

1.15

Bonding in Methane and
Orbital Hybridization

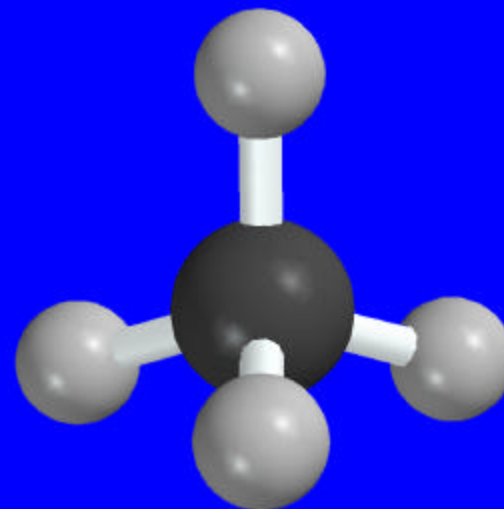
Structure of Methane

tetrahedral

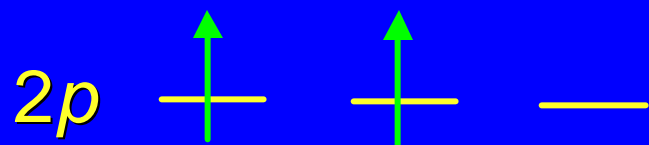
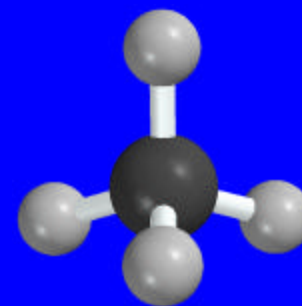
bond angles = 109.5°

bond distances = 110 pm

but structure seems inconsistent with
electron configuration of carbon

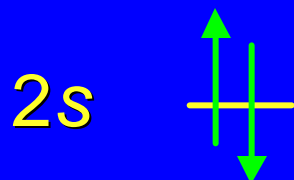


Electron configuration of carbon



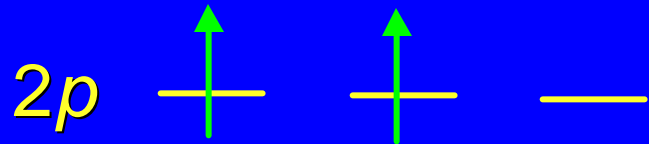
only two unpaired electrons

should form σ bonds to only two hydrogen atoms

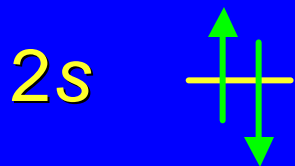


bonds should be at right angles to one another

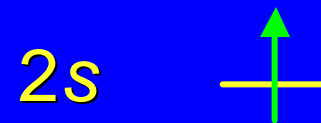
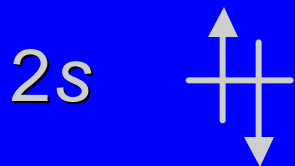
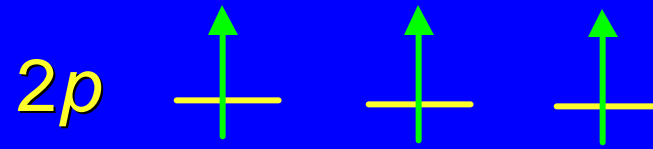
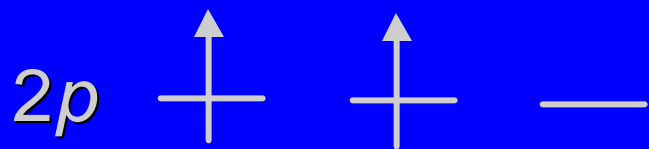
sp^3 Orbital Hybridization



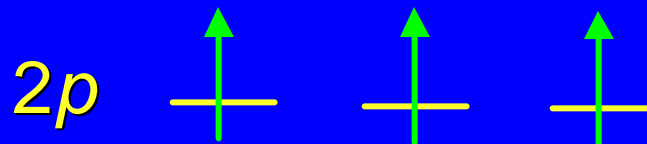
Promote an electron from the $2s$
to the $2p$ orbital



sp^3 Orbital Hybridization



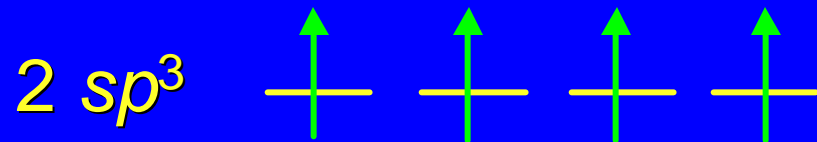
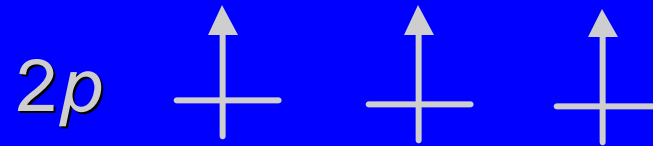
sp^3 Orbital Hybridization



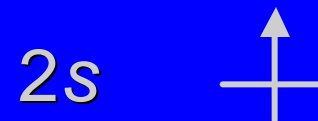
Mix together (hybridize) the $2s$ orbital and the three $2p$ orbitals



sp^3 Orbital Hybridization

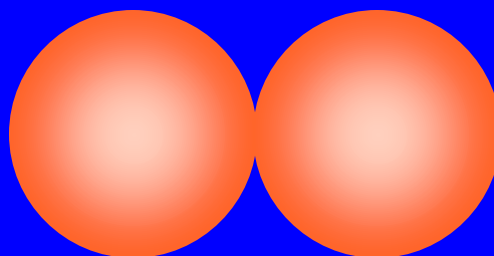


4 equivalent half-filled orbitals are consistent with four bonds and tetrahedral geometry

