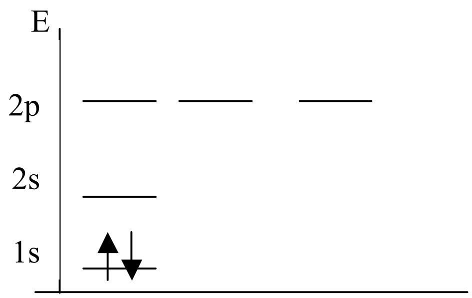
Ionic Bonding

Lithium fluoride is an example of ionic bonding in which positive and negative species are bonded to each other. Li could lose $1e^-$ from 2s orbital to become isoelectronic to He (as Li^+) and F could gain $1e^-$ to become isoelectronic to Ne (as F^-).

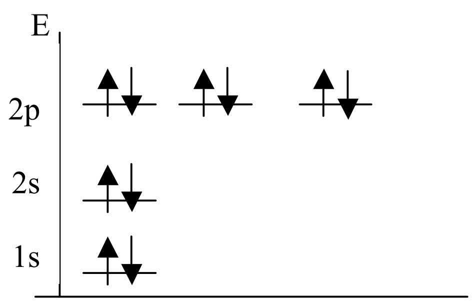
$$Li^o + F^o \rightarrow \underset{\text{Loss of } 1e^-}{Li^+} + \underset{\text{Gain of } 1e^-}{F^-}$$

Isoelectronic = Same electron configuration

Li^+ (cation) Isoelectronic with He

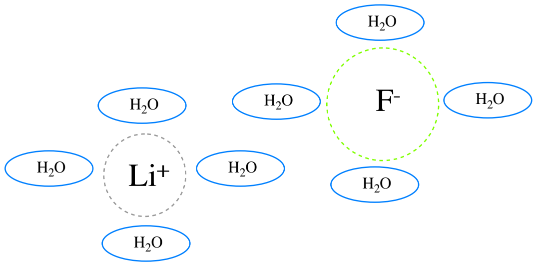


F^- (anion) Isoelectronic with Ne

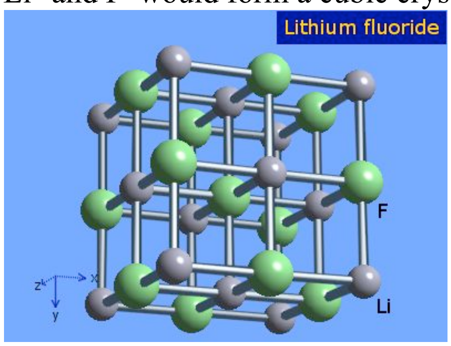


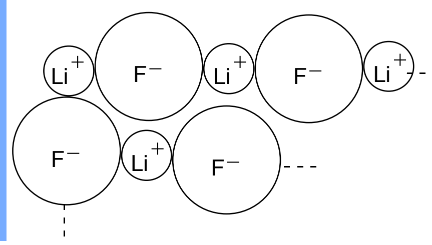
In space, Li^+ and F^- would be attracted to each other

In solution, Li^+ and F^- might be separated due to solvation (e.g. water would surround)



In a solid, Li^+ and F^- would form a cubic crystalline solid





Electronegativity

- Desire of atoms for electrons
- Electronegativity increases from left to right across the period in the periodic table (atoms get stronger attraction as the nuclear charge increases
- Electronegativity increases from bottom to top in the group (Distance between nucleus and valence shell decreases)

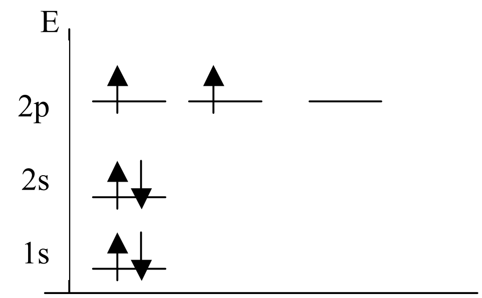
Covalent Bonding

- Sharing of electrons between the atoms
- More common in organic chemistry

Electronic configuration of carbon (C):

- Atomic number = 6
- Atomic weight = 12

Carbon (C)



- Carbon needs to gain or lose $4e^-$ to get an inert gas configuration, but this would result in unfavourable charge buildup:

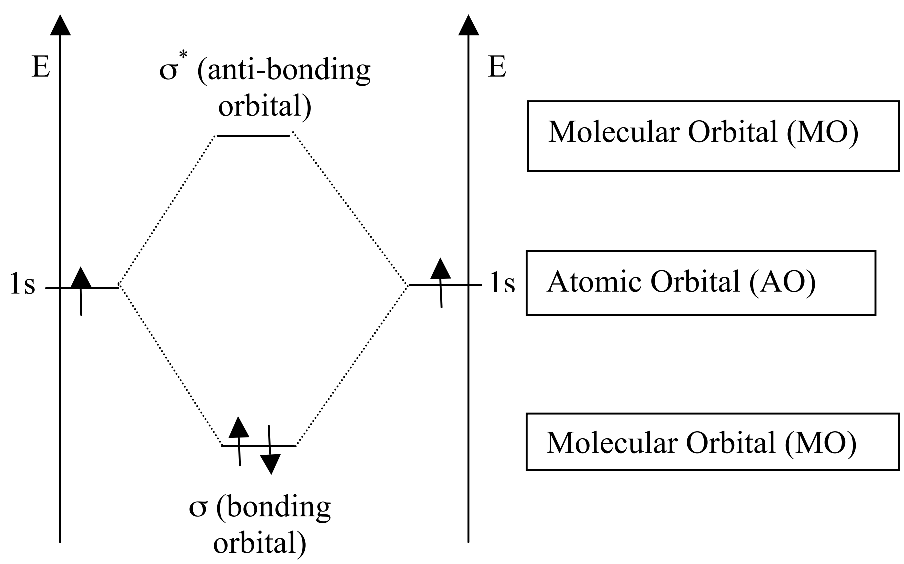
- C^{4+} is isoelectronic with He

- C^{4-} is isoelectronic with Ne

- So, carbon makes up to 4 bonds to <u>share</u> $4e^-$ (covalent bonding)

<u>Energetics of Forming Bonds</u>

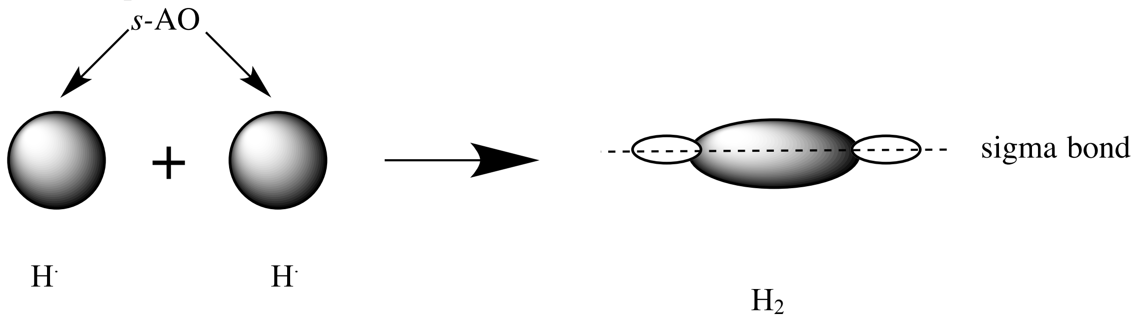
e.g. H_2



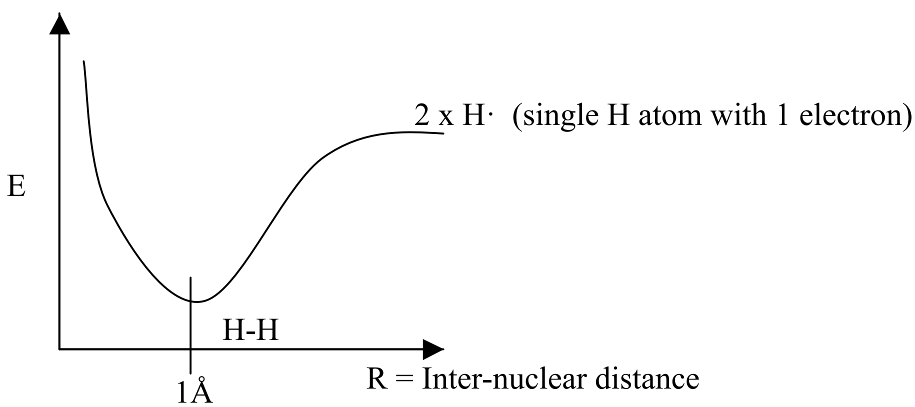
As two hydrogen atoms come together, molecular hydrogen (H_2) is formed

