

# Bonding in Methane and Orbital Hybridization

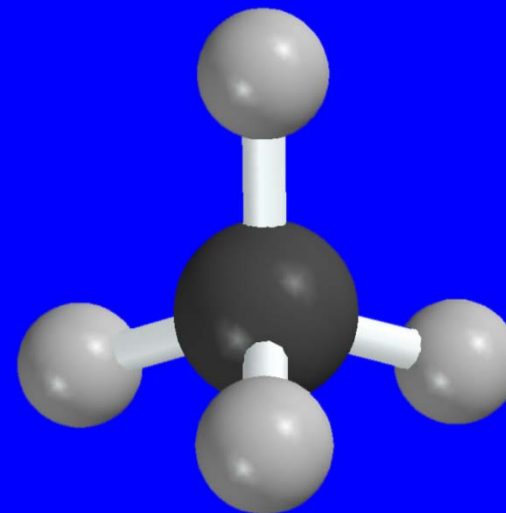
## *Structure of Methane*

tetrahedral

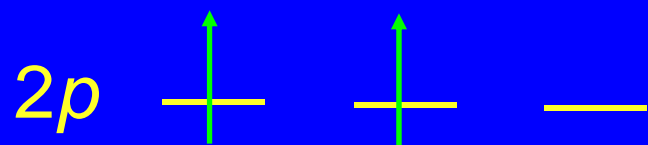
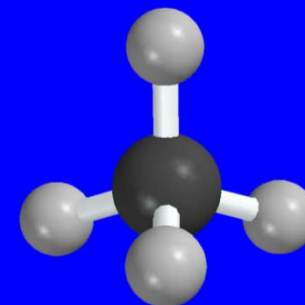
bond angles =  $109.5^\circ$

bond distances = 110 pm

but structure seems inconsistent with  
electron configuration of carbon

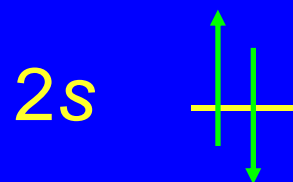


## *Electron configuration of carbon*



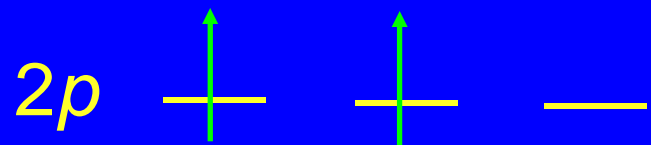
only two unpaired electrons

should form  $\sigma$  bonds to only two hydrogen atoms

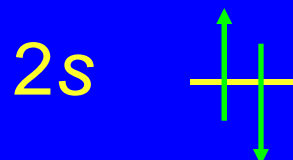


bonds should be at right angles to one another

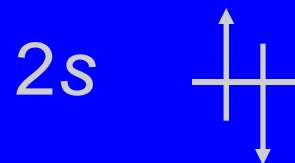
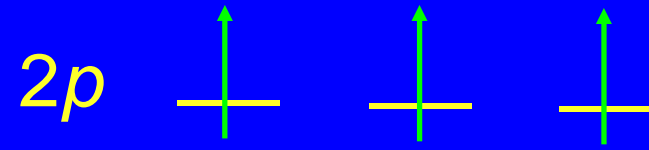
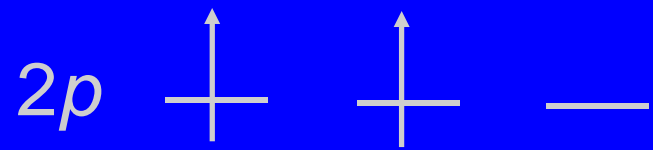
## $sp^3$ Orbital Hybridization



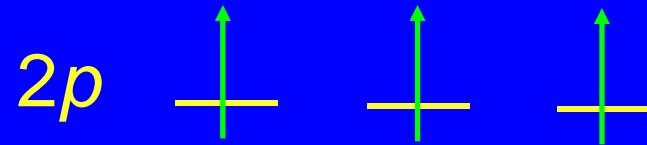
Promote an electron from the  $2s$   
to the  $2p$  orbital



# $sp^3$ Orbital Hybridization



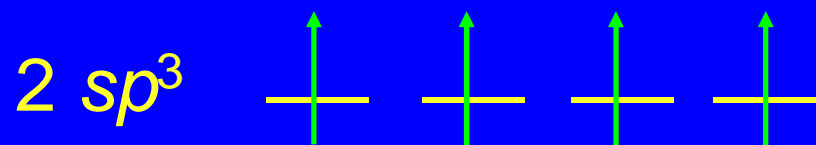
## $sp^3$ Orbital Hybridization



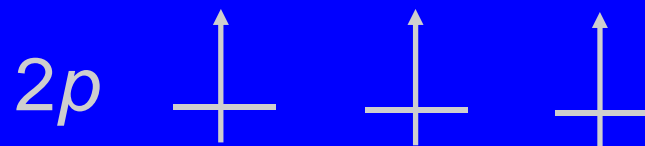
Mix together (hybridize) the  $2s$  orbital and the three  $2p$  orbitals



## $sp^3$ Orbital Hybridization

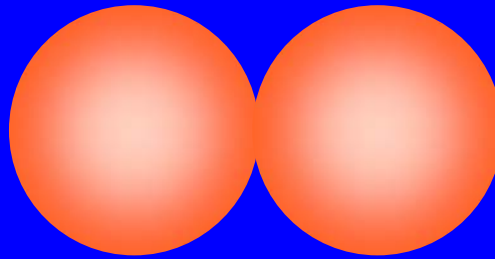


4 equivalent half-filled orbitals are consistent with four bonds and tetrahedral geometry