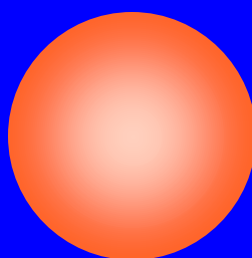


Shapes of orbitals

p

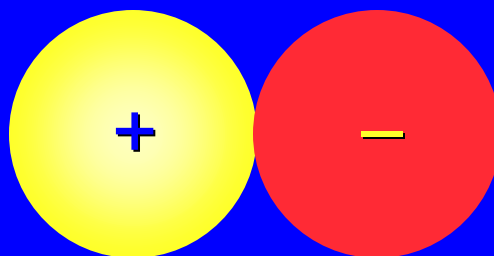


s

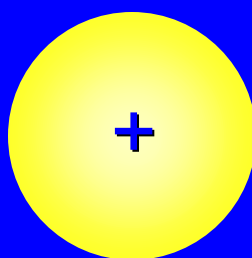


Nodal properties of orbitals

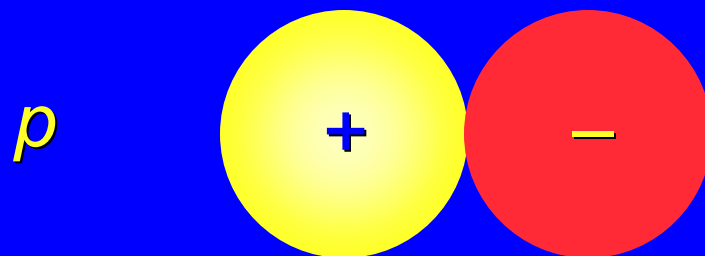
p



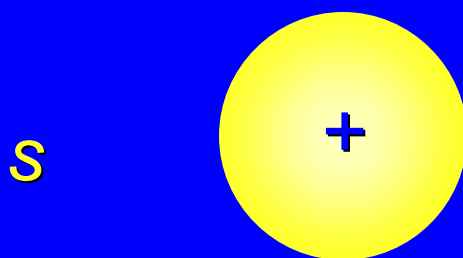
s



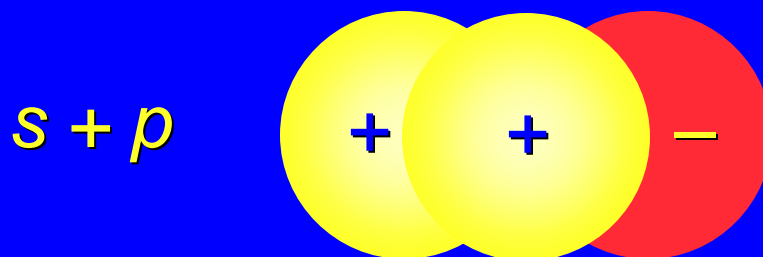
Shape of sp^3 hybrid orbitals



take the s orbital and place it on
top of the p orbital



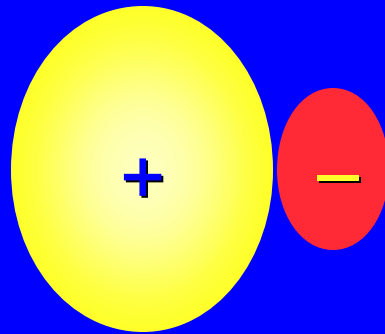
Shape of sp^3 hybrid orbitals



reinforcement of electron wave in
regions where sign is the same
destructive interference in regions of
opposite sign

Shape of sp^3 hybrid orbitals

sp hybrid



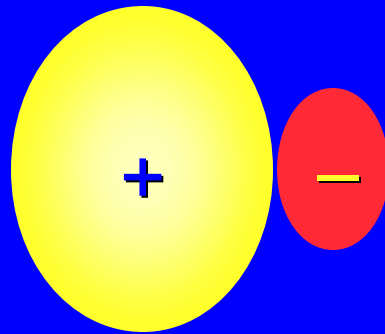
orbital shown is sp hybrid

analogous procedure using three s orbitals
and one p orbital gives sp^3 hybrid

shape of sp^3 hybrid is similar

Shape of sp^3 hybrid orbitals

sp hybrid



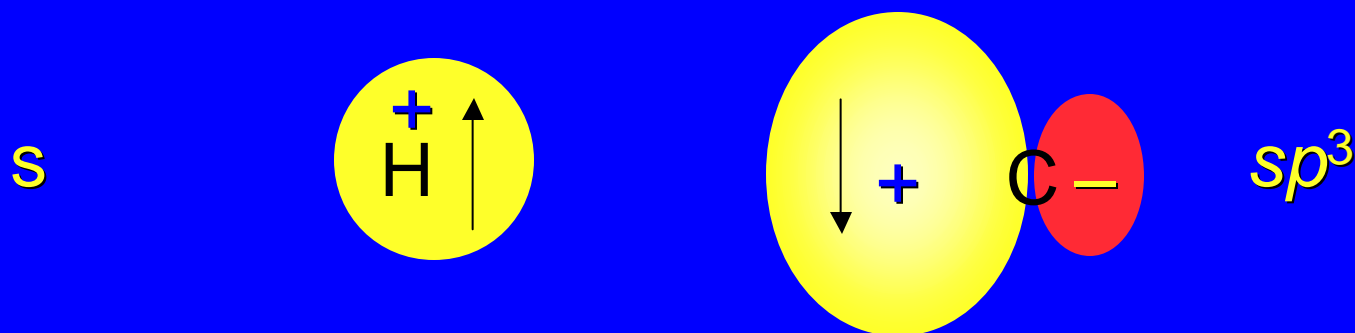
hybrid orbital is not symmetrical

higher probability of finding an electron on one side of the nucleus than the other

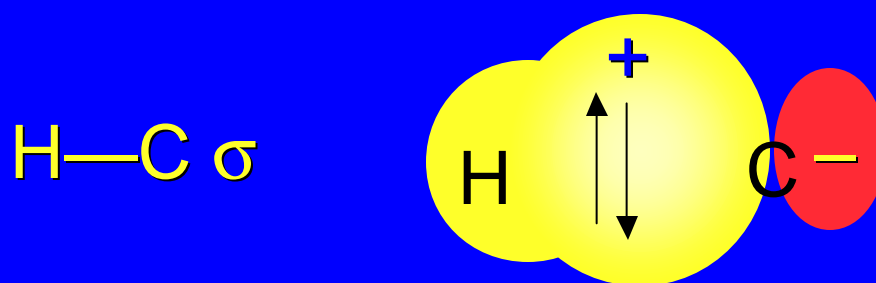
leads to stronger bonds

The C—H s Bond in Methane

In-phase overlap of a half-filled $1s$ orbital of hydrogen with a half-filled sp^3 hybrid orbital of carbon:



gives a s bond.



