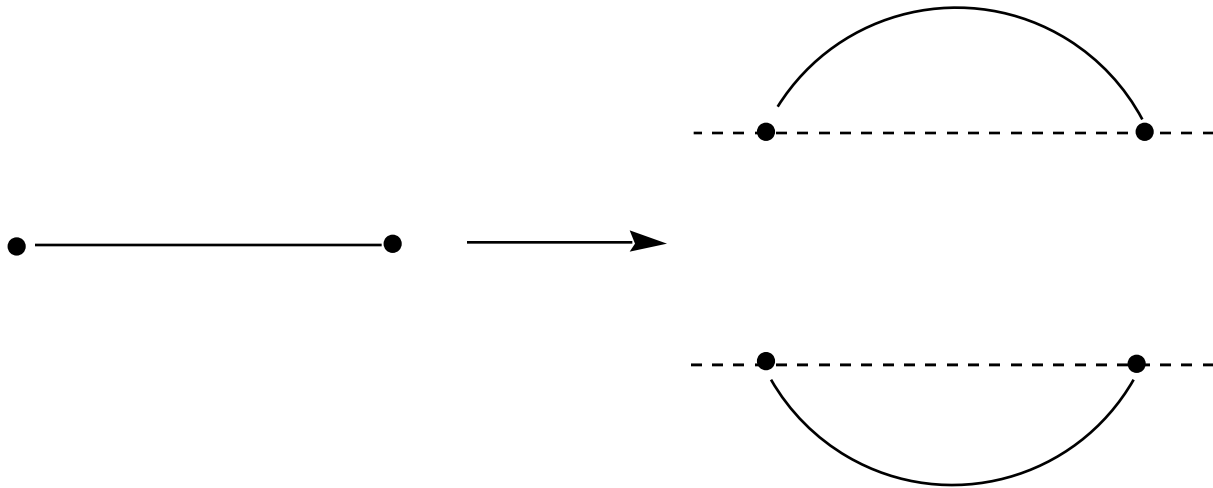


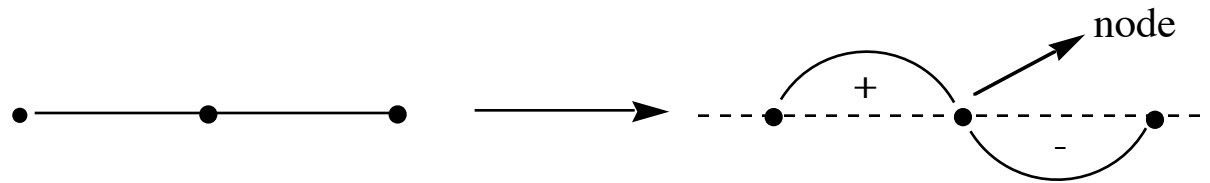
Bonding

Conceptually easier to view bonding if one considers electrons as waves

consider a 2-D standing wave



If we constrain another point of the string we obtain the first harmonic



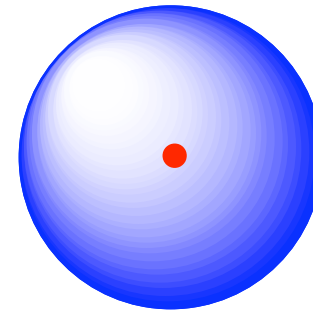
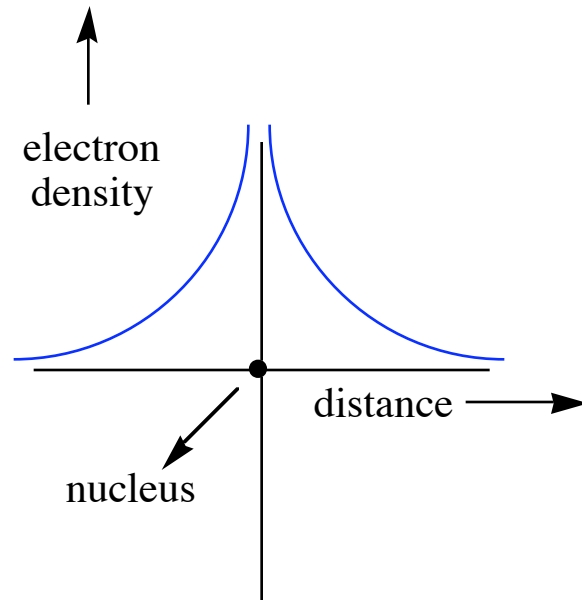
the sign is arbitrary

important point is the change in sign (called a node)

