Grade 12 Chemistry

Structure and Properties of Matter

Class 7

Formal Charge

- Draw the Lewis structure of HCN, you will realize that you can draw two structures
- Formal charges tells you the “best” way the atoms share their electrons, when charges = 0 or as small as possible

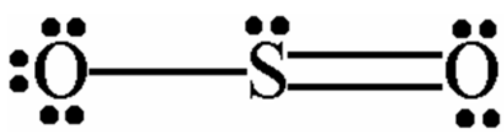
Formal Charge = $V - \frac{1}{2}B - L$

V = # of valence electrons
B = # of bonding electrons
L = # of LP electrons

- Rules for Formal Charges:
  - For molecules, the sum of the charges must add up to zero
  - For cations, the sum of formal charges must equal the positive charge. For anions, the sum of formal charges must equal the negative charge
- Sometimes there is more than one acceptable Lewis structure
  - No formal charges are preferable
  - Small formal charges are better than large formal charges
  - The negative formal charge should be on the more electronegative atom

Checkpoint

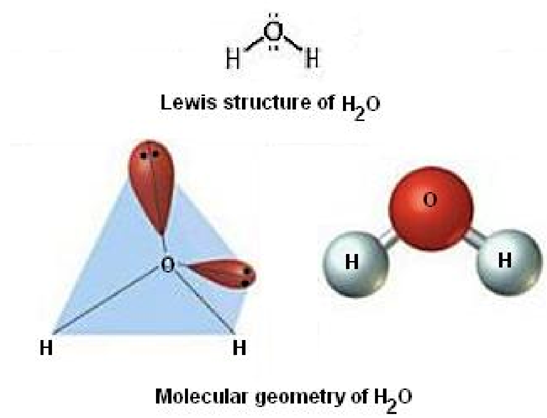
- Calculate the formal charge for SO_2



- From Class 5, check ClON again using Formal Charges

Molecular Geometry

- Allows chemists to visualize the molecule in a 3D representation
- 1857, Gillespie and Nyholm developed a model for predicting the shape of molecules using the VSEPR theory



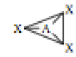
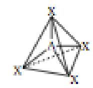
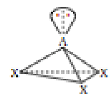
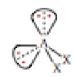
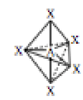
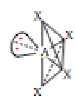
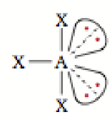
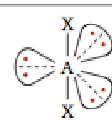
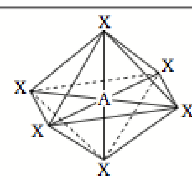
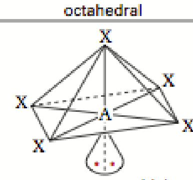
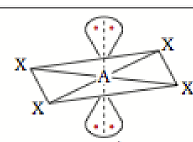
The VSEPR Model

- **V**alence **S**hell **E**lectron-**P**air **R**epulsion Model
- Used to predict shapes of simple molecules
- Rule: Electron pairs, whether bonding or nonbonding, attempt to move as far apart as possible
- Lone Pair (LP) will spread out more than a Bonding Pair (BP); repulsion is greatest in a LP

Decreasing Repulsion:

LP-LP > LP-BP > BP-BP

Table 4.2 Common Molecular Shapes and Their Electron Group Arrangements

Number of electron groups	Geometric arrangement of electron groups	Type of electron pairs	VSEPR notation	Name of Molecular shape	Example
2	linear	2 BP	AX_2	X—A—X linear	BeF_2
3	trigonal planar	3 BP	AX_3	 trigonal planar	BF_3
3	trigonal planar	2 BP, 1 LP	AX_2E	 angular	$SnCl_2$
4	tetrahedral	4 BP	AX_4	 tetrahedral	CF_4
4	tetrahedral	3 BP, 1LP	AX_3E	 trigonal pyramidal	PCl_3
4	tetrahedral	2 BP, 2LP	AX_2E_2	 angular	H_2S
5	trigonal bipyramidal	5 BP	AX_5	 trigonal bipyramidal	$SbCl_5$
5	trigonal bipyramidal	4 BP, 1LP	AX_4E	 seesaw	$TeCl_4$
5	trigonal bipyramidal	3 BP, 2LP	AX_3E_2	 T-shaped	BrF_3
5	trigonal bipyramidal	2 BP, 3LP	AX_2E_3	 linear	XeF_2
6	octahedral	6 BP	AX_6	 octahedral	SF_6
6	octahedral	5 BP, 1LP	AX_5E	 square pyramidal	BrF_5
6	octahedral	4 BP, 2LP	AX_4E_2	 square planar	XeF_4

Predicting Molecular Shape

1. Draw a preliminary Lewis structure of the molecule
2. Count the number of bonding pairs attached to the central atom – all BP (single, double, triple) are counted as one group
3. Count the number of lone pairs on the central atom
4. Use the VSEPR chart to determine the shape