Justification for Orbital Hybridization

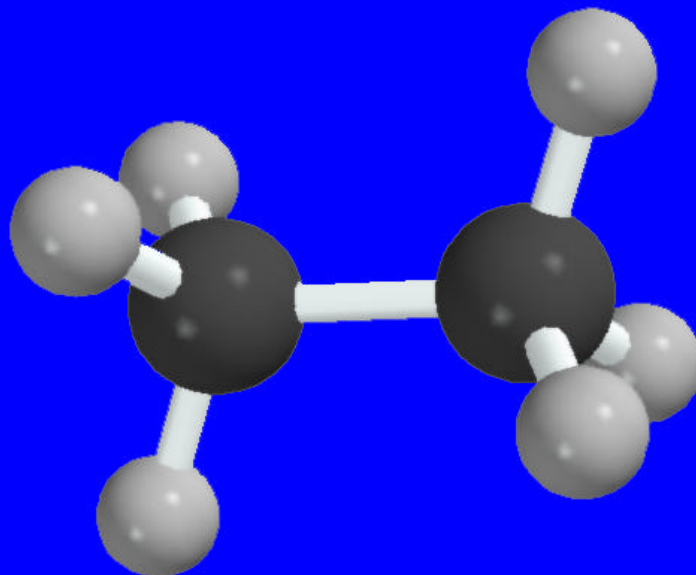
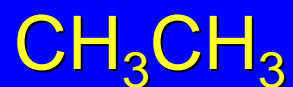
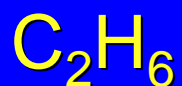
consistent with structure of methane

allows for formation of 4 bonds rather than 2

bonds involving sp^3 hybrid orbitals are stronger than those involving s - s overlap or p - p overlap

1.16
*sp*³ Hybridization
and Bonding in Ethane

Structure of Ethane

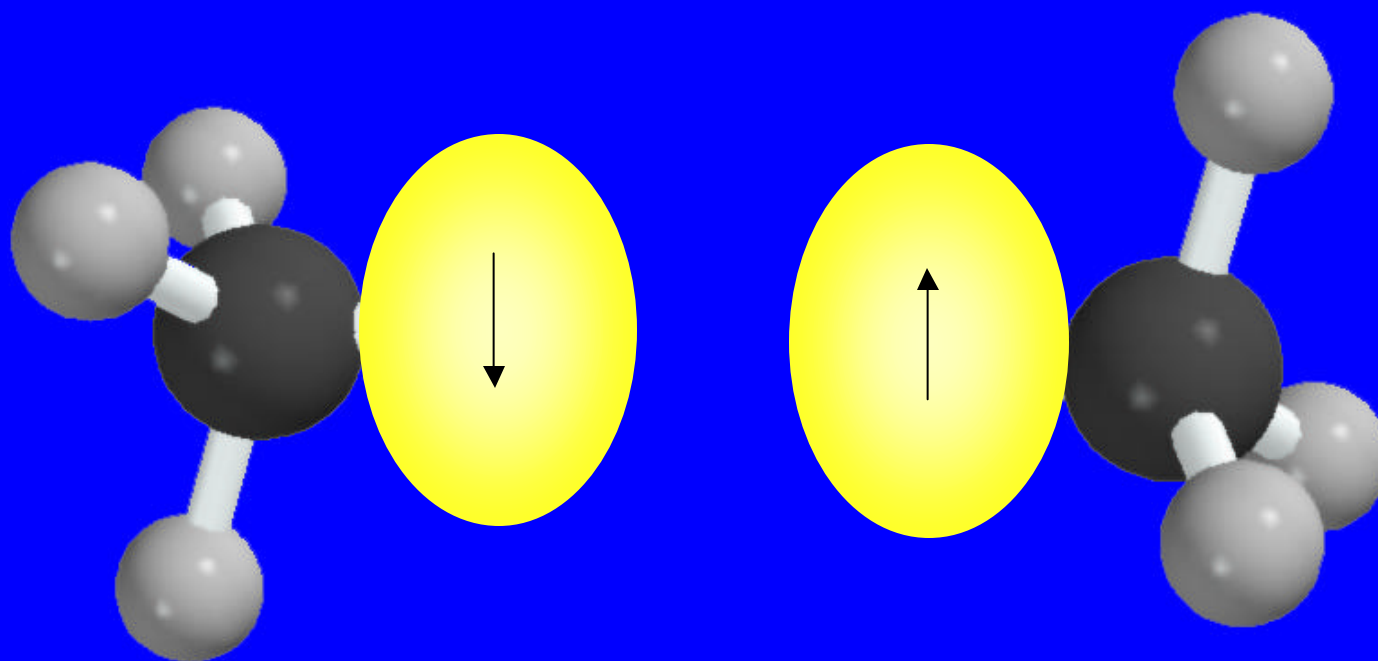


tetrahedral geometry at each carbon

C—H bond distance = 110 pm

C—C bond distance = 153 pm

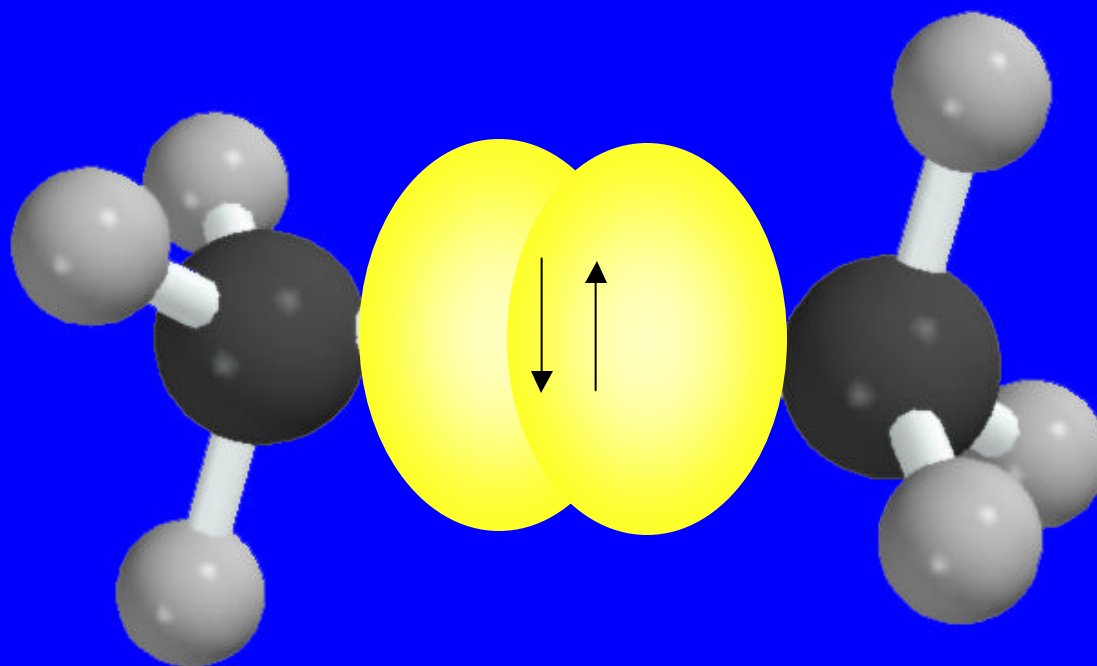
The C—C σ Bond in Ethane



In-phase overlap of half-filled sp^3 hybrid orbital of one carbon with half-filled sp^3 hybrid orbital of another.