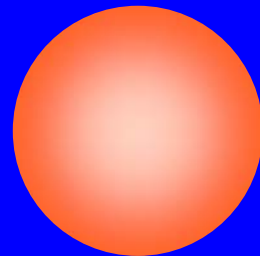


# Shapes of orbitals

*p*



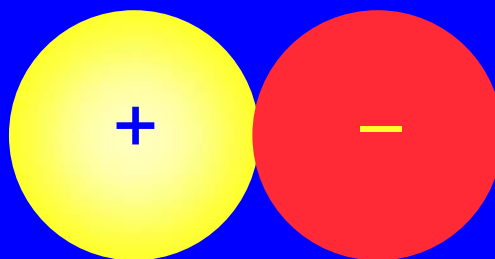
*s*



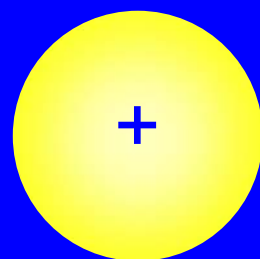


## *Nodal properties of orbitals*

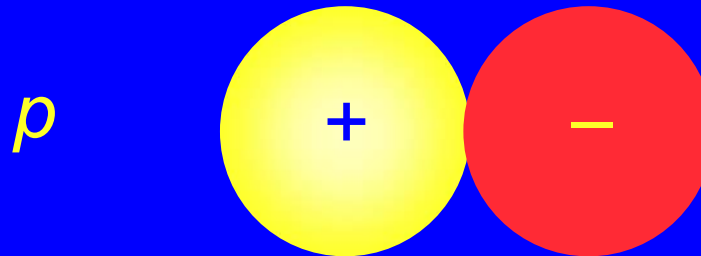
*p*



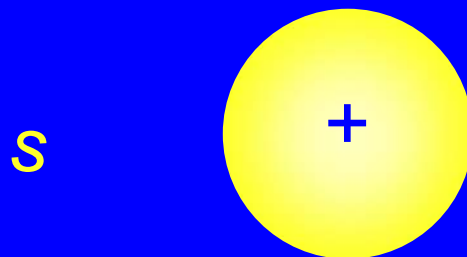
*s*



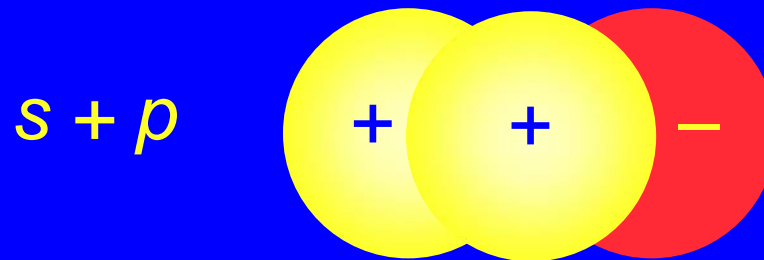
## *Shape of $sp^3$ hybrid orbitals*



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



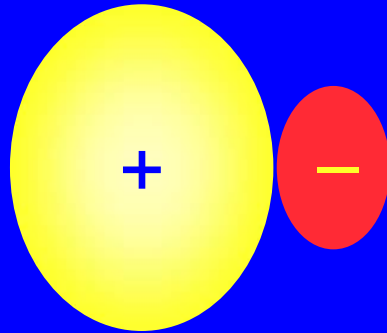
## *Shape of $sp^3$ hybrid orbitals*



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



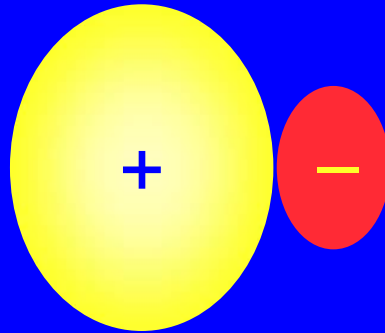
orbital shown is  $sp$  hybrid

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



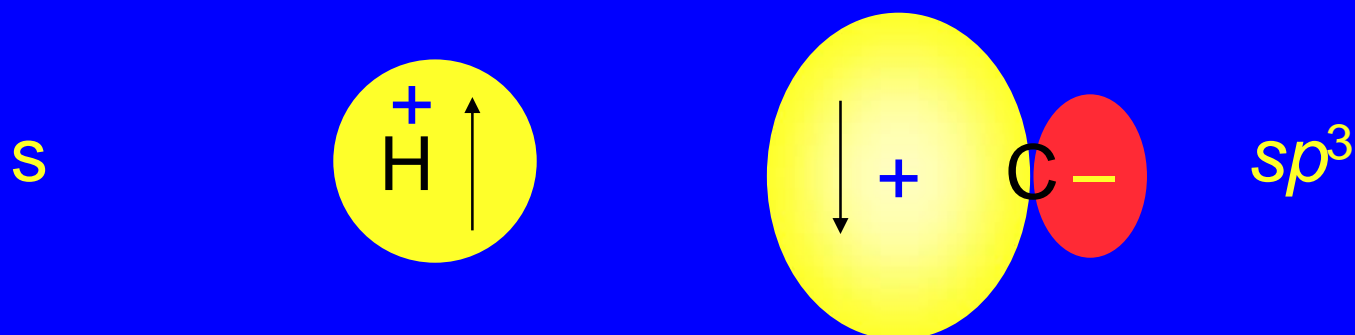
hybrid orbital is not symmetrical

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

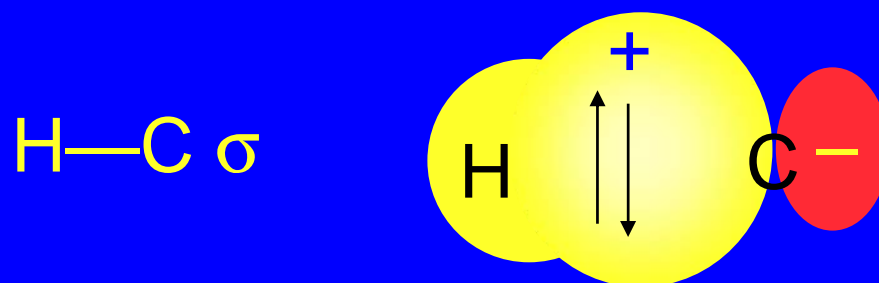
leads to stronger bonds

## The C—H $\sigma$ 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  $\sigma$  bond.



## *Justification for Orbital Hybridization*

consistent with structure of methane

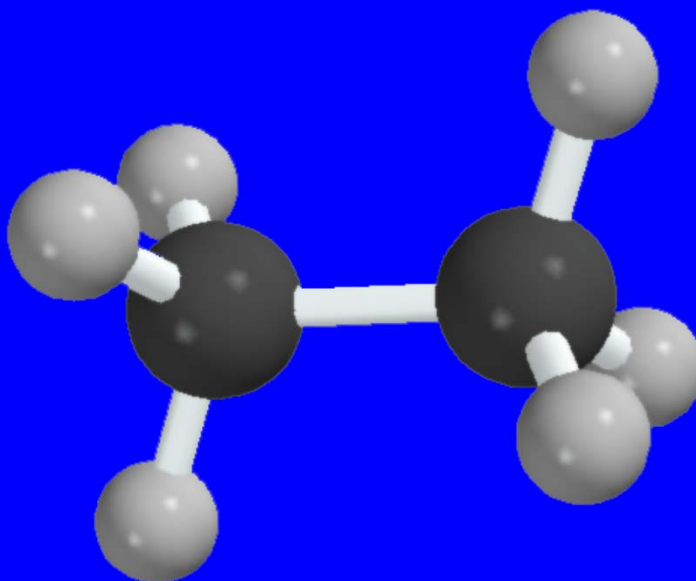
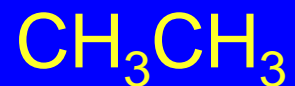
allows for formation of 4 bonds rather than 2