Checkpoint

Predict the molecular shape of:

a) H_3O^+
b) SF_6
c) BrF_5

Bond Order

- Bond Order – Number of bonding pairs of electrons between two atoms

$$\text{Bond Order} = \frac{\text{Number of Bonds}}{\text{Number of Bonding Groups}}$$

- If bond order = 0, molecule cannot form
- Higher bond order indicates more attraction and more stability
- Bond order does not need to be an integer (resonance)

Checkpoint

Determine the Bond Order for:

a) HCN

b) NO_3^-

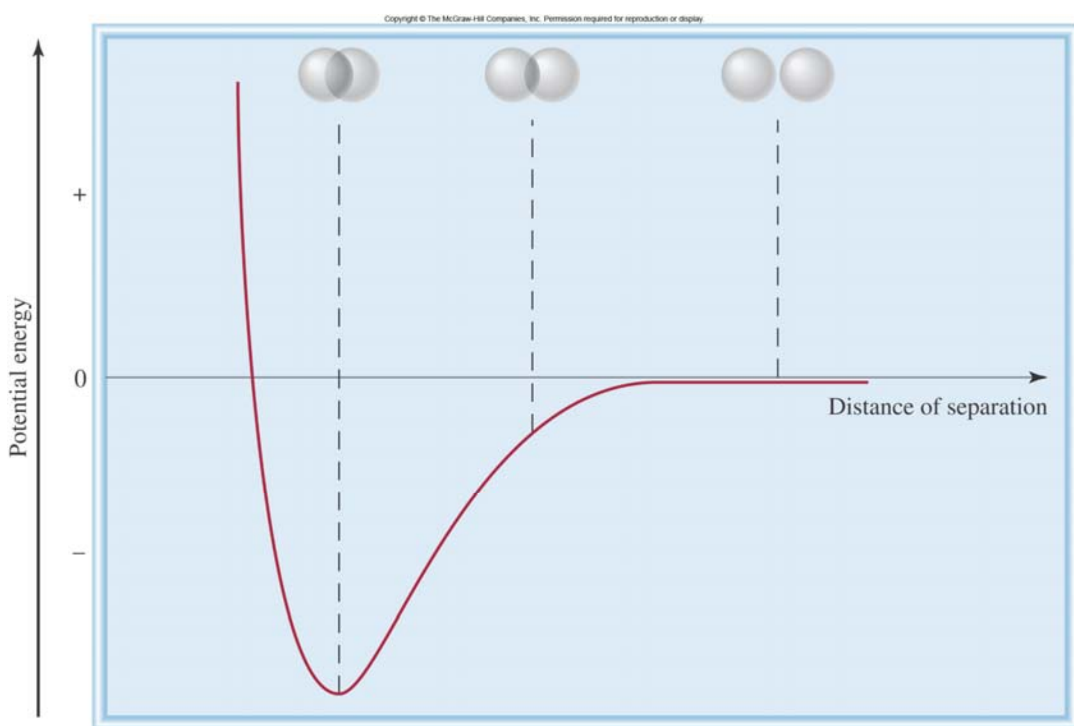
c) O_2

Valence Bond Theory

- Lewis theory does not clearly explain why chemical bonds exist; does not explain differences in bond length

  H-H = 74pm   F-F = 142pm

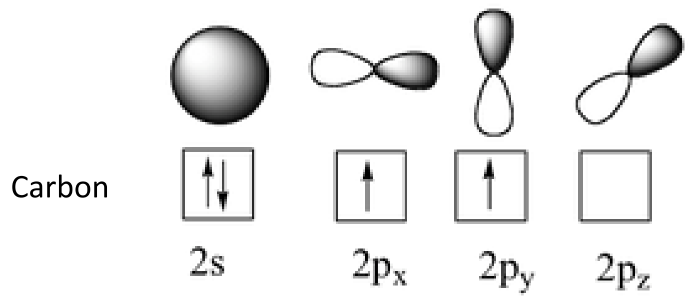
- Valence Bond Theory assumes that the electrons in a molecule occupy atomic orbitals of the individual atoms