Overlap is along internuclear axis to give a σ bond.

The C—C σ Bond in Ethane



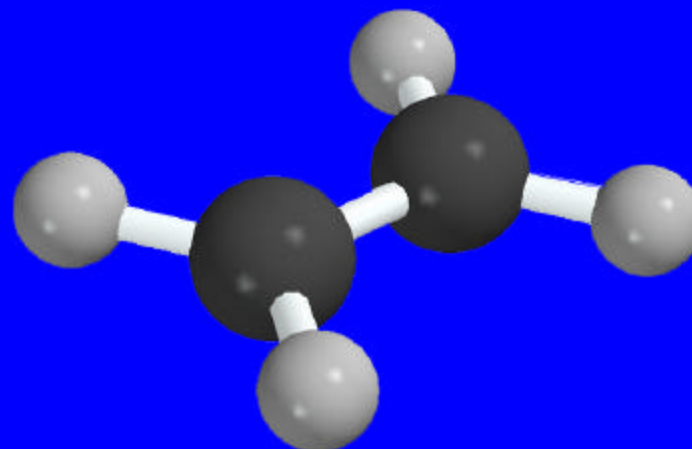
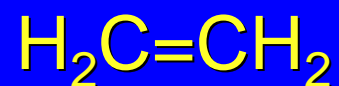
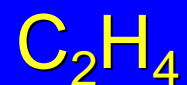
In-phase overlap of half-filled sp^3 hybrid orbital of one carbon with half-filled sp^3 hybrid orbital of another.

Overlap is along internuclear axis to give a σ bond.

1.17

sp^2 Hybridization
and Bonding in Ethylene

Structure of Ethylene

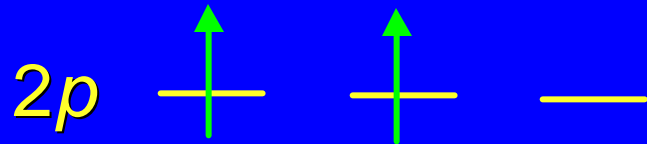


planar

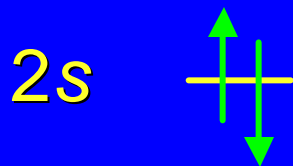
bond angles: close to 120°

bond distances: C—H = 110 pm
C=C = 134 pm

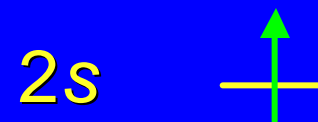
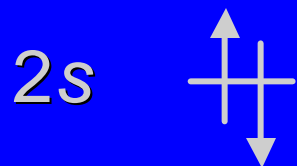
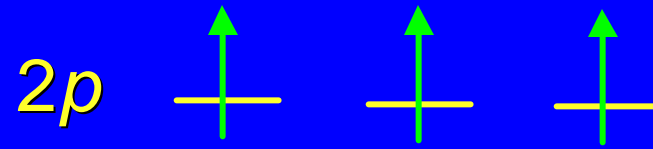
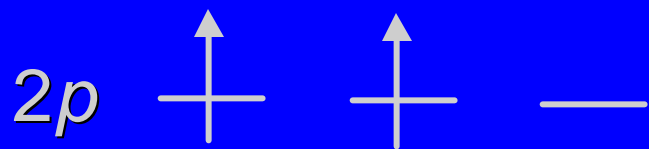
sp^2 Orbital Hybridization



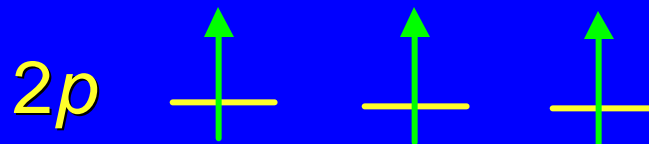
Promote an electron from the $2s$
to the $2p$ orbital