$H^{\cdot} \longrightarrow H{:}H \longleftarrow {}^{\cdot}H$

Orbital representation:



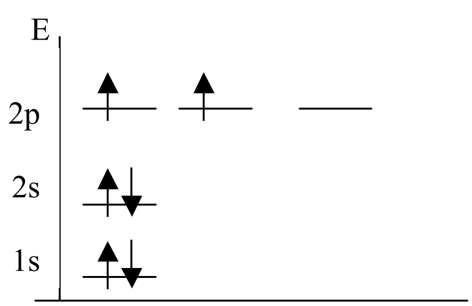
Energy diagram of two hydrogen atoms interacting to form a bond:



1Å is the average H-H bond distance

Electronic configuration of carbon (C):
- Atomic number = 6
- Atomic weight = 12

<u>Carbon (C)</u>



- Carbon needs to gain or lose $4e^-$ to get an inert gas configuration, but this would result in unfavourable charge buildup:

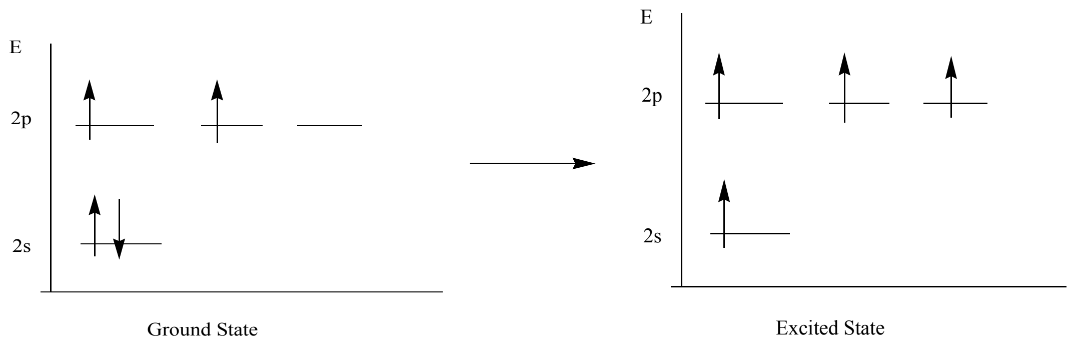
- C^{4+} is isoelectronic with He

- C^{4-} is isoelectronic with Ne

- So, carbon makes up to 4 bonds to <u>share</u> $4e^-$ (covalent bonding)

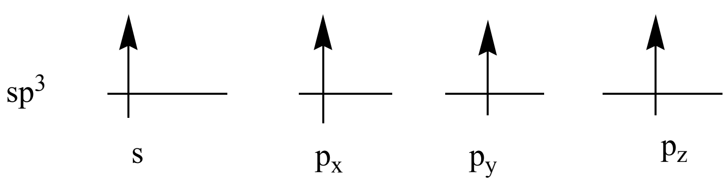
Hybridization:

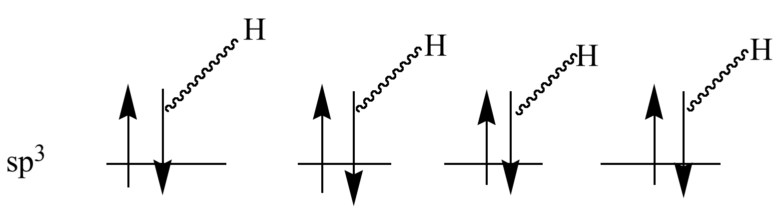
- Mixing of atomic orbitals (with the wrong geometry for bonding) to form hybrid orbitals with the correct geometry for bonding

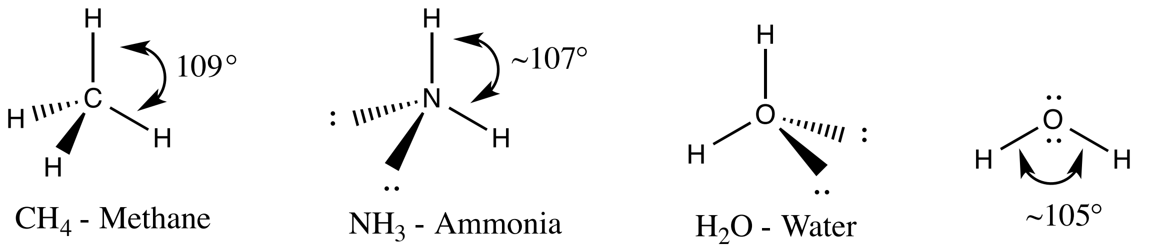


sp^3 Hybridization

- Single bonds
- Tetrahedral geometry
- Angle between two H atoms in methane: 109°, close to that with other elements
- Often free rotation around single bonds
- Overlap of atomic orbitals with s component gives sigma molecular orbital (bond)