Hybridization of Atomic Orbitals

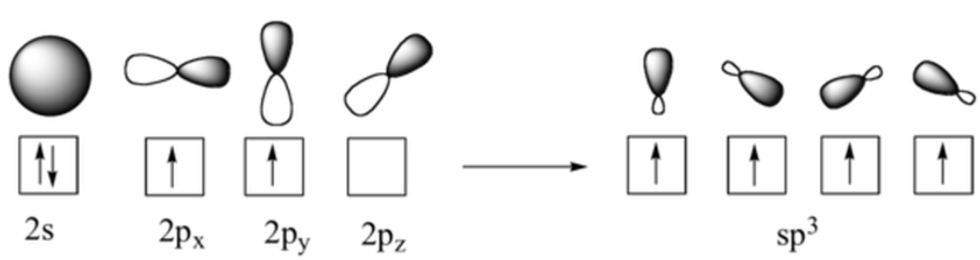
sp^3 Hybridization

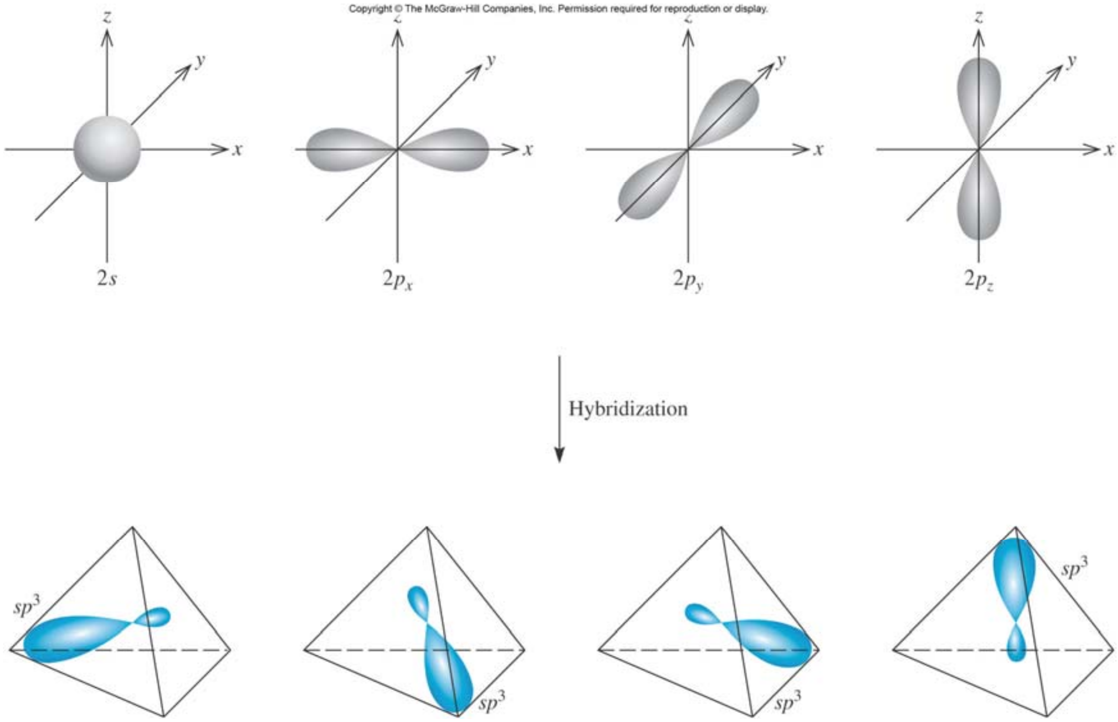
- Consider the CH_4 molecule:

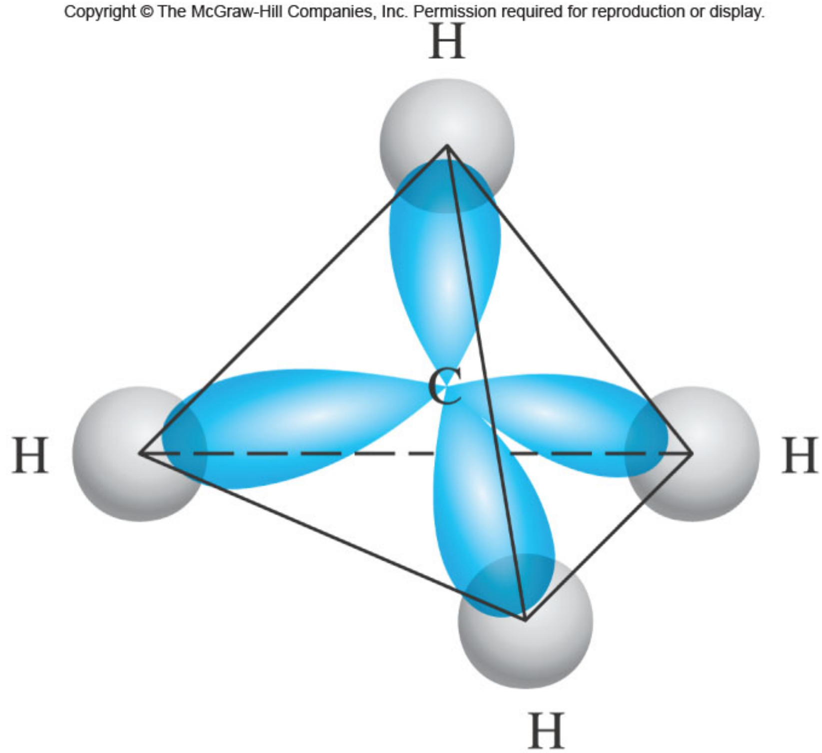


- This carbon can only form two bonds with hydrogen since there are only 2 electrons

- To account for the four C-H bonds, we must excite an electron from the 2s orbital to the 2p orbital
  - However this will result in 3 bonds with hydrogen that are the same lengths and 1 bond with hydrogen that is different
- All bonds are 109.5° so hybridization must have occurred between the *s* and *p*-orbitals