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

$sp^3$  Hybridization  
and Bonding in Ethane



## Structure of Ethane

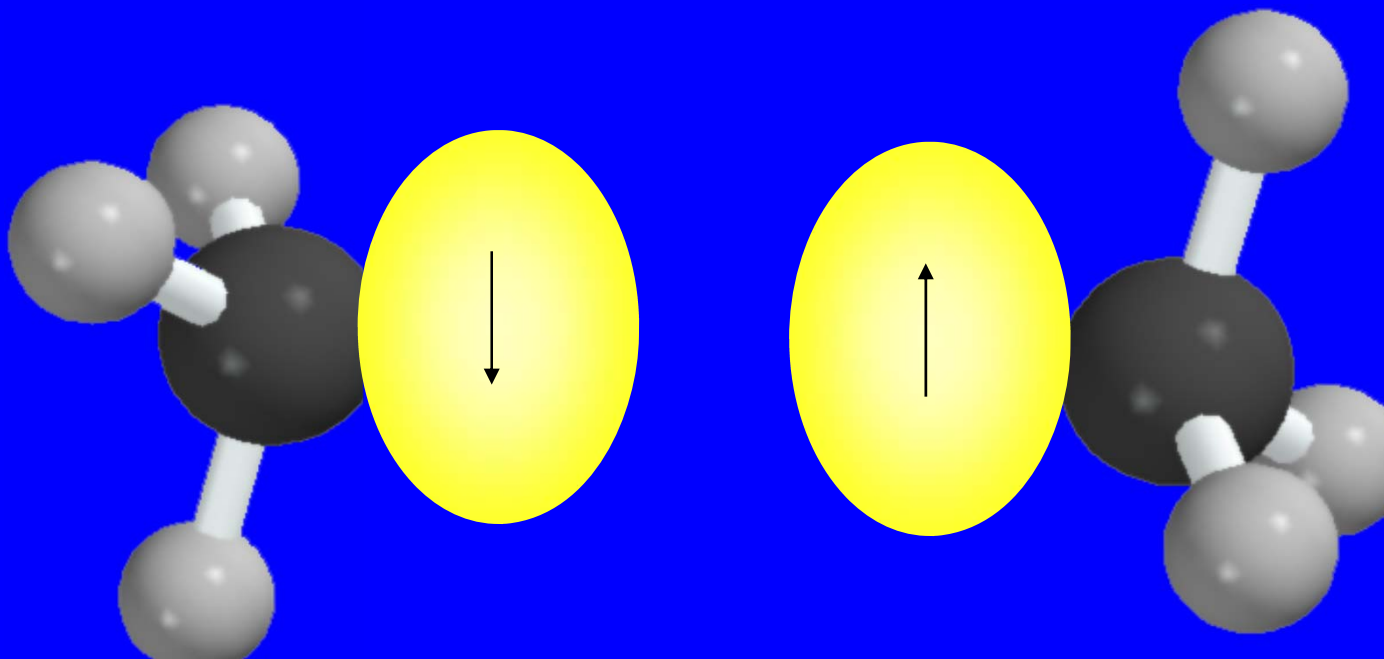


tetrahedral geometry at each carbon

C—H bond distance = 110 pm

C—C bond distance = 153 pm

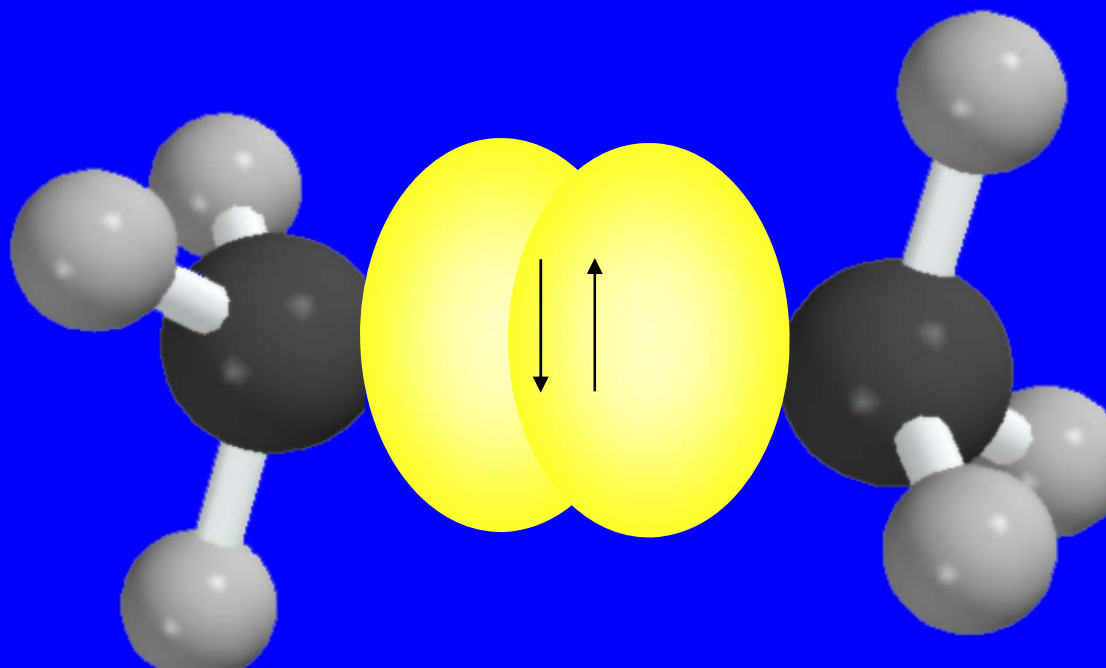
## *The C—C $\sigma$ Bond in Ethane*



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  $\sigma$  bond.

