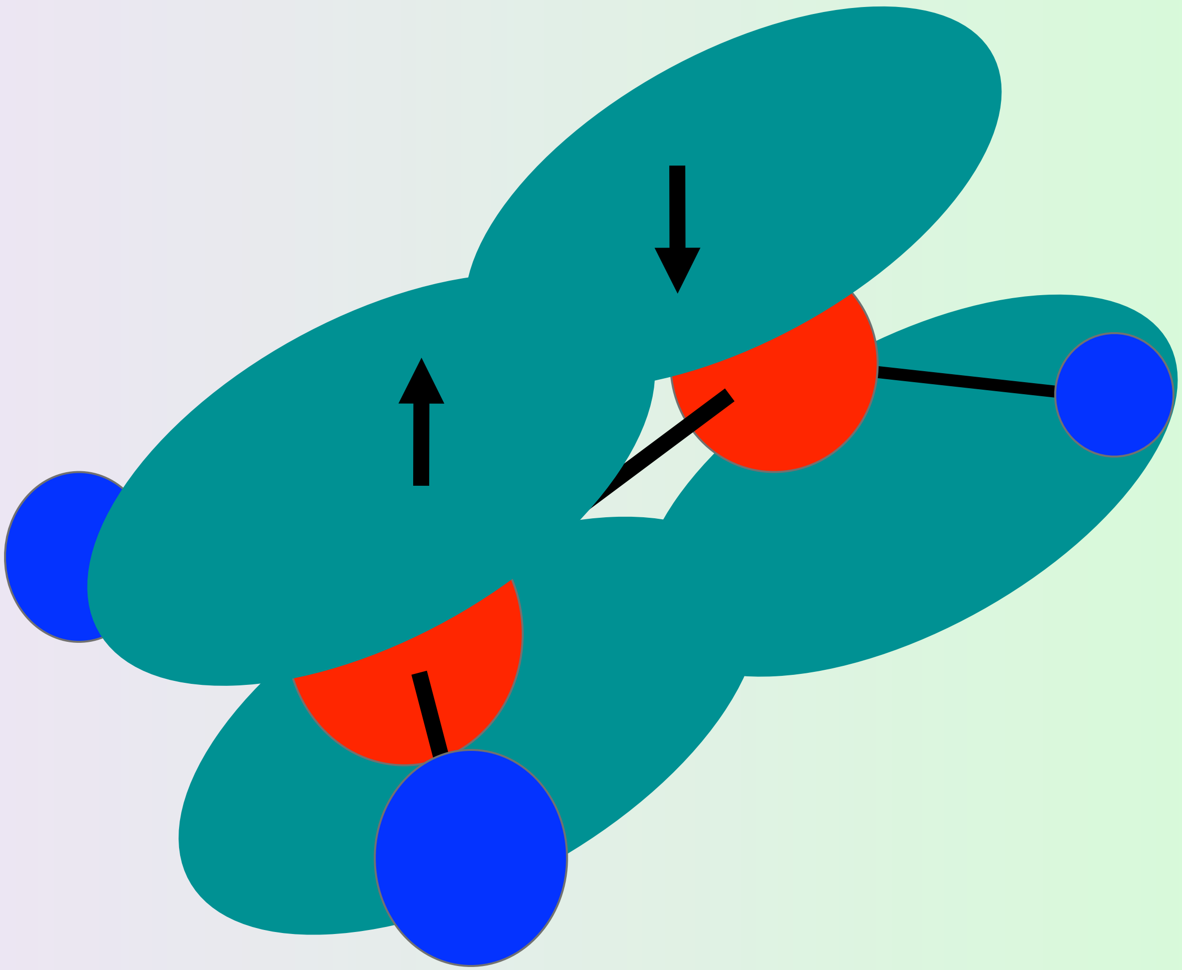
π –Bonding in Ethylene

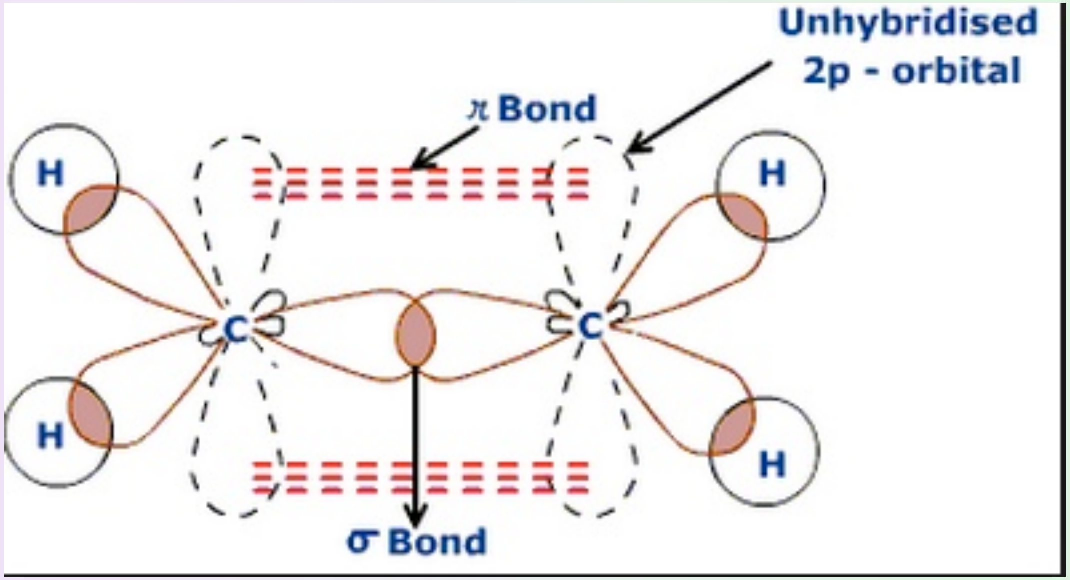


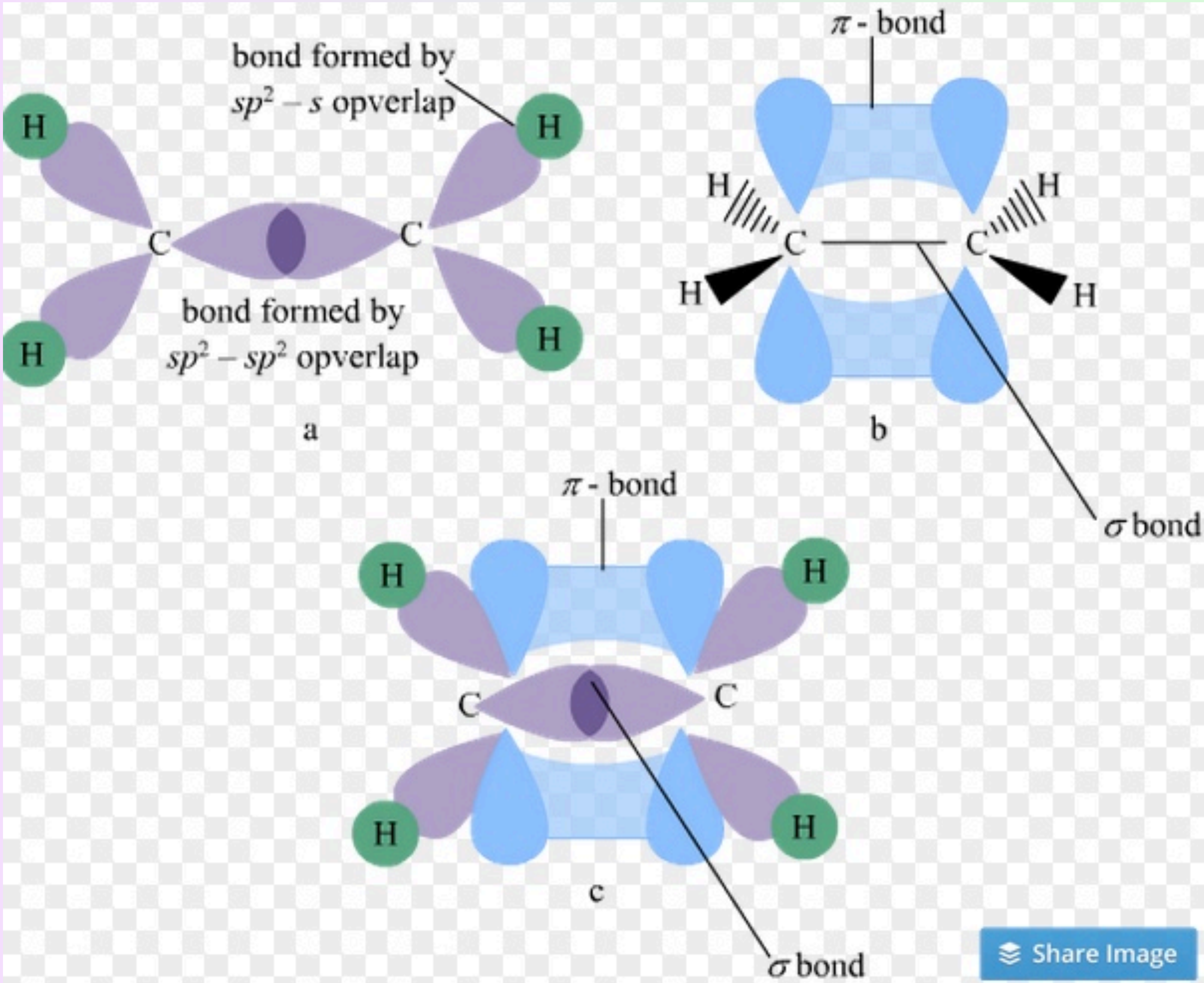
π –Bonding in Ethylene