Wave Function of s Orbital

in 2-D

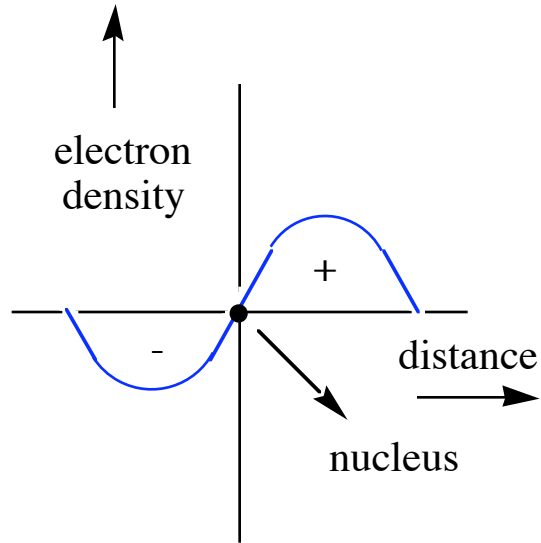
in 3-D



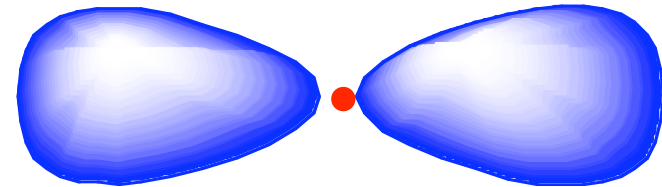
no node: same sign throughout sphere
electron density diminishes further from nucleus

Wave Function of p Orbital

in 2-D



in 3-D

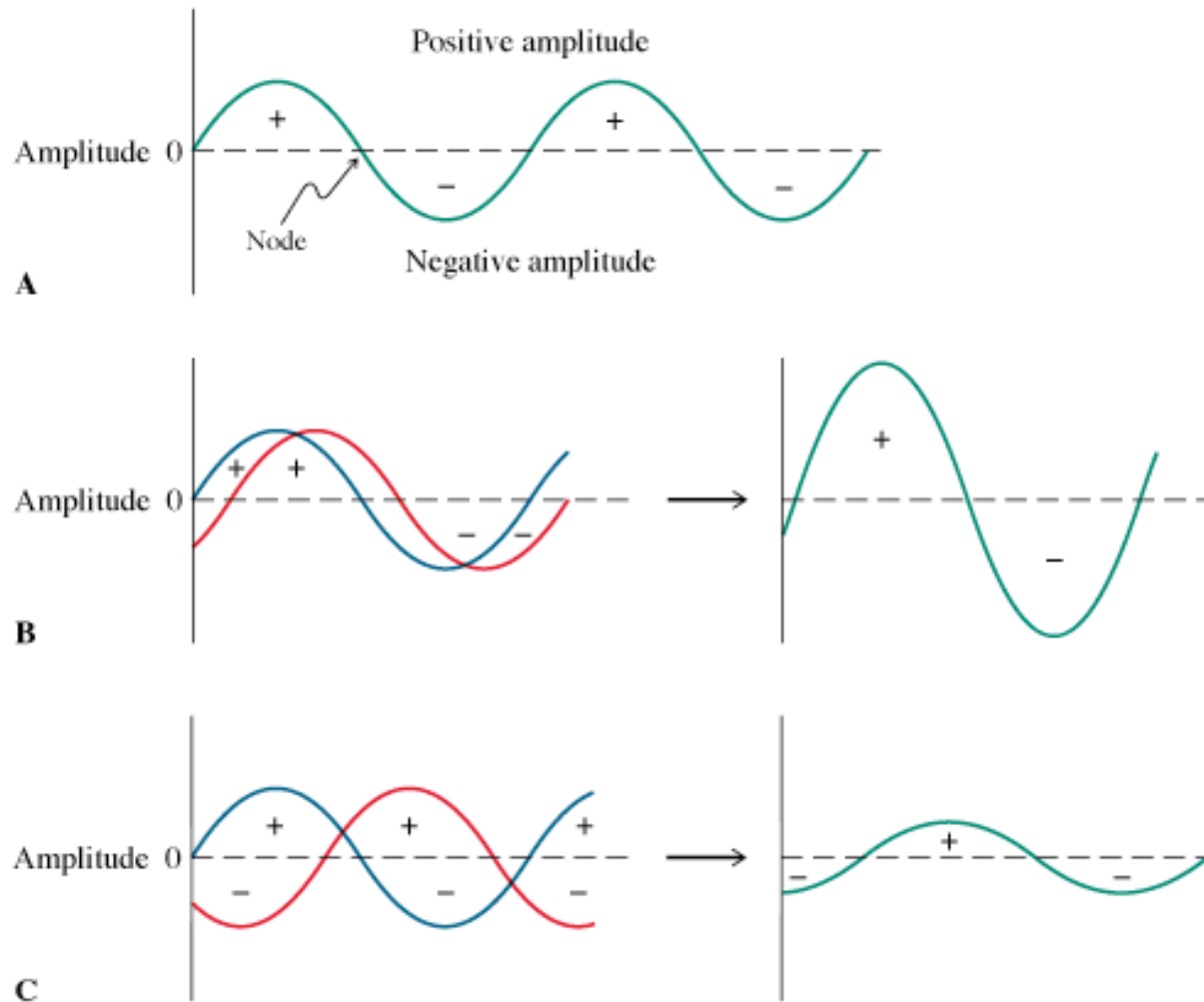


Important Points:

density is zero at nucleus

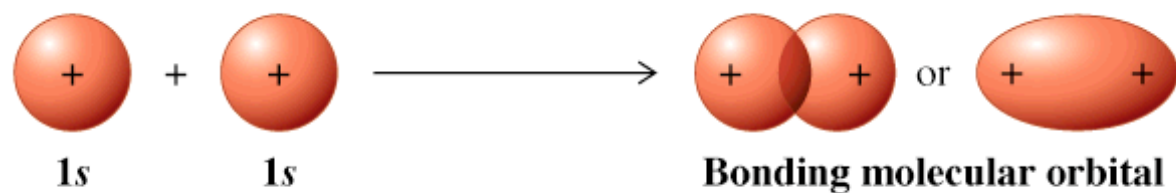
the lobes on opposite sides of the nucleus are out of phase

Combination of Two Waves

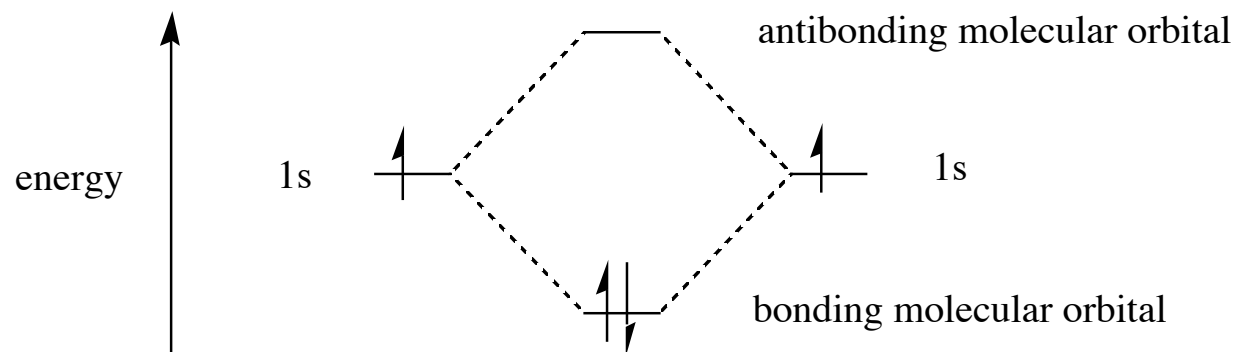


In a bond the wave functions are added

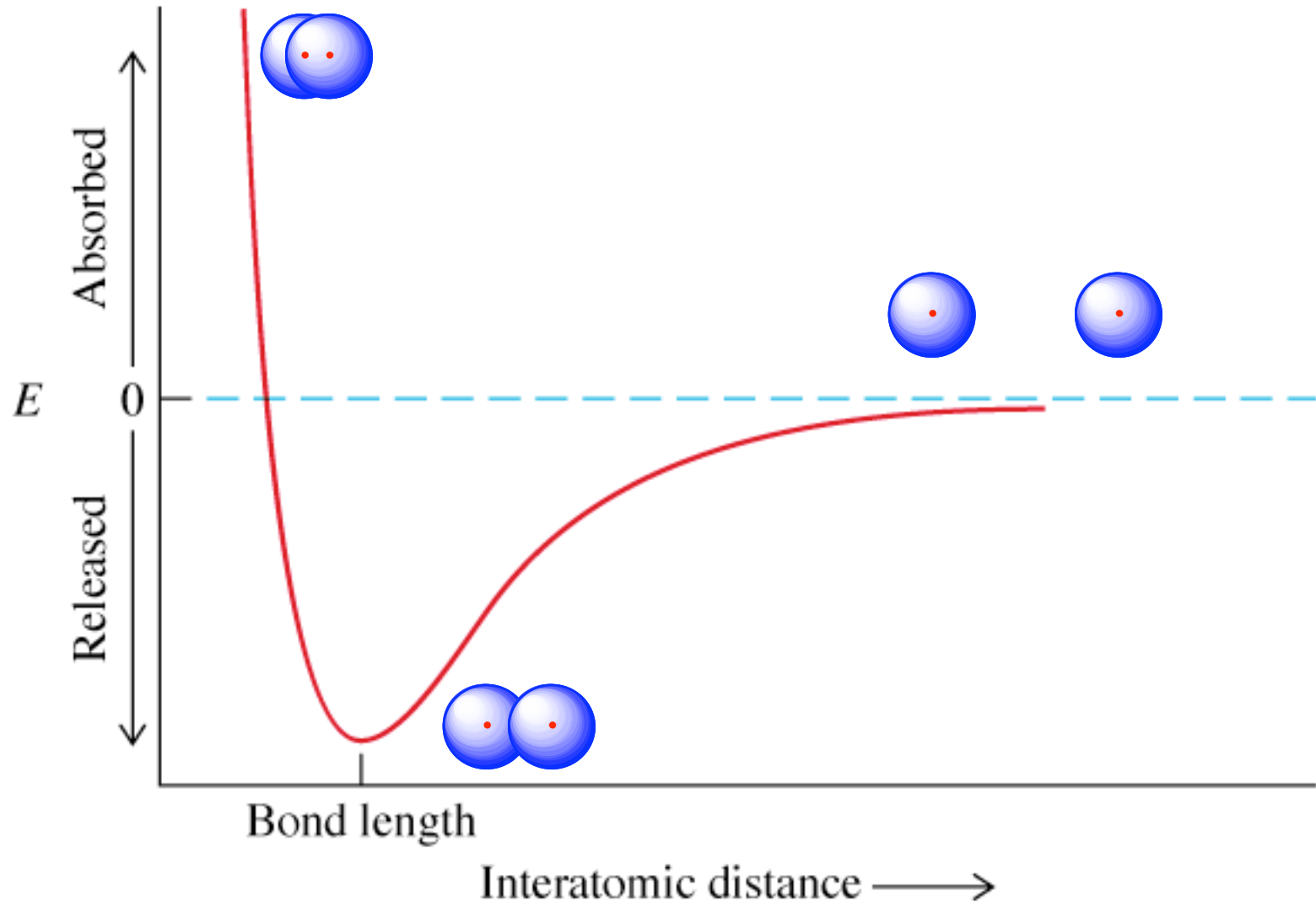
Combination of Atomic Orbitals



Forms Molecular Orbitals



Energy Gain in a Covalent Bond



BOND FORMATION

Bonds are formed by a combination of orbitals

orbitals - location of electrons (on time average)

described by the wave function

phase - describes the sign of an orbital