## *The C—C $\sigma$ Bond in Ethane*

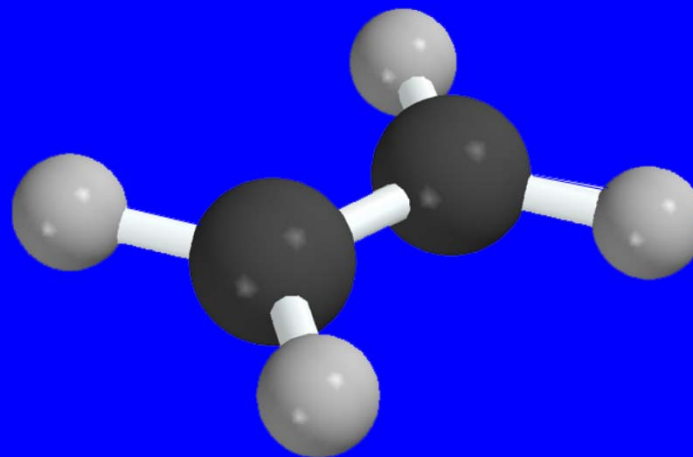
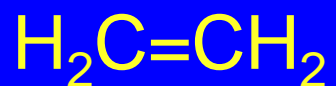


In-phase overlap of half-filled  $sp^3$  hybrid orbital of one carbon with half-filled  $sp^3$  hybrid orbital of another.

Overlap is along internuclear axis to give a  $\sigma$  bond.

$sp^2$  Hybridization  
and Bonding in Ethylene

## *Structure of Ethylene*

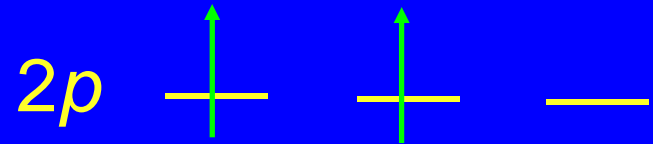


planar

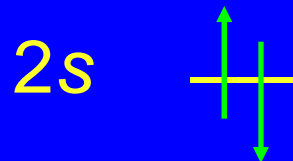
bond angles: close to  $120^\circ$

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

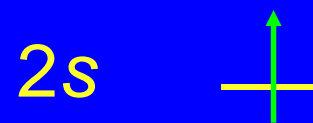
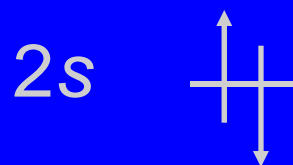
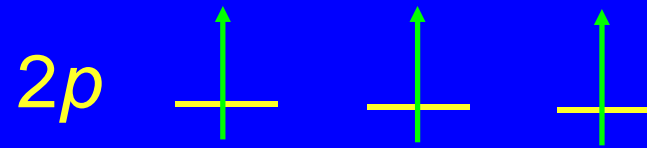
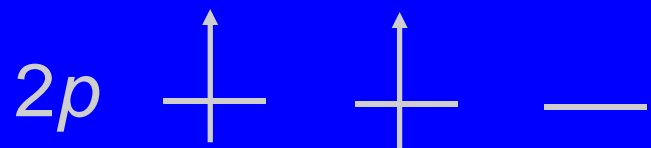
## $sp^2$ Orbital Hybridization



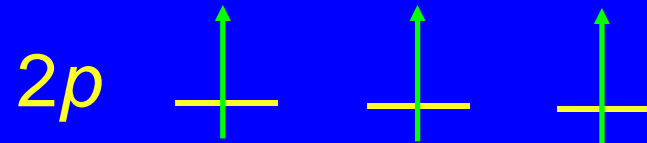
Promote an electron from the  $2s$   
to the  $2p$  orbital