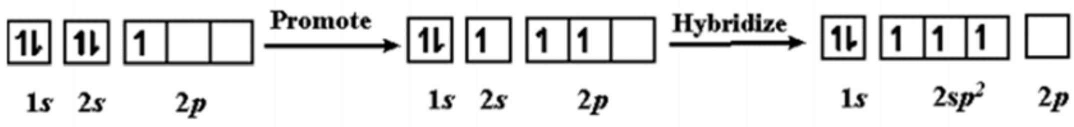

z
y
x
2s
2px
2py
2pz
Hybridization
sp3
sp3
sp3
sp3


H
C
H
H
H

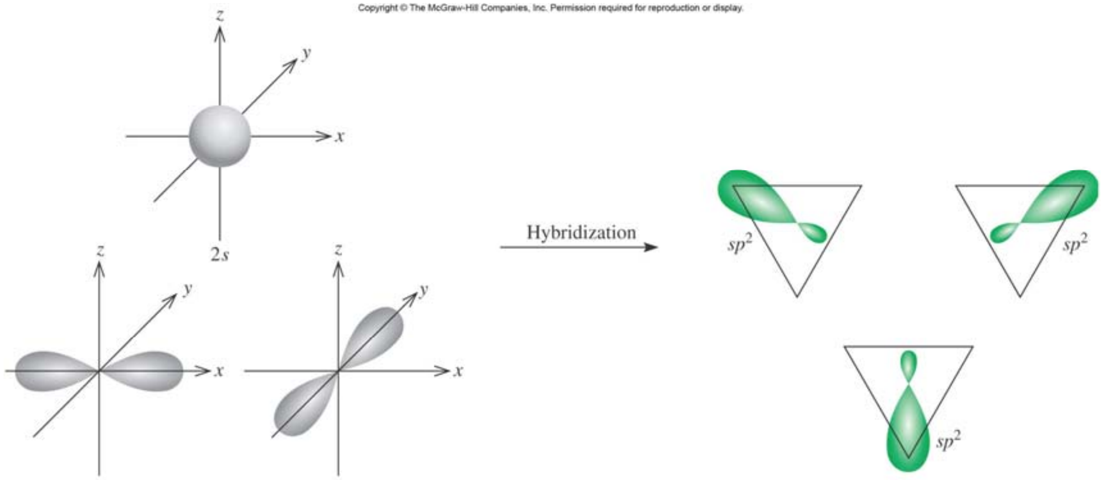
sp^2 Hybridization

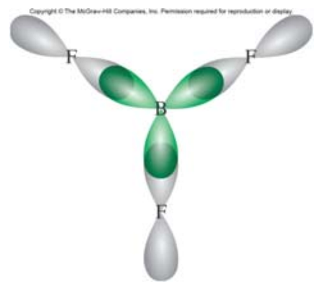
- Consider BF_3: hybridized 1s and 2p orbitals

Boron



- The sp^2 orbitals lie in the same plane and the angle between them is 120°

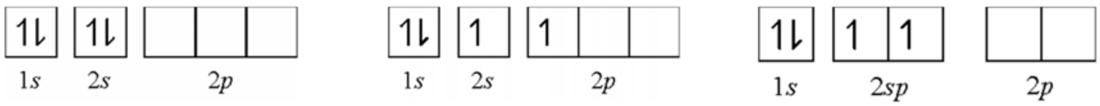




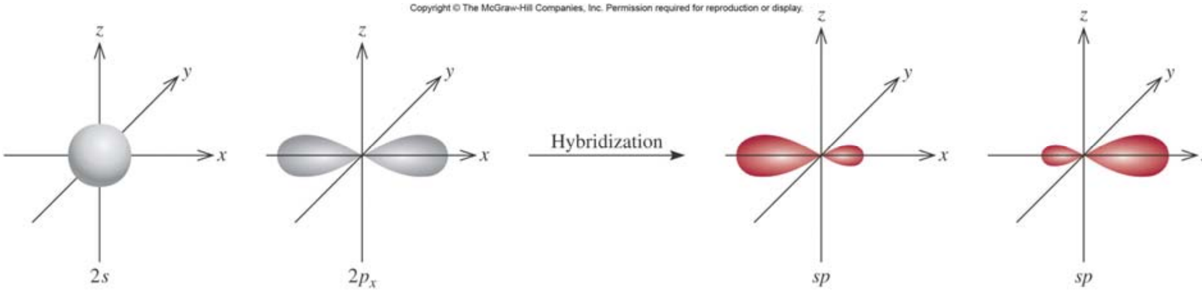
sp Hybridization

- Consider $BeCl_2$: hybridization of 1s and 1p

Beryllium



- The two hybrid orbitals lie on the same plane so the angle is 180°
- The bonds within Be-Cl are formed between Be sp hybrid orbital and Cl 3p orbital