when two atomic orbitals of like phase overlap in space they can form a bonding region

where the electrons can reside

this bond lowers the energy of the structure by shielding the nucleus of the two atoms

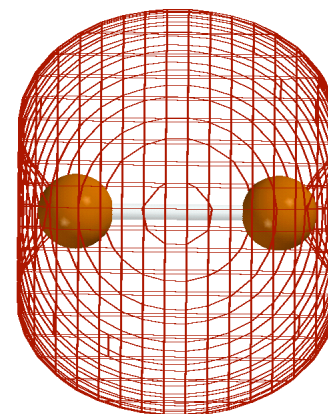
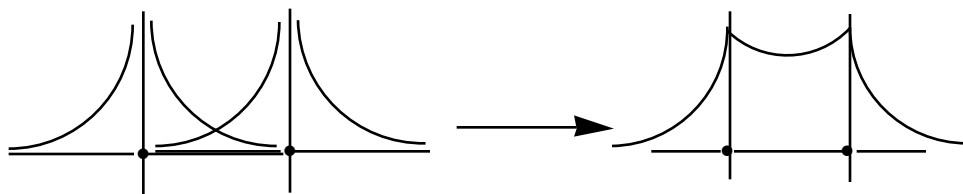
always get same number of molecular orbitals as atomic orbitals used

Organic compounds are described in terms of two types of bonds

(σ sigma and π pi bonds)

σ BONDS

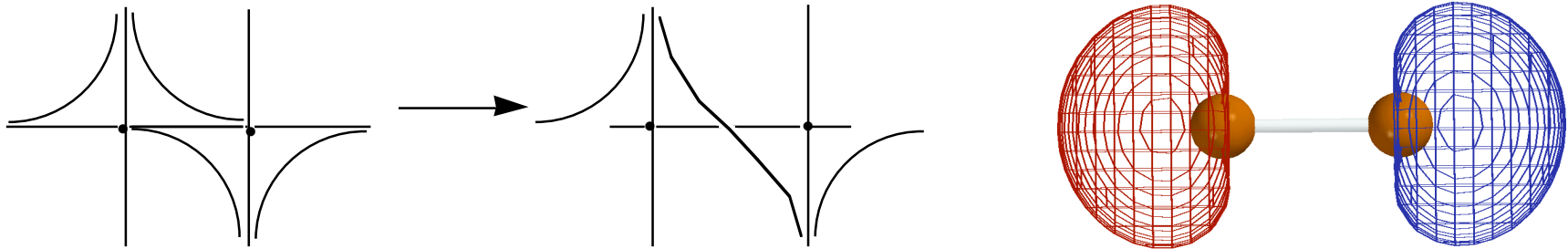
Bonding electron density is symmetric along the internuclear axis