sp^2 Orbital Hybridization



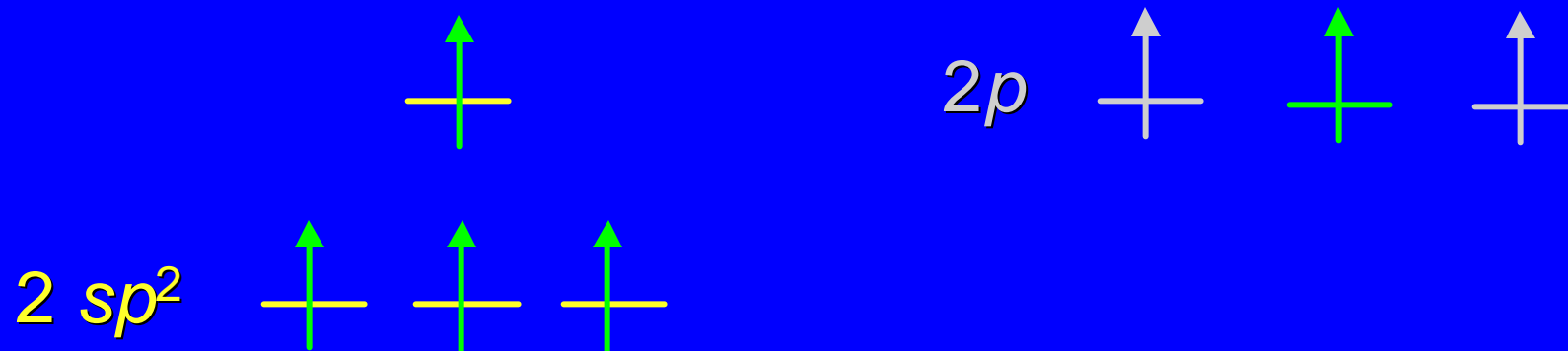
sp^2 Orbital Hybridization



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



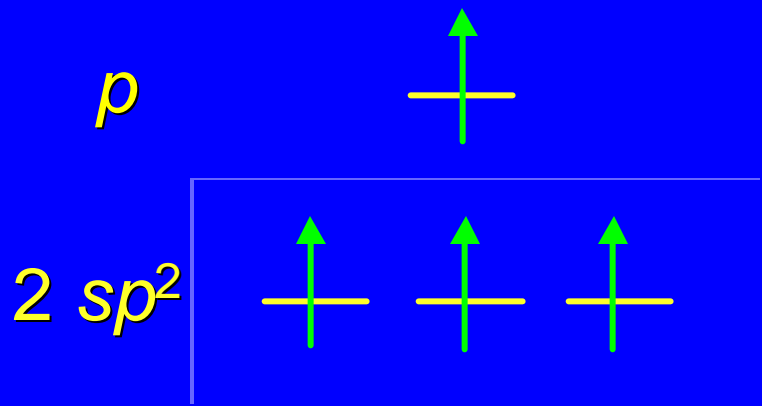
sp^2 Orbital Hybridization



3 equivalent half-filled sp^2 hybrid orbitals plus 1 p orbital left unhybridized

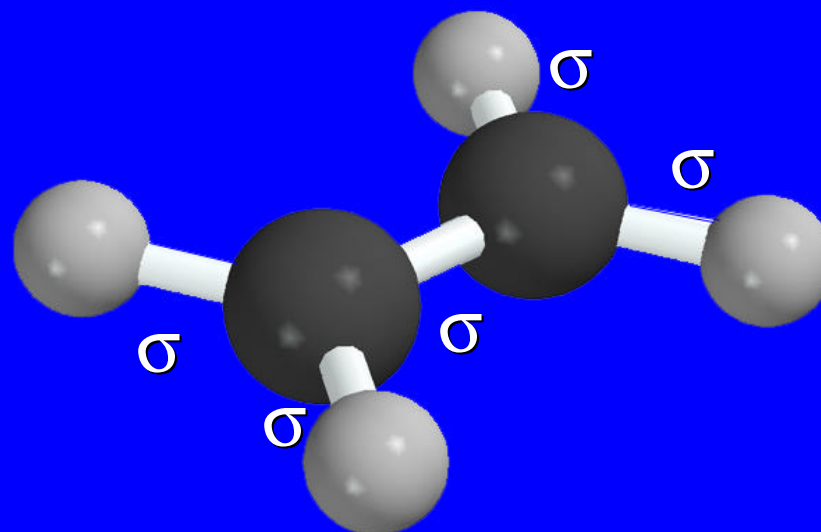
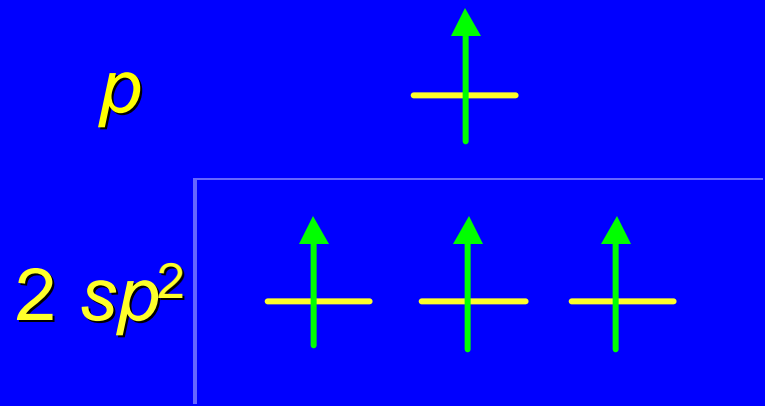


sp^2 Orbital Hybridization

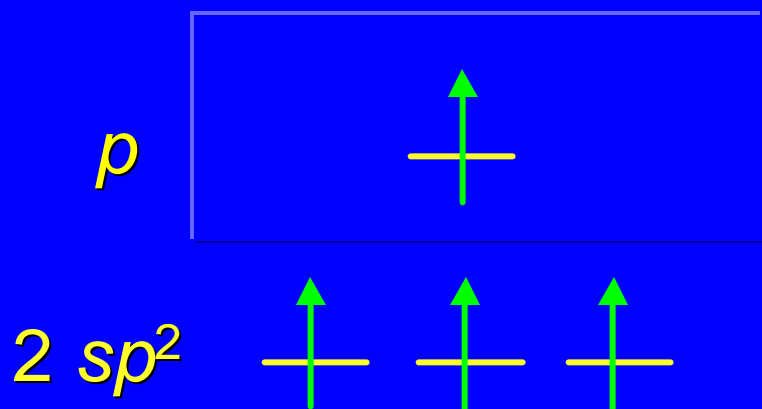


2 of the 3 sp^2 orbitals are involved in σ bonds to hydrogens; the other is involved in a σ bond to carbon