# $sp^2$ Orbital Hybridization



## $sp^2$ Orbital Hybridization

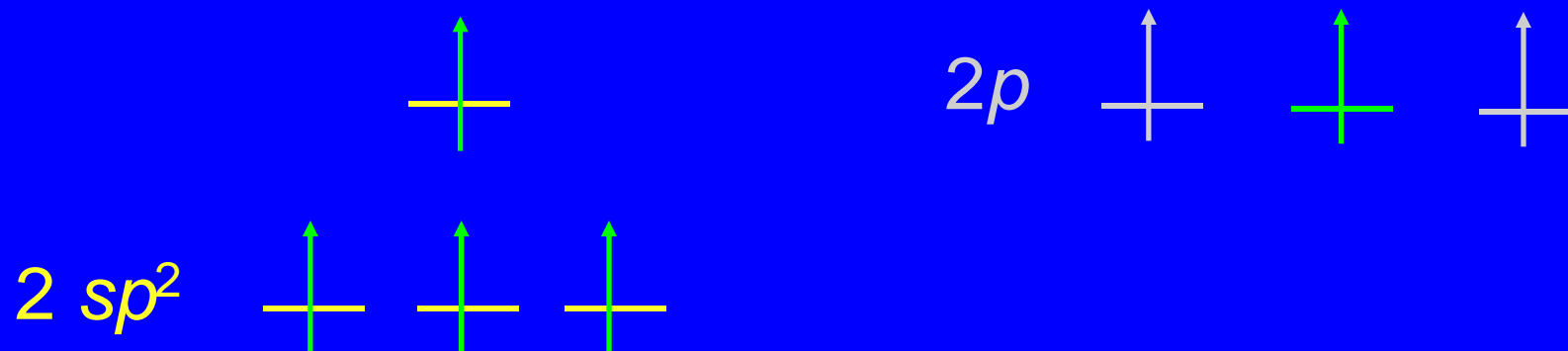


Mix together (hybridize) the  $2s$  orbital and two of the three  $2p$  orbitals





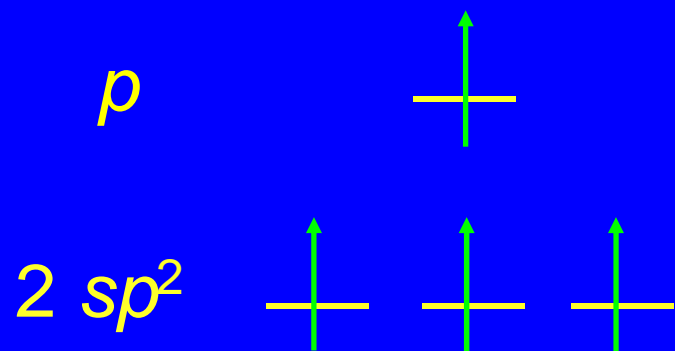
# $sp^2$ Orbital Hybridization



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

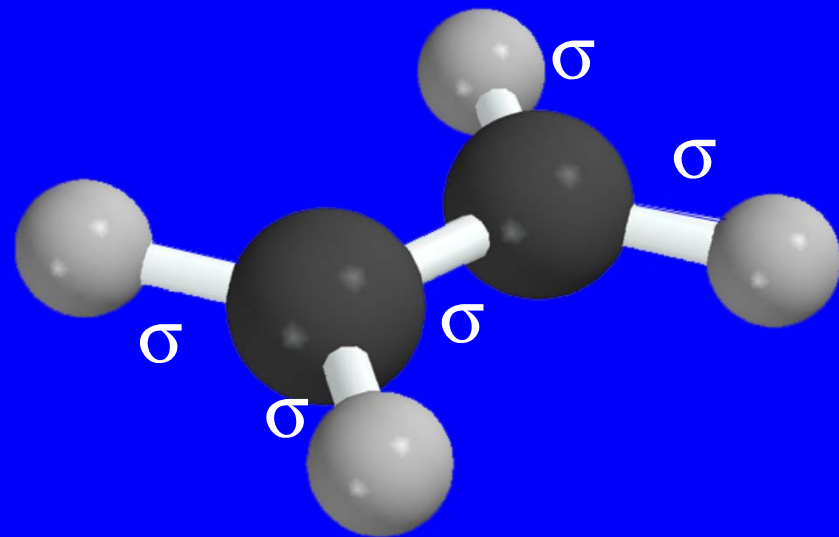
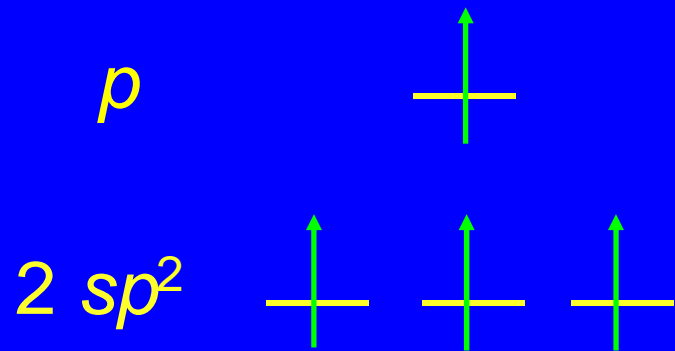


## $sp^2$ Orbital Hybridization

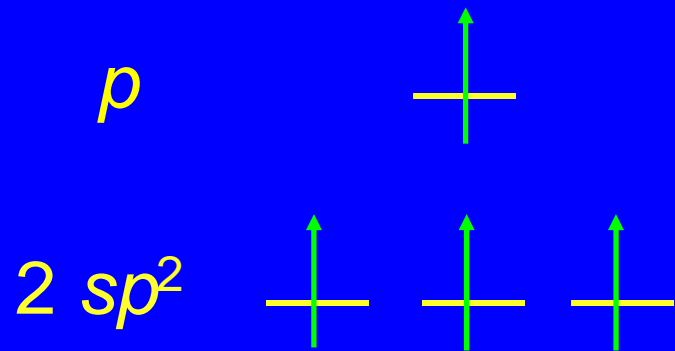


2 of the 3  $sp^2$  orbitals are involved in  $\sigma$  bonds to hydrogens; the other is involved in a  $\sigma$  bond to carbon