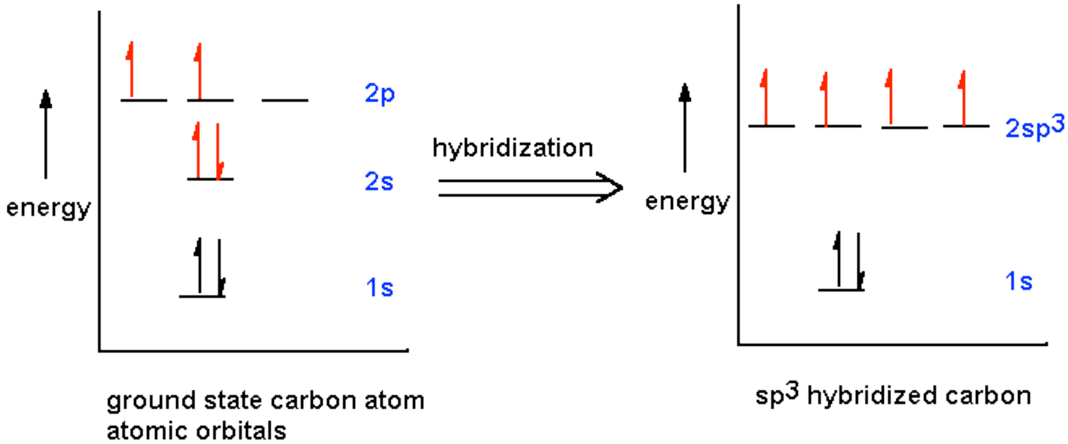
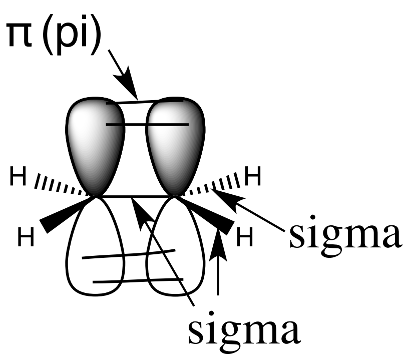
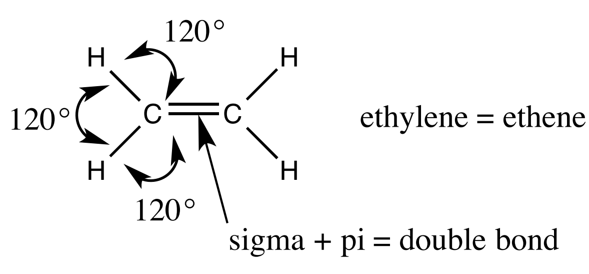


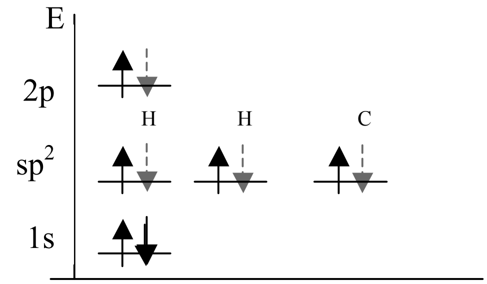
Figure: Hybridization of 2nd shell *s* (one) orbitals and *p* (three) orbitals of carbon

sp² Hybridization

- Double bonds
- Planar geometry
- Angle between two atoms: 120°
- No free rotation around double bonds
- Overlap of atomic orbitals with s component gives sigma molecular orbital (bond)
- Overlap of p atomic orbitals with s component gives pi molecular orbital (bond)

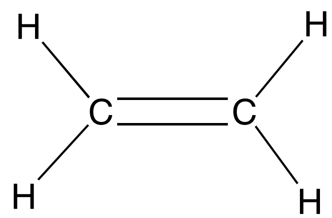






Molecular Orbital

- Linear combination of atomic orbitals
- Combination of atomic orbitals of s- character gives molecular orbital called sigma molecular orbital (σ)
- Combination of atomic orbitals of p-character gives molecular orbital called pi molecular orbital (π)