sp^2 Orbital Hybridization

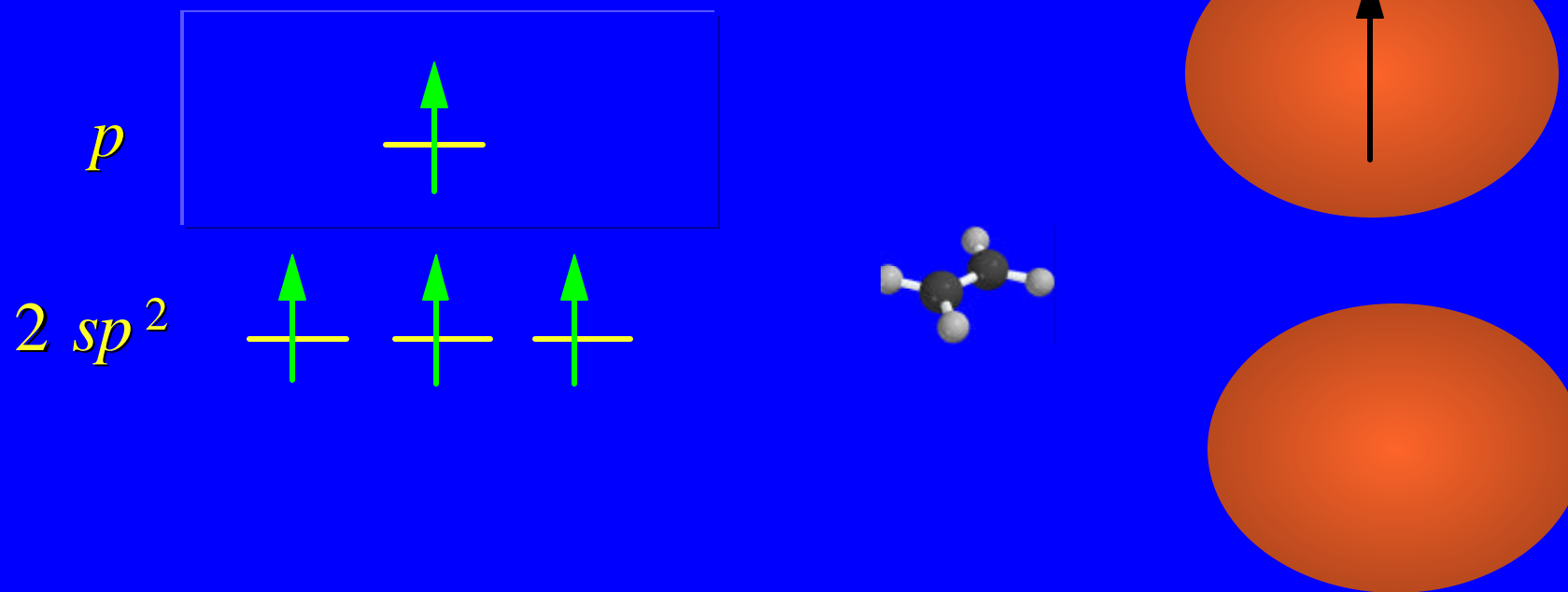


p Bonding in Ethylene



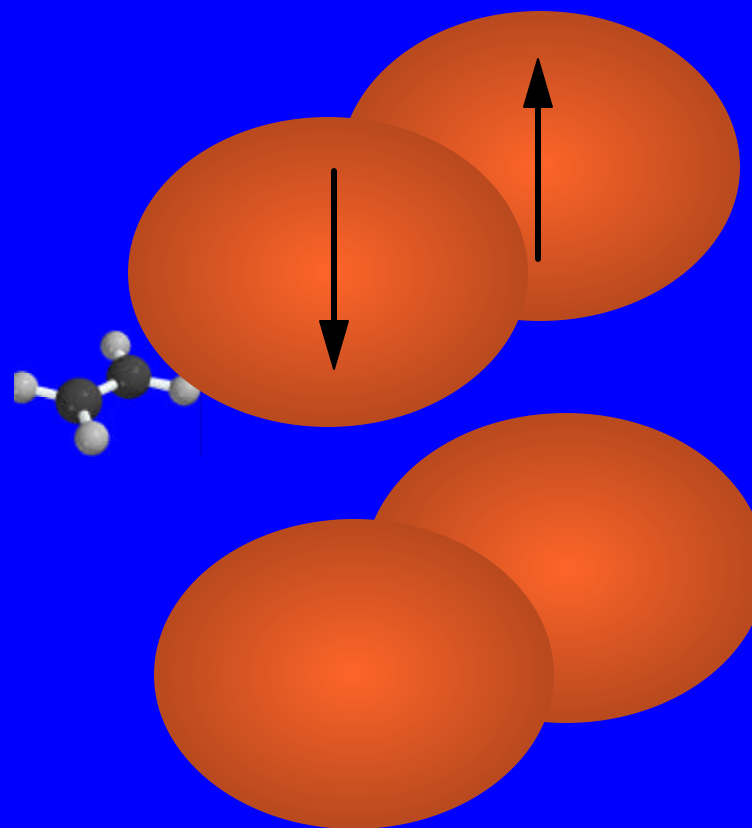
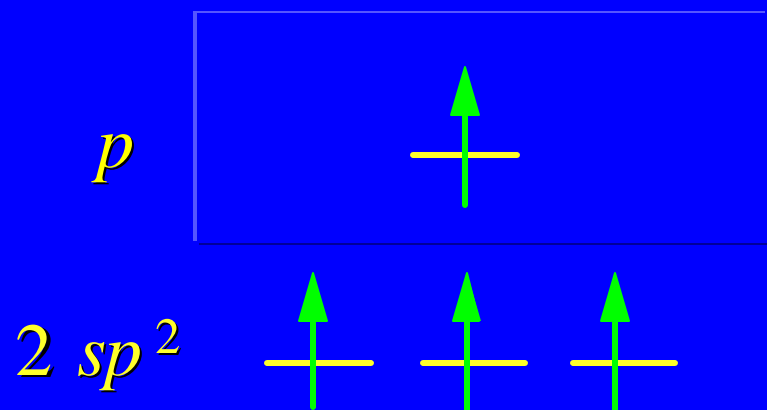
the unhybridized *p* orbital of carbon is involved in π bonding to the other carbon

***p** Bonding in Ethylene*



each carbon has an unhybridized 2 p orbital
axis of orbital is perpendicular to the plane of the σ bonds

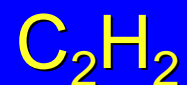
***p** Bonding in Ethylene*



side-by-side overlap of half-filled
 p orbitals gives a π bond
double bond in ethylene has a
 σ component and a π component

1.18
sp Hybridization
and Bonding in Acetylene

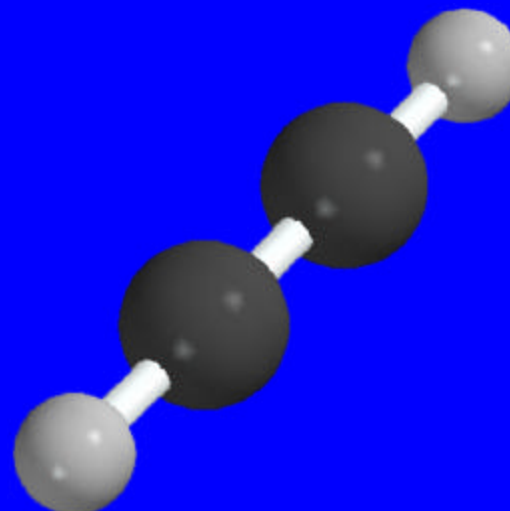
Structure of Acetylene



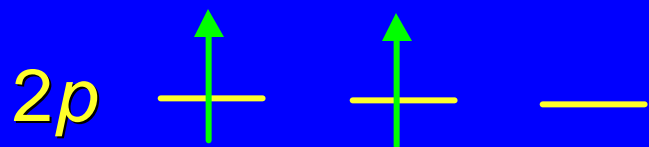
linear

bond angles: 180°

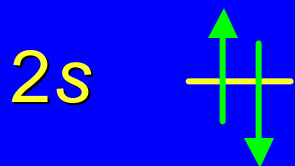
bond distances: C—H = 106 pm
CC = 120 pm