# $sp^2$ Orbital Hybridization

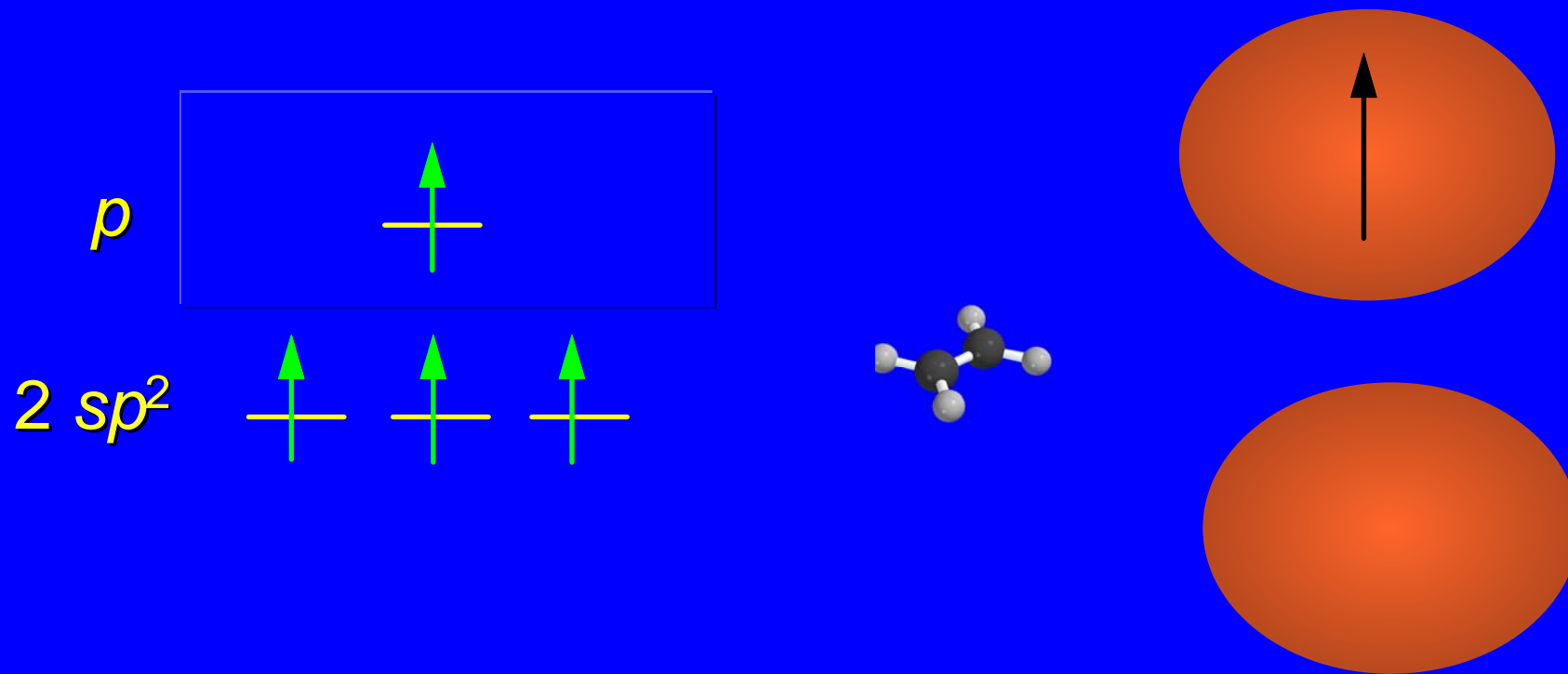


## $\pi$ Bonding in Ethylene



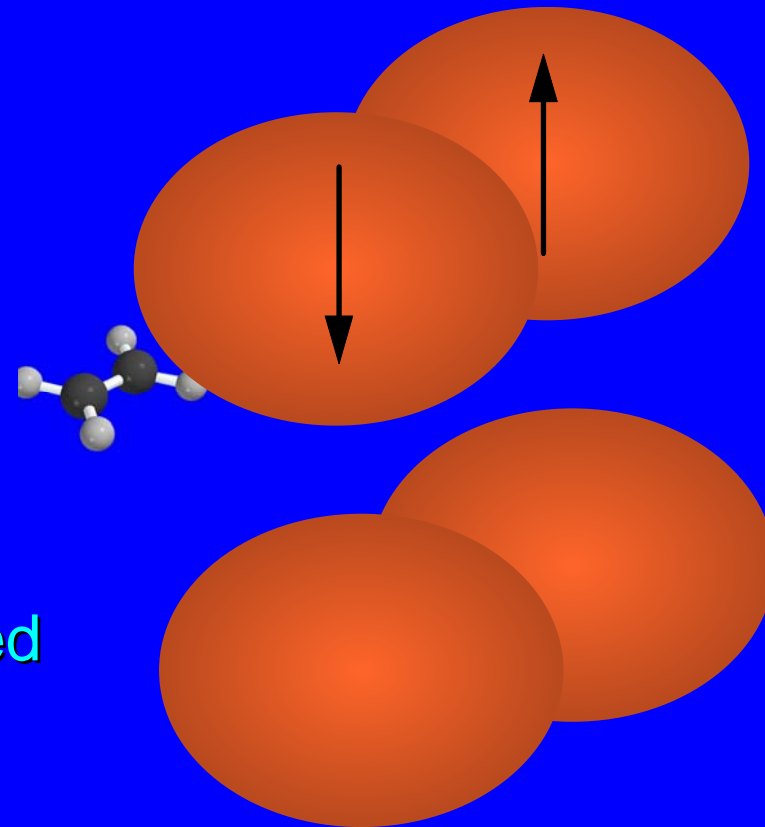
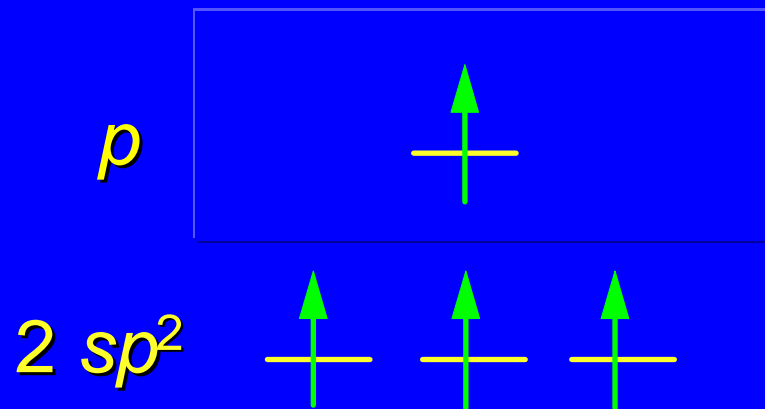
the unhybridized  $p$  orbital of carbon is involved in  $\pi$  bonding to the other carbon

## $\pi$ Bonding in Ethylene



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

## $\pi$ Bonding in Ethylene



side-by-side overlap of half-filled  
 $p$  orbitals gives a  $\pi$  bond  
double bond in ethylene has a  
 $\sigma$  component and a  $\pi$  component

1.18  
*sp* Hybridization  
and Bonding in Acetylene

## *Structure of Acetylene*

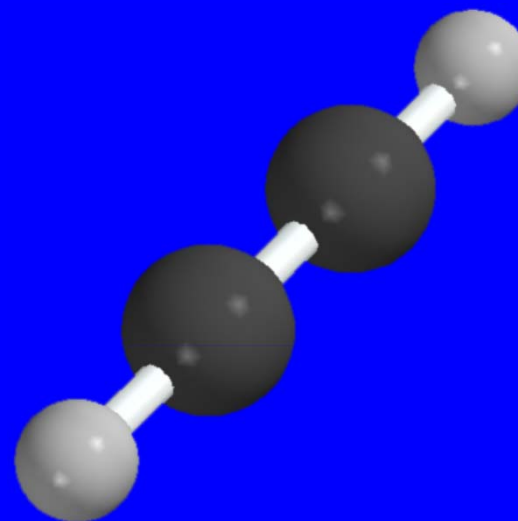


linear

bond angles:  $180^\circ$

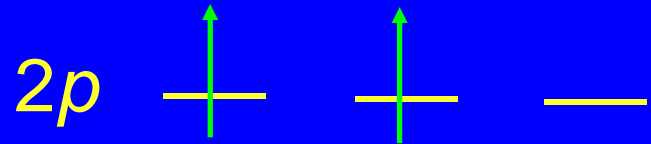
bond distances: C—H = 106 pm

CC = 120 pm

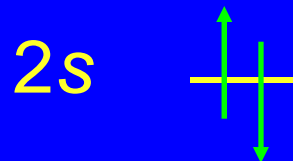




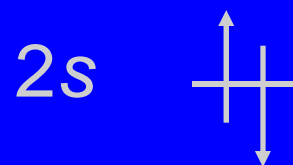
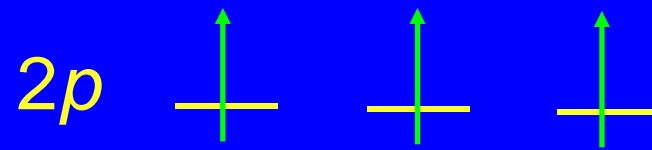
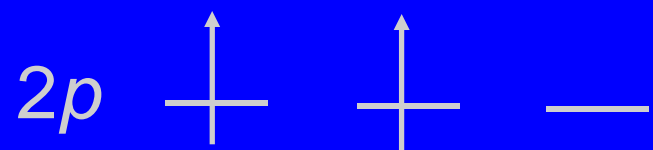
## *sp Orbital Hybridization*