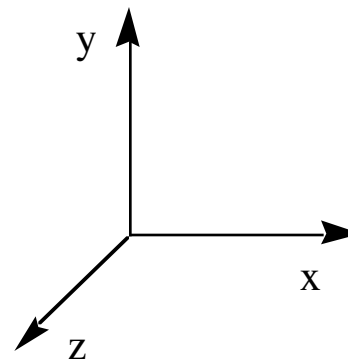
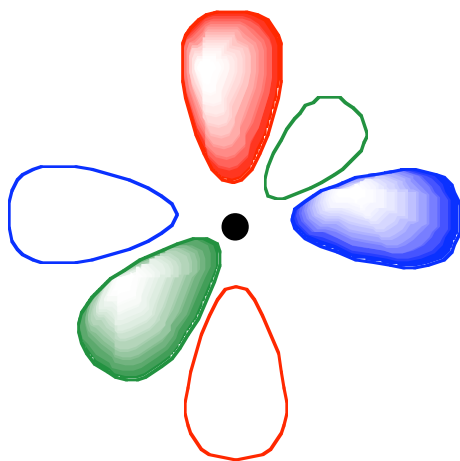
Since we combined two orbitals we need to obtain two molecular orbitals

we obtain one bonding and one antibonding

antibonding is obtained by subtracting the two wave functions



Remember that there are 3 p orbitals

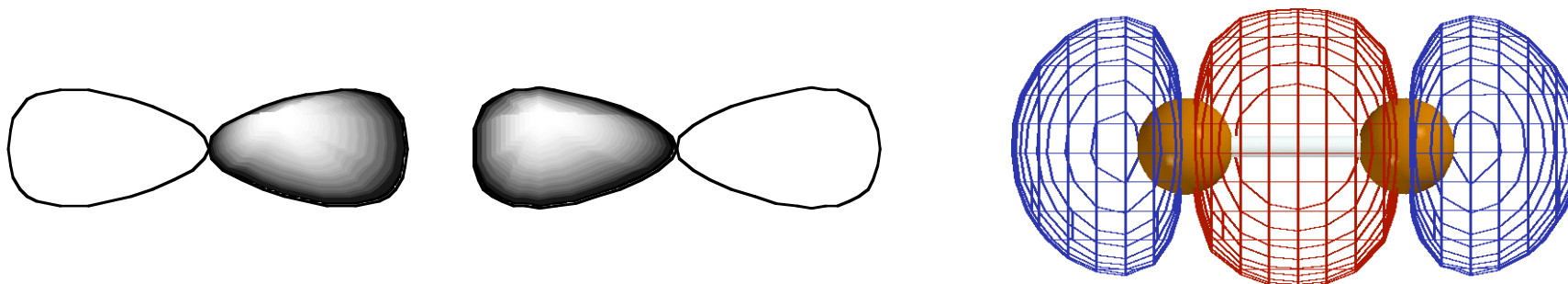


- each one perpendicular to the other two

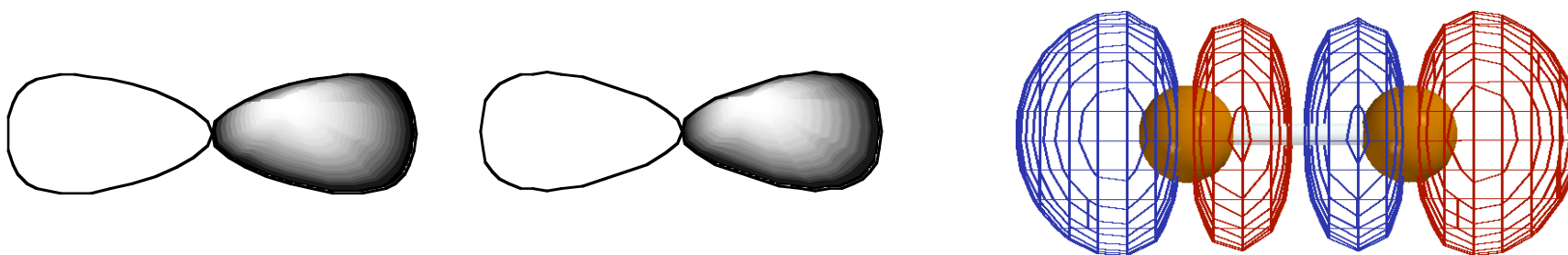
this geometry allows the p orbital to form a different type of bond