How to tell if an atom is sp^3, sp^2 or sp

- Draw the Lewis dot structure of the molecule
- Count the number of bonding sites
  - Single bond = 1 site
  - Double bonds = 1 site
  - Triple bonds = 1 site
- Count the number of lone pairs
- 2 bonding sites = sp
- 3 bonding sites = sp^2
- 4 bonding sites = sp^3

Checkpoint

Determine the hybridization state of the central (underlined) atom in the following molecules:

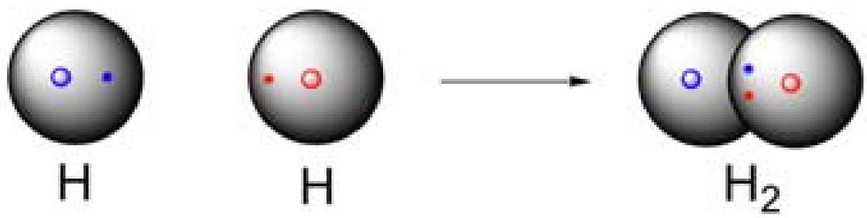
a) $\underline{Be}H_2$

b) $\underline{Al}I_3$

c) $\underline{P}F_3$

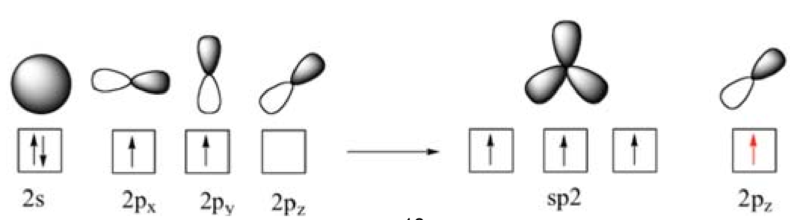
Sigma (σ) Bonds

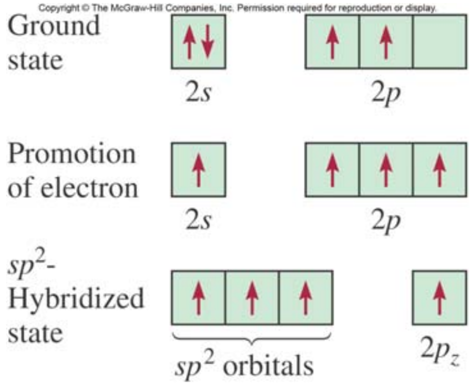
- Sigma Bonds = single bonds; covalent bonds formed by orbitals overlapping end to end with the electron density concentrated between the nuclei of the bonding atoms