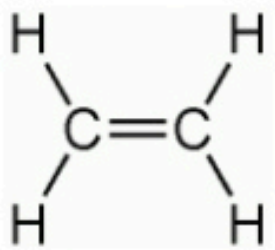


π –Bonding in Ethylene

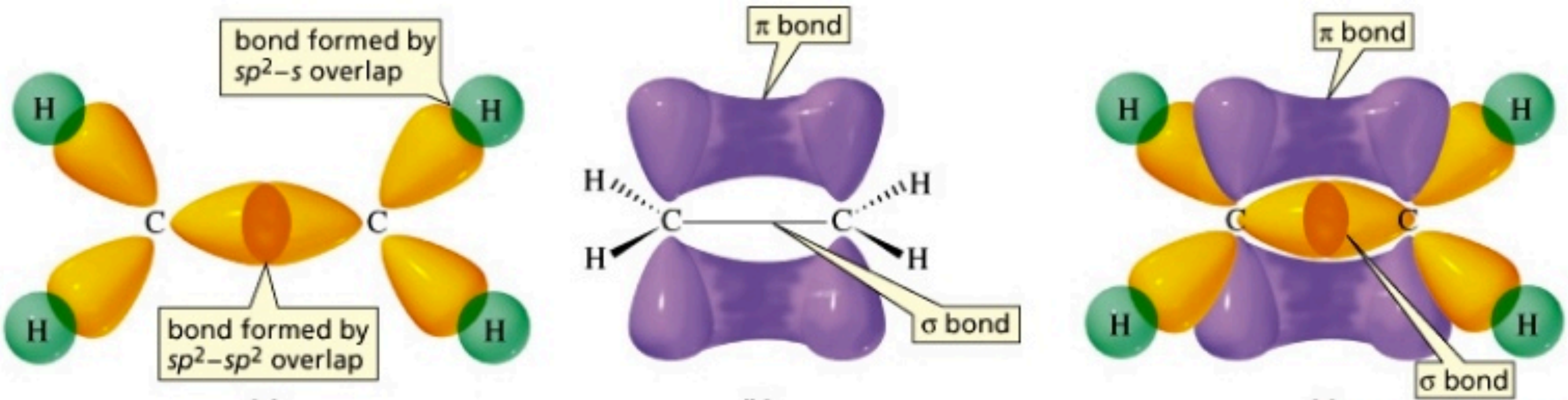



Unhybridised
2p - orbital
π Bond
H
H
C
C
H
H
σ Bond


bond formed by
sp² – s opverlap
H
H
H
H
C
C
bond formed by
sp² – sp² opverlap
a
π - bond
H
H
C
C
H
H
b
σ bond
π - bond
H
H
C
C
H
H
c
σ bond
Share Image



Ethylene (Ethene)



(a) (b) (c)

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