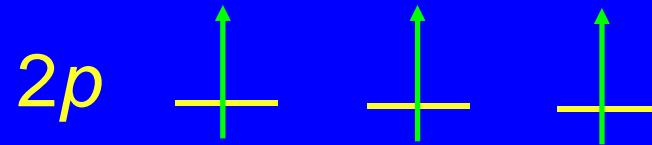
Promote an electron from the 2s  
to the 2p orbital



# sp Orbital Hybridization



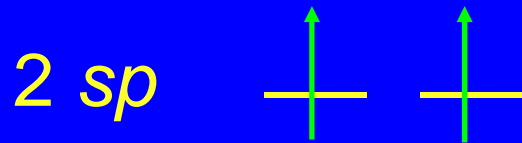
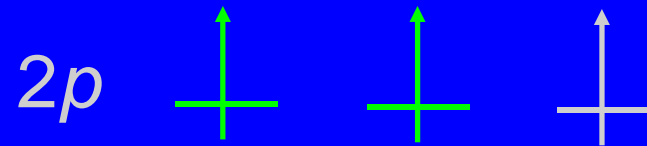
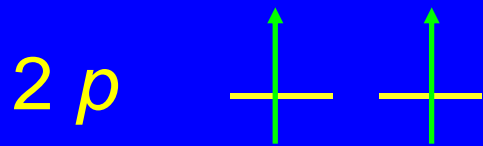
## *sp Orbital Hybridization*



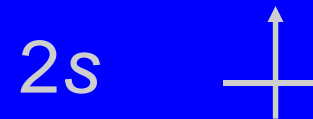
Mix together (hybridize) the 2s orbital and one of the three 2p orbitals



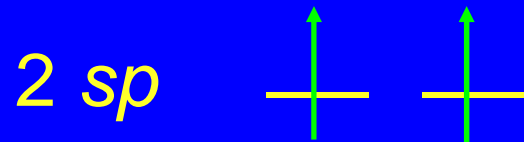
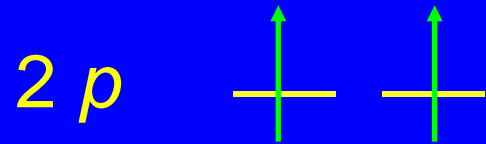
## sp Orbital Hybridization



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

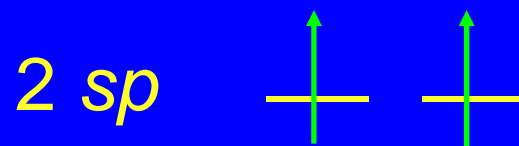
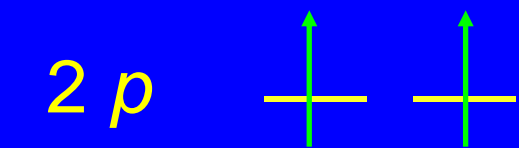


## *sp Orbital Hybridization*

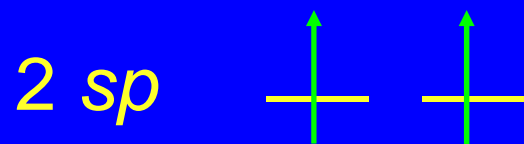
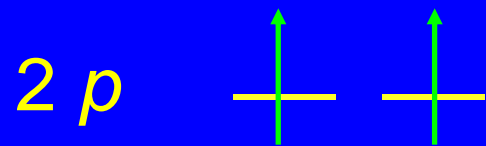


1 of the 2  $sp$  orbitals  
is involved in a  $\sigma$  bond  
to hydrogen; the other  
is involved in a  $\sigma$  bond  
to carbon

# *sp Orbital Hybridization*

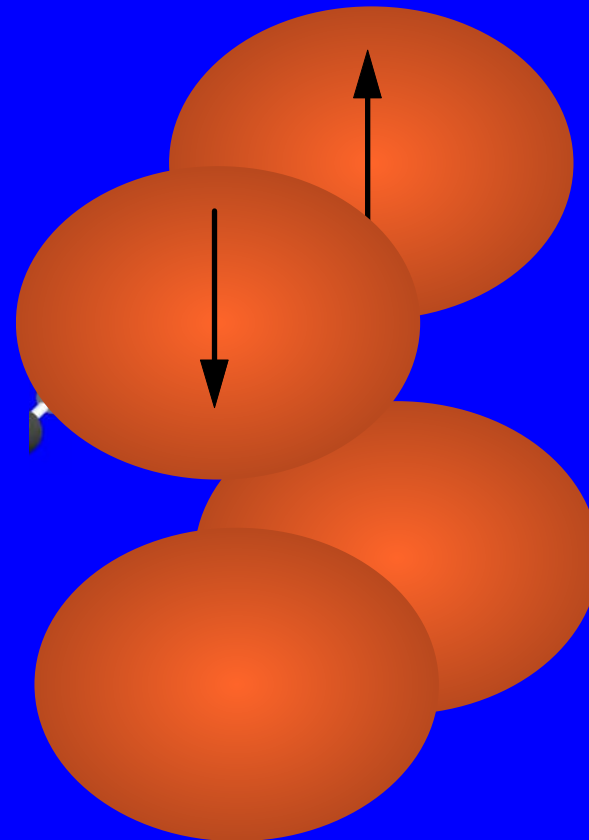
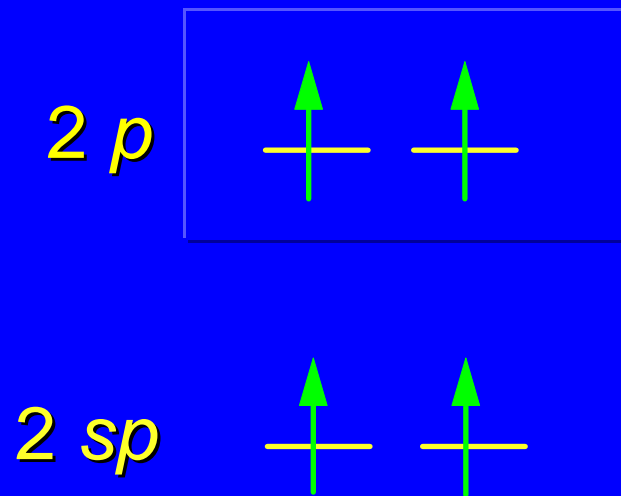