P Orbitals Can Also Form σ Bonds

Likewise need to add and subtract two p orbitals to obtain the molecular orbitals



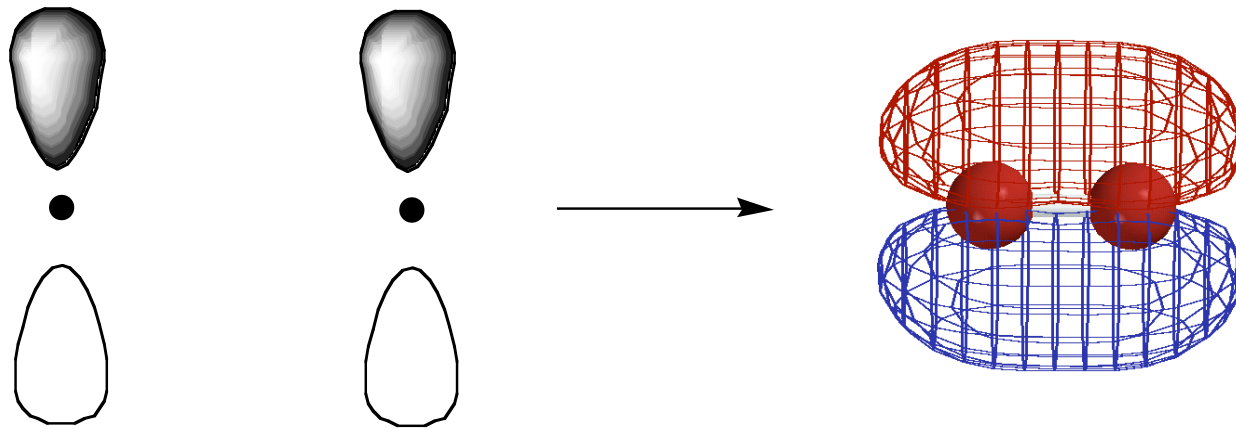
Bonding Molecular Orbital



Antibonding Molecular Orbital

Only Consider the $2p_y$ Orbital

if two of these orbitals are brought together a different type of bond can form



π bond

internuclear axis has a nodal plane

s orbitals can only form σ bonds

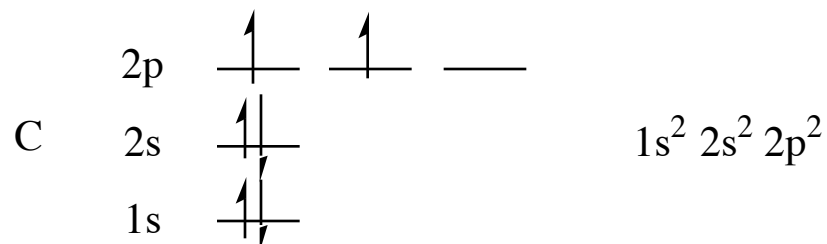
p orbitals can form σ or π bonds

Hybrid Orbitals

If we only used s and p orbitals to form bonds then the bond angles would always be 90°

Also could not fill atoms' valence shell with covalent bonds

consider carbon



In a covalent bond electrons are shared between two atoms
(each atom donates one to the sharing)

with carbon there are only two unpaired valence electrons
therefore two covalent bonds are possible

An atom can combine its atomic orbitals to form hybridized orbitals

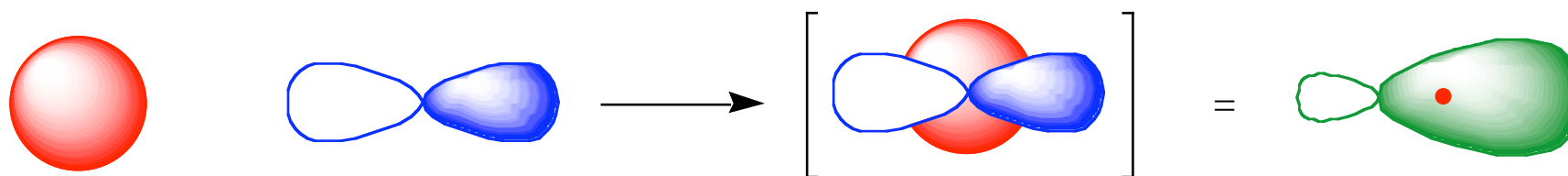
same rules apply as for combining to form molecular orbitals

- 1) get same number of hybridized orbitals as starting orbitals
- 2) shape of hybridized orbitals is obtained by mathematical addition of the wave functions for the atomic orbitals