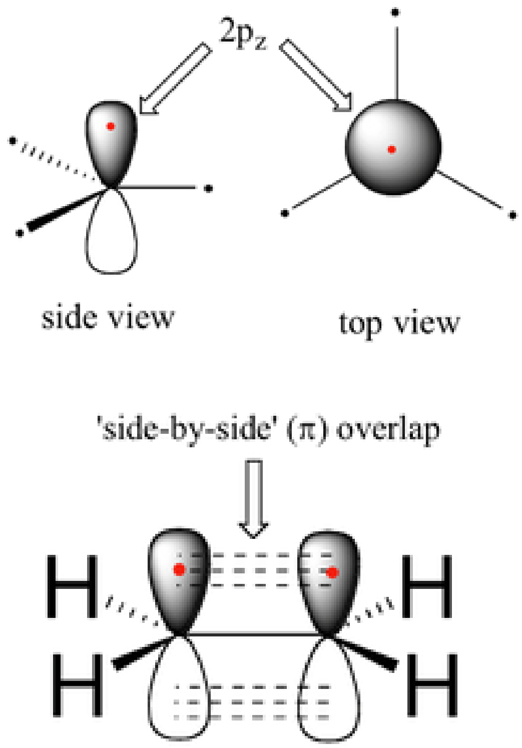


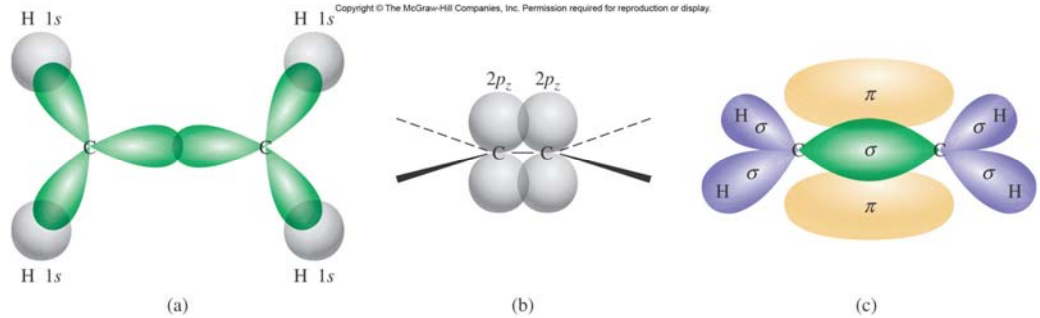
Pi (π) Bonds

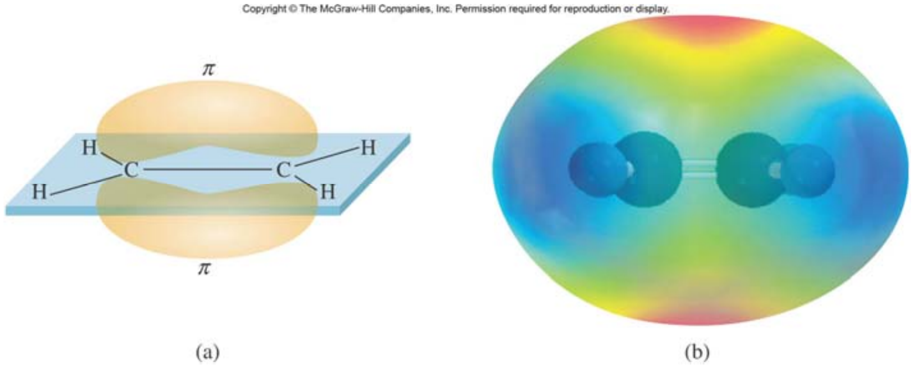
- Pi bonds = double or triple bonds; covalent bond formed by sideways overlapping orbitals with electron density concentrated above and below the plane of the nuclei
- Consider ethene: Formed from the side-by-side overlap of the two unhybridized $2p_z$ orbitals from each carbon



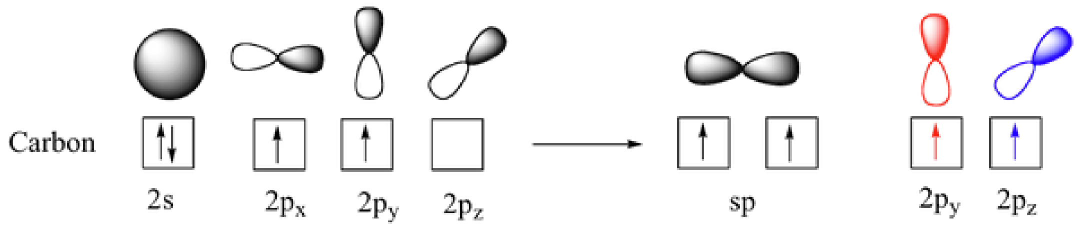

Ground state
2s
2p
Promotion of electron
2s
2p
sp2-Hybridized state
sp2 orbitals
2pz

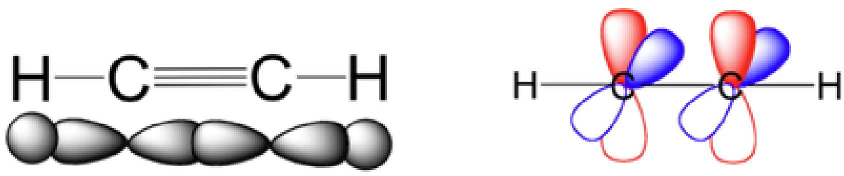

2pz
side view
top view
'side-by-side' (π) overlap
H
H
H
H


H 1s
H 1s
H 1s
H 1s
C
C
2pz 2pz
C C
π
σ
H
π
(a)
(b)
(c)


π
H
C
C
H
H
H
π
(a)
(b)

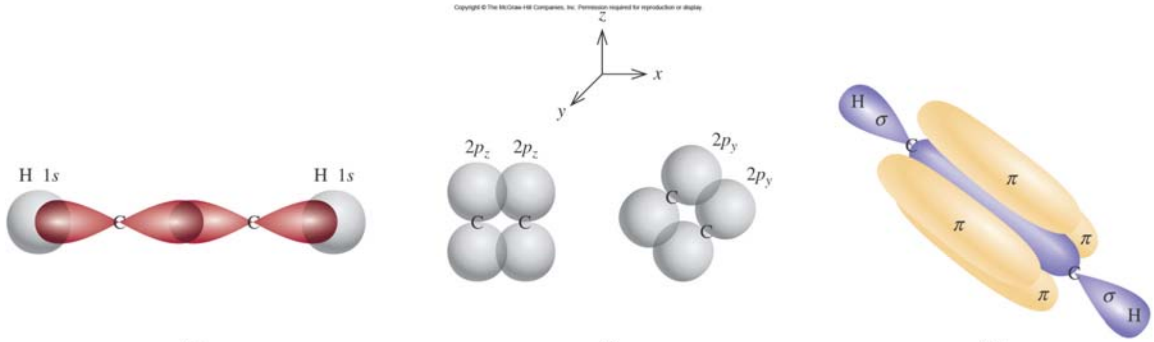
- Consider ethyne where the carbons are sp-hybridized