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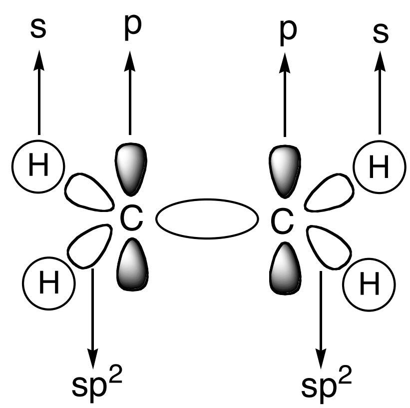
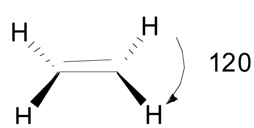
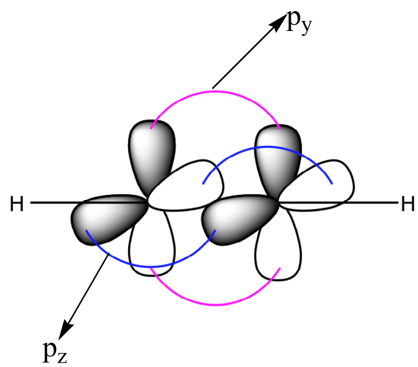




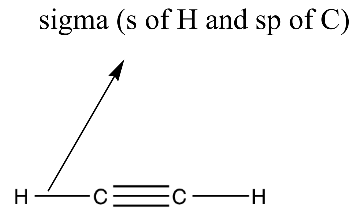
- When atomic orbitals overlap they form molecular orbitals.
- Double bond contains one σ bond and one π bond.
- σ bond has free rotation.
- π bond fixes geometry, does not allow for rotation around the double bond.

sp Hybridization

- Triple bonds
- Linear geometry
- No free rotation around triple bonds



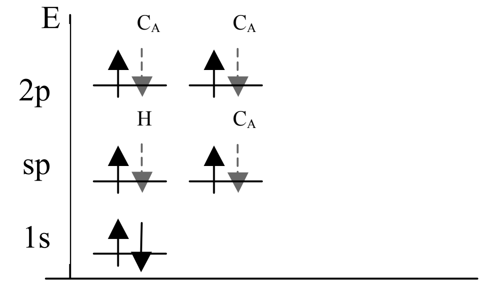
Triple bond:
One sigma bond between the carbons plus two pi bonds formed through p_y and p_z



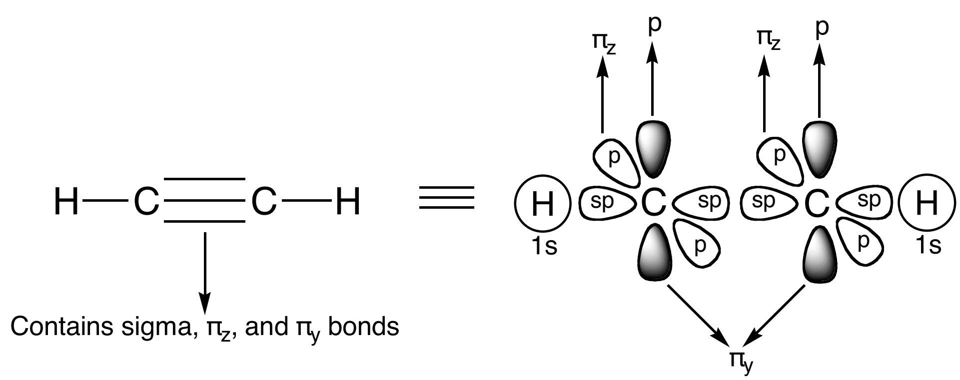
acetylene = ethyne

<u>sp Hybridization</u>

- Triple bonds
- Linear geometry
- No free rotation around triple bonds
- Angle between two atoms: 180^o



e.g.) Acetylene/Ethyne



<u>Representation of Molecules</u>

- Show only electrons in outer (valence) shell
- Non-bonding electrons may or may not be shown
- Use element symbols, but carbon can be represented by point of angle or end of line
- Hydrogens and bonds to them from carbon are optional; show others.

- Each line in a structure represents 2 e^-
- Solid wedge ( ): Toward you / out of the page
- Dashed wedge ( ): Away from you / into the page