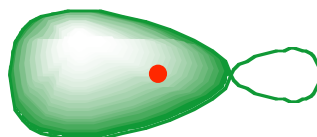
the name (designation) of hybridized orbitals merely refers to the number and type of atomic orbitals used in formation

sp Orbital

combine one s orbital with one p orbital

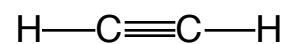


if the orbitals are subtracted then an identical hybridized orbital is obtained
directed 180° from the first



Realize that if one s orbital and one p orbital are hybridized two p orbitals remain

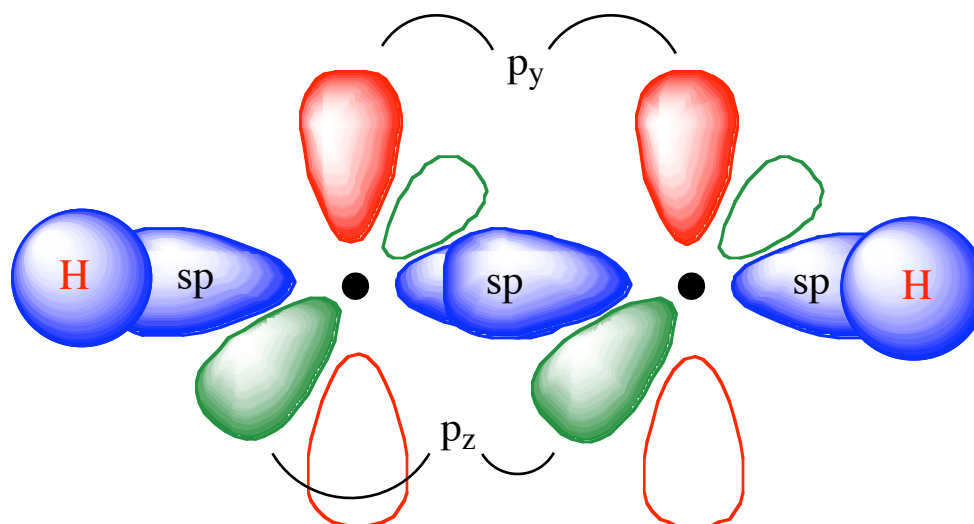
consider acetylene:



- when looking at a Lewis dot multiple bond structure only one σ bond can be between two atoms

- therefore the additional bonds are always π bonds

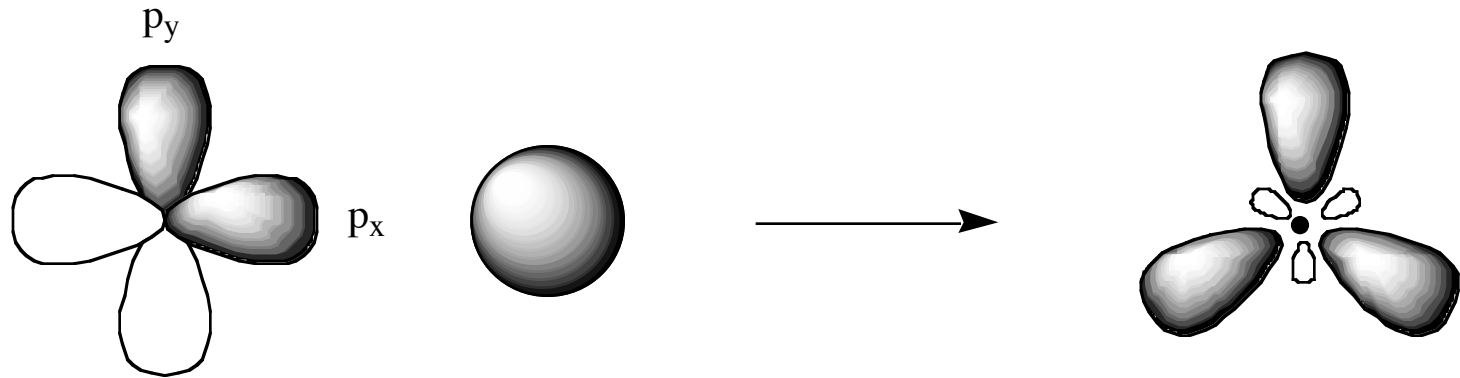
Bonding View of Acetylene



the two hybridized sp orbitals form σ bonds with the other carbon and a hydrogen
the remaining p orbitals form two additional π bonds