## $\pi$ Bonding in Acetylene



the unhybridized  $p$  orbitals of carbon are involved in separate  $\pi$  bonds to the other carbon

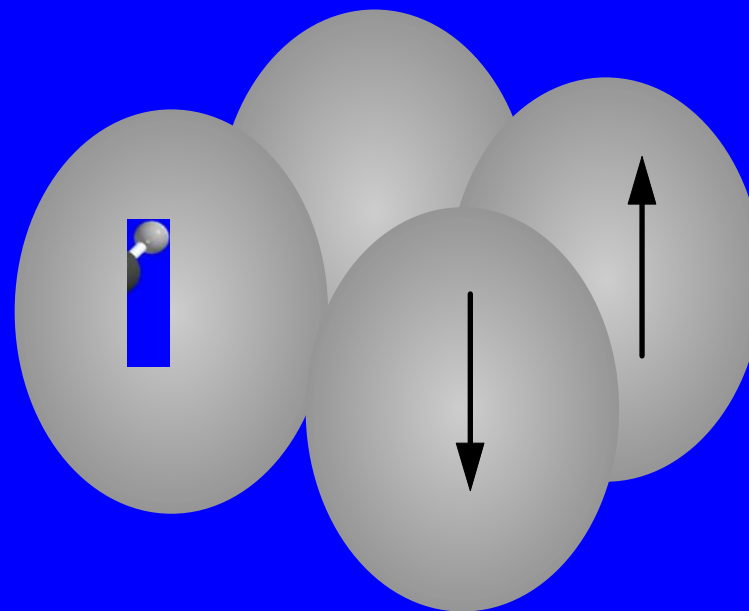
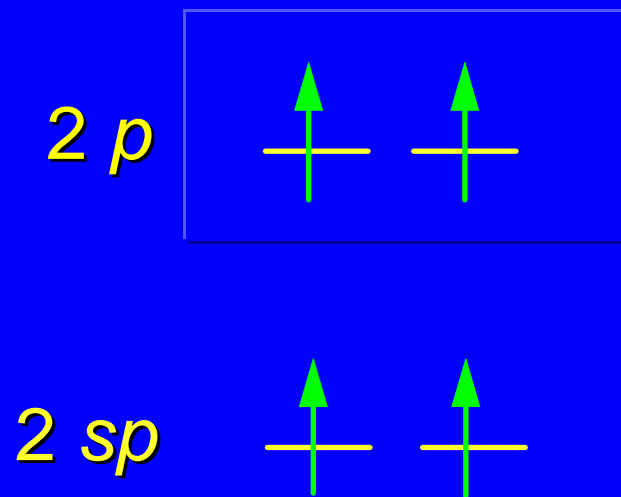
## $\pi$ Bonding in Acetylene



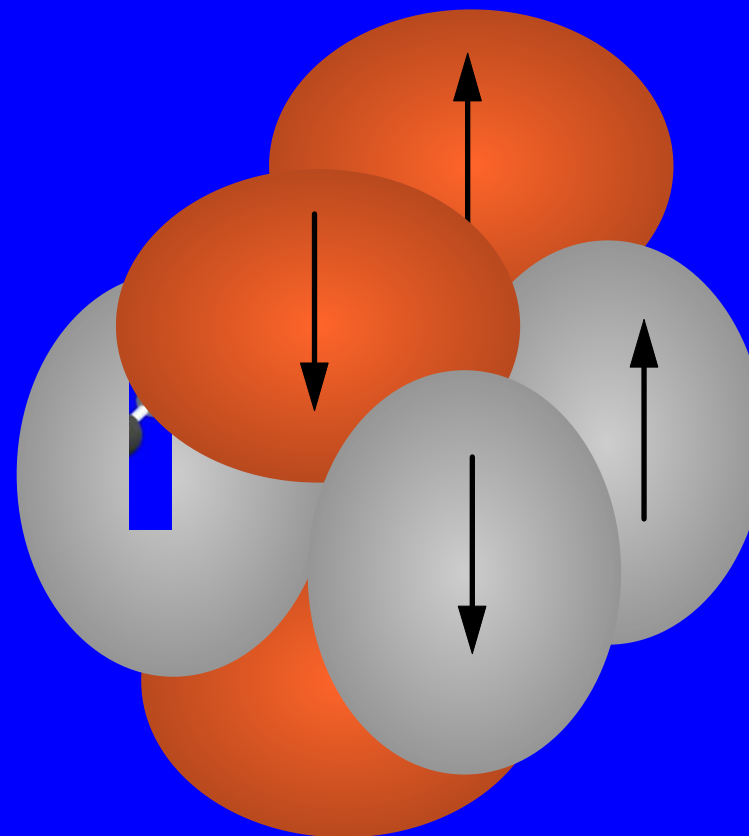
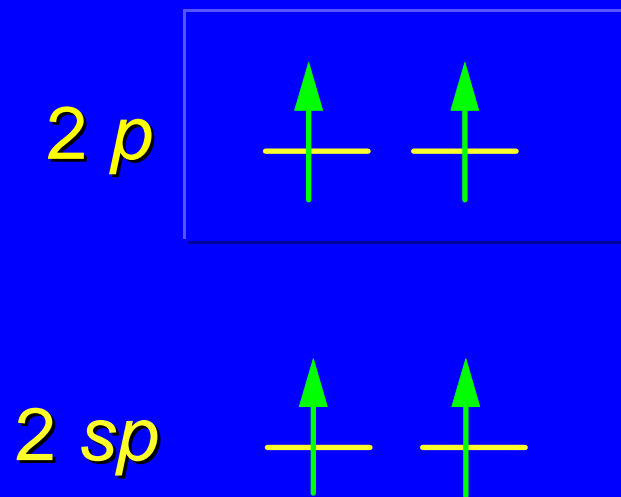
one  $\pi$  bond involves one of the  $p$  orbitals on each carbon  
there is a second  $\pi$  bond perpendicular to this one



# $\pi$ Bonding in Acetylene



# $\pi$ Bonding in Acetylene



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