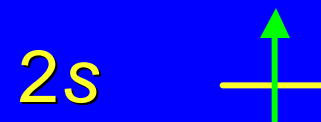
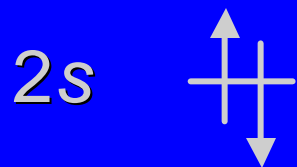
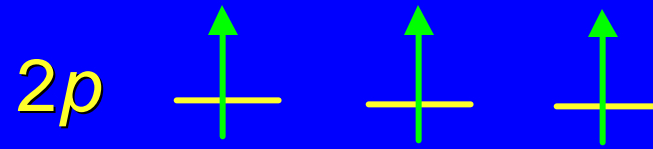
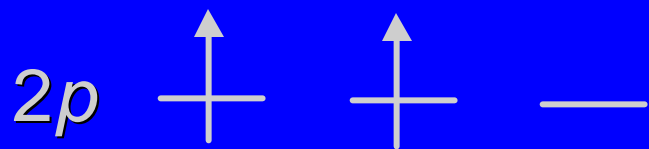
sp Orbital Hybridization



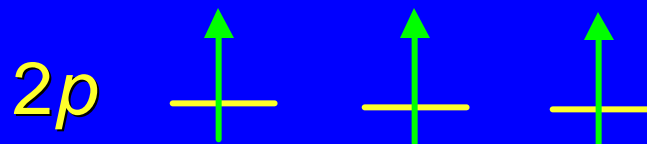
Promote an electron from the 2s
to the 2p orbital



sp Orbital Hybridization



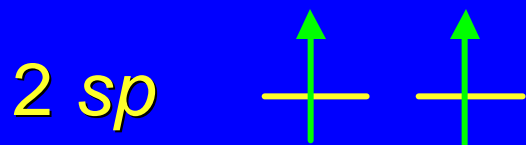
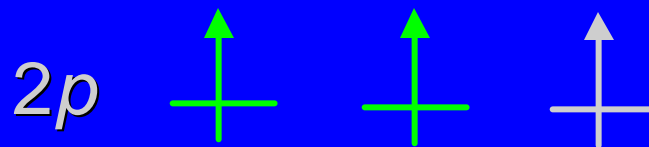
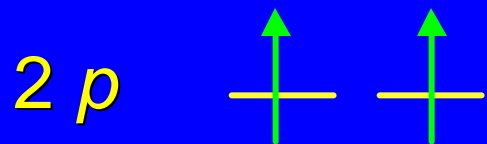
sp Orbital Hybridization



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



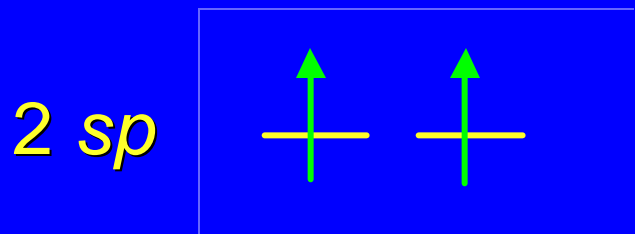
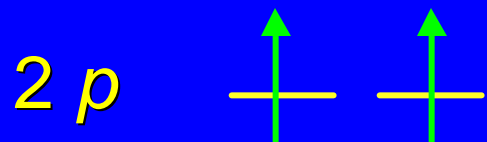
sp Orbital Hybridization



2 equivalent half-filled
sp hybrid orbitals plus
2 *p* orbitals left
unhybridized

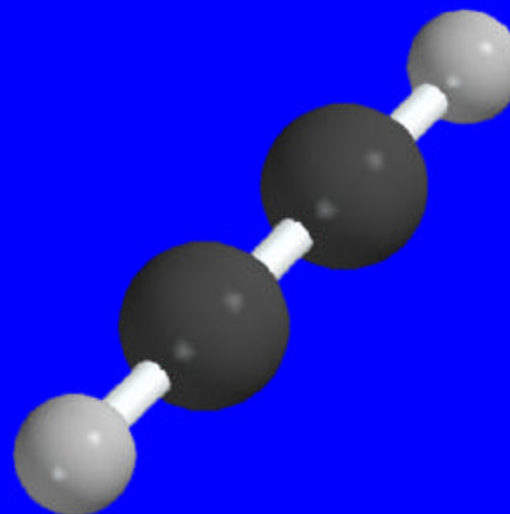
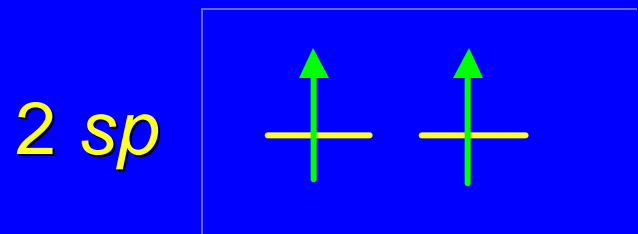
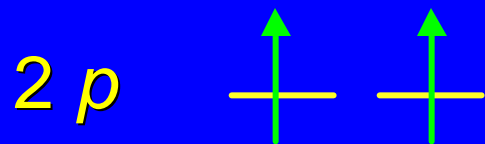


sp Orbital Hybridization



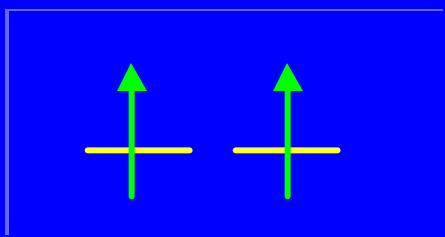
1 of the 2 sp orbitals is involved in a σ bond to hydrogen; the other is involved in a σ bond to carbon

sp Orbital Hybridization



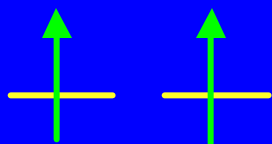
p Bonding in Acetylene

2 *p*



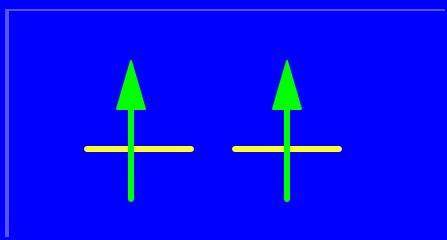
the unhybridized *p* orbitals of carbon are involved in separate π bonds to the other carbon