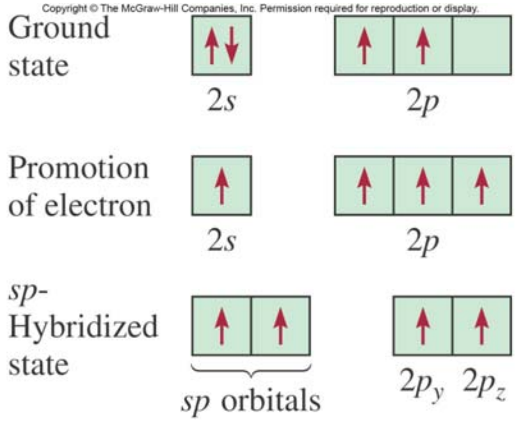


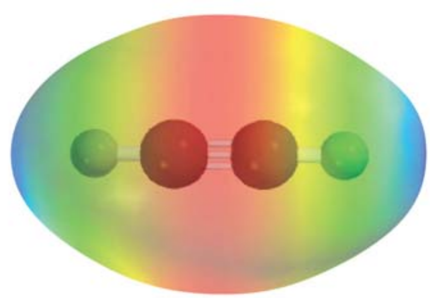
σ bonding framework

π overlap



(a) (b) (c)

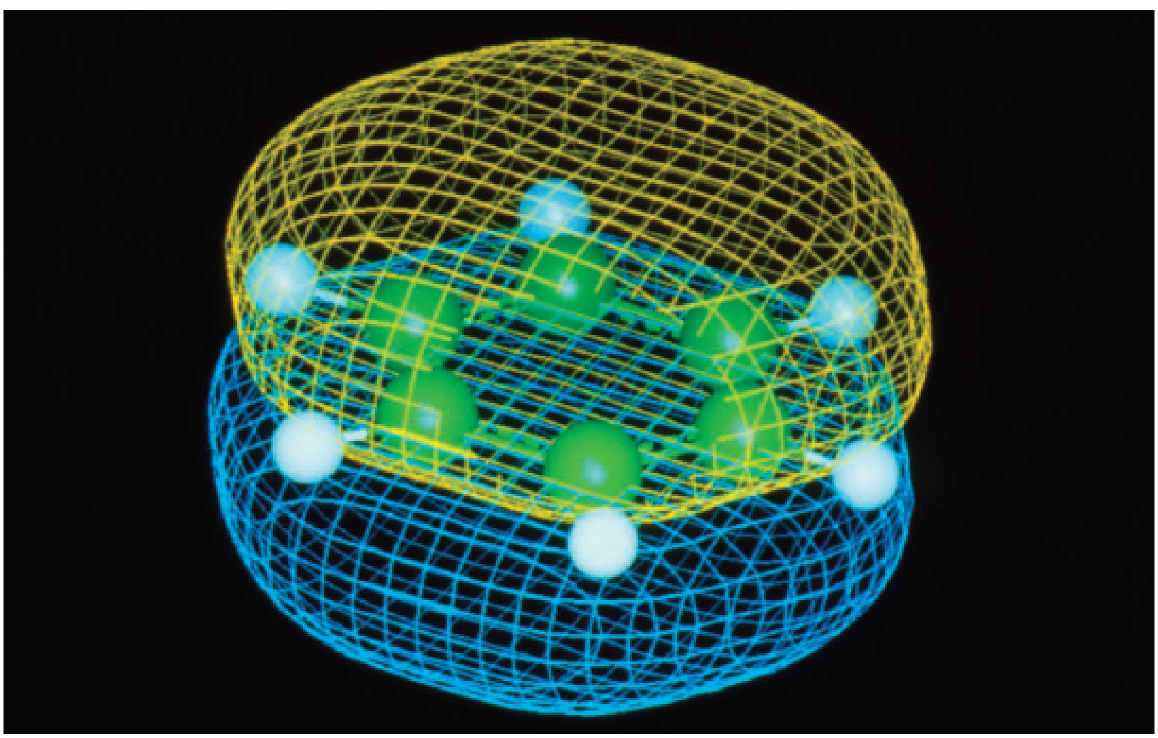




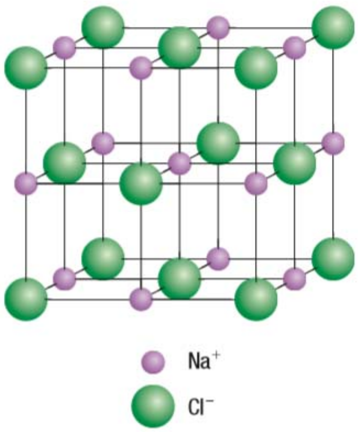
(d)

Checkpoint

- Draw the picture of the following molecules using valence bond theory and state the number of sigma bonds and pi bonds.
  a) Magnesium hydride
  b) Aluminum trihydride
  c) Methanal (Formaldehyde)
  d) Benzene