sp^2 Hybridization

- can also hybridize by combining two p orbitals and one s orbital

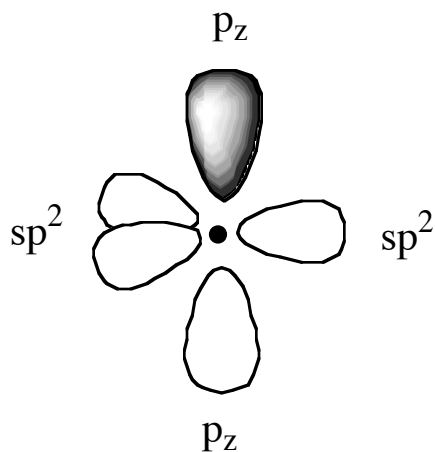


look in the x-y plane
 p_z is coming in and out of the plane

three sp^2 orbitals

all three sp^2 orbitals are in the same plane
(120° apart from one another)

the remaining p orbital is perpendicular to this plane

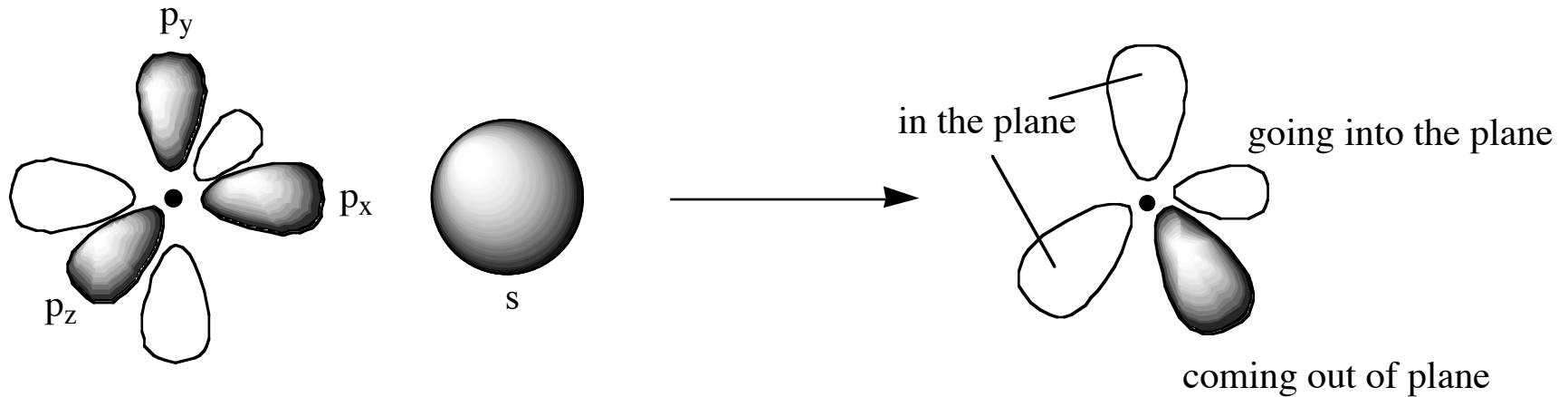


the hybridized sp^2 orbitals can form σ bonds

the p_z orbital can form a π bond

sp^3 Hybridization

To form four equivalent bonds carbon can hybridize all of its valence shells
(three p and one s to form four sp^3)



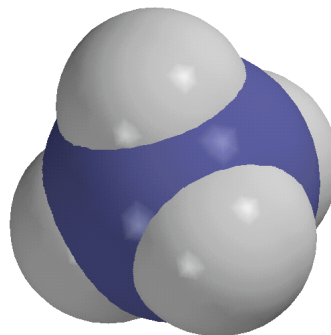
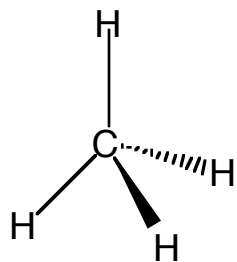
the four sp^3 hybridized orbitals have a bond angle of 109.5°

How to View 3-Dimensional Objects

organic chemists use a wedge and dash line system to designate stereochemistry

wedge line - object is pointing out of the plane

dash line - object is pointing into the plane



In Summary:

s orbitals can only form σ bonds

p orbitals can form either σ or π bonds

hybridized orbitals form σ bonds

multiple bonds are formed with one σ bond and additional π bonds (from p orbitals)

lone pair of electrons often go into hybridized orbitals

(unless they are involved in resonance!)

Why do atomic orbitals hybridize?

allows some atoms to form more covalent bonds (energetic basis)

allows atoms to form bonds at different angles

Molecular geometry is therefore dependent upon the type of hybridization undertaken

How to Determine Molecular Structure

- determine number of σ bonds from an atom
- determine number of lone pair of electrons on an atom
(only count lone pairs localized on atom,
lone pairs in resonance must go into an atomic p orbital)
- the addition of the above two numbers equals the number of
hybridized orbitals required
- remaining atomic orbitals are used to form multiple bonds