2 *sp*

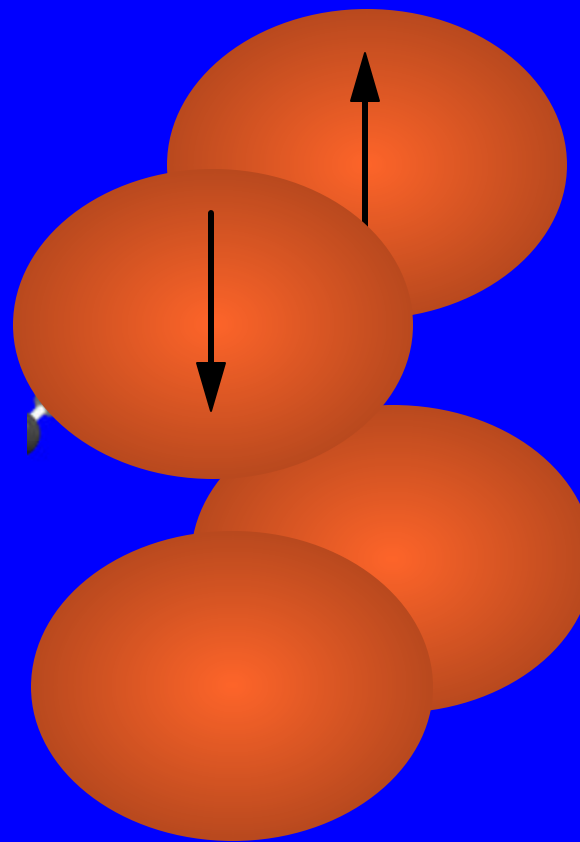
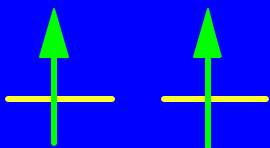


***p** Bonding in Acetylene*

$2p$



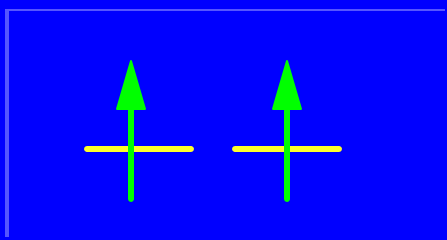
$2sp$



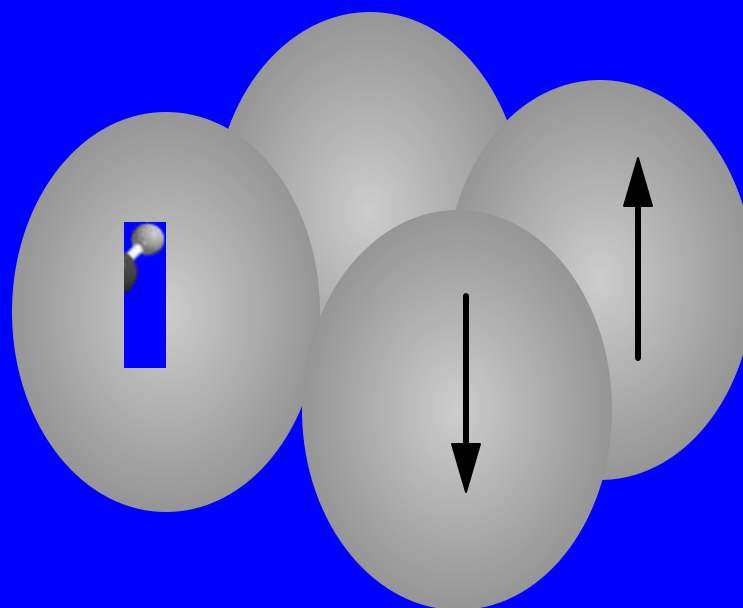
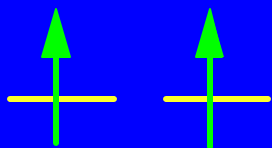
one π bond involves one of the p orbitals on each carbon
there is a second π bond perpendicular to this one

***p** Bonding in Acetylene*

2 p

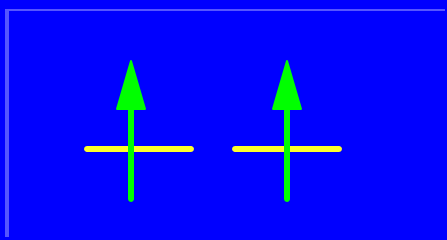


2 sp

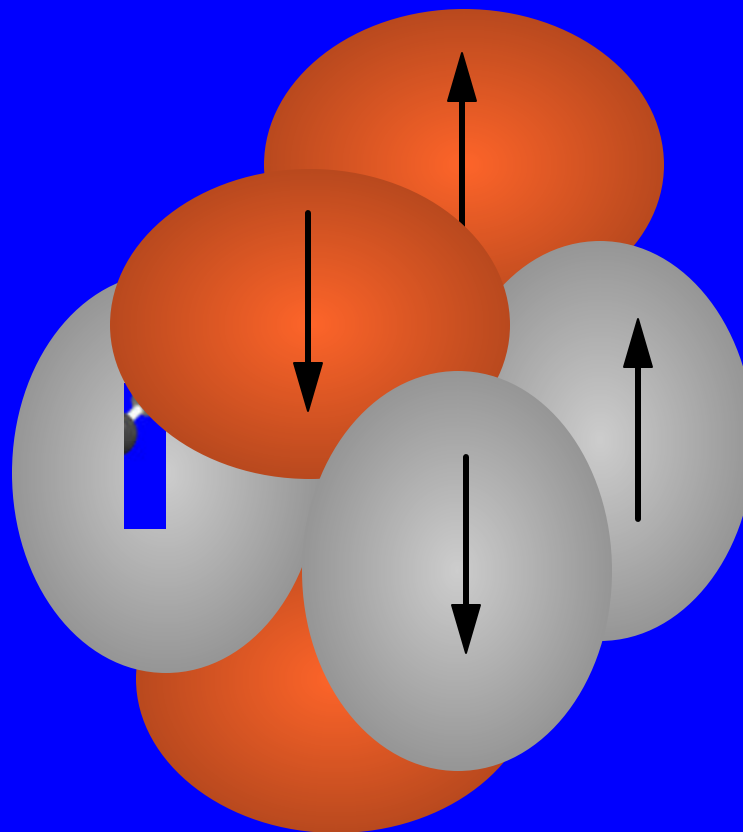
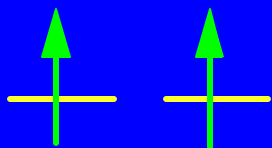


***p** Bonding in Acetylene*

2 p



2 sp



1.19

Which Theory of
Chemical Bonding is Best?

Three Models

Lewis

most familiar—easiest to apply

Valence-Bond (Orbital Hybridization)

provides more insight than Lewis model
ability to connect structure and reactivity
to hybridization develops with practice

Molecular Orbital

potentially the most powerful method
but is the most abstract
requires the most experience to use
effectively