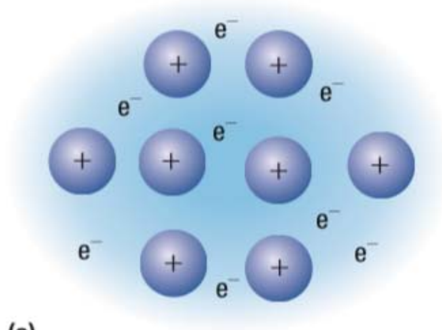


Structure and Properties of Solids

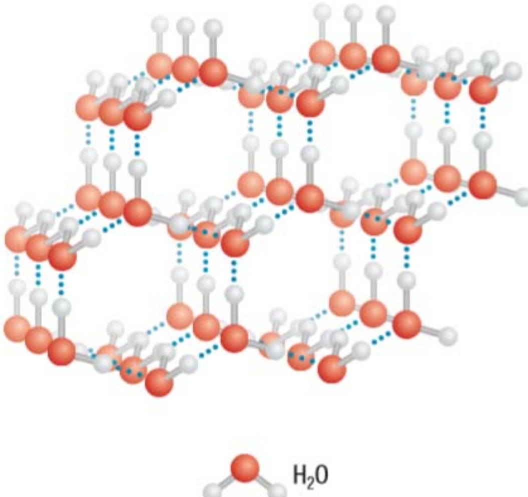


- **Ionic Crystals** – the interaction of a metal and a non-metal with the alternating packing of positive and negative ions
- Properties:
  - Hard, brittle solid
  - Does not conduct electricity as a solid
  - High melting points due to strong ionic bonds

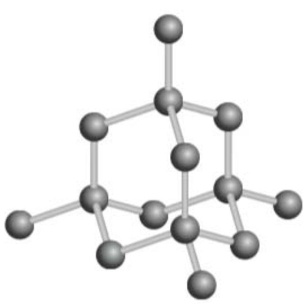
- **Metallic Crystals** – a solid with closely packed metal atoms held together by electrostatic interaction and free-moving electrons
- Based on "Electron Sea Theory" – valence electrons are free to move while the nucleus remains fixed
- Properties:
  - Low ionization energies
  - Malleable
  - Conducts electricity
  - Hard



(a)

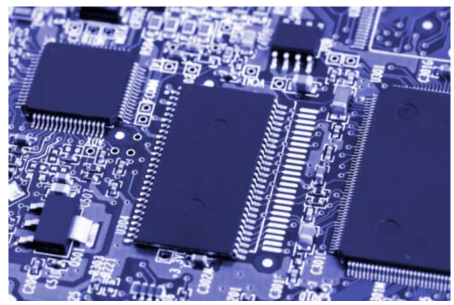


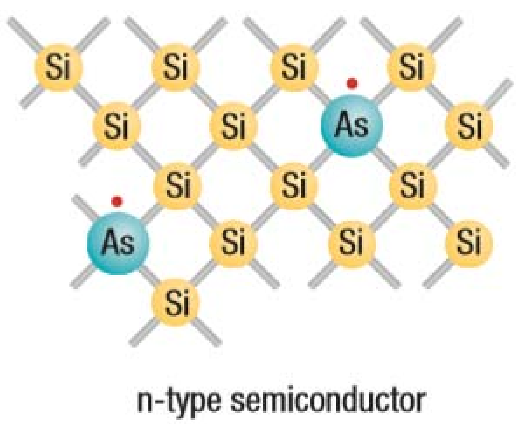
- **Molecular Crystals** – held together by dispersion forces, dipole-dipole forces and hydrogen bonds
- Ex: H_2O, I_2, P_4 and S_8
- Properties:
  – Do not conduct electricity
  – Lower melting points
  – Less hard than ionic crystals

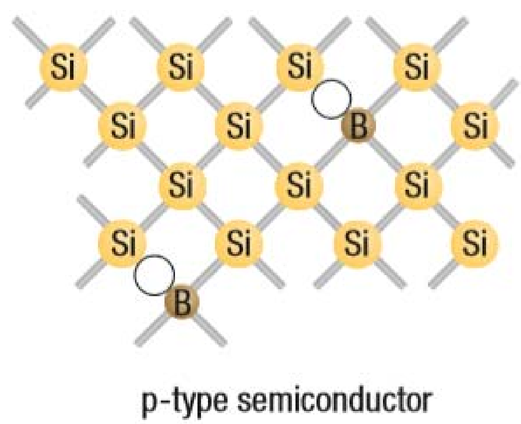


- **Covalent Network Crystals** – held together by covalent bonds in an interwoven network
- Ex: Diamond, Quartz (SiO_2)
- Properties:
  – High melting points
  – Extreme hardness
  – Do not conduct electricity

- **Semiconductors** – covalent crystals such as Si or Ge that conduct small amounts of electricity in standard conditions
- Doping – process of adding arsenic or boron to the covalent crystals to increase conductivity
- Two Types:
  - N-type semiconductors
  - P-type semiconductors







High temperatures cause additional electrons in **arsenic** (5 valence electrons) to excite to another level

Boron (3 valence electrons) has 1 less valence electron than silicon which allows electrons to move in and fill the hole