BONDING THEORIES

SCH4U1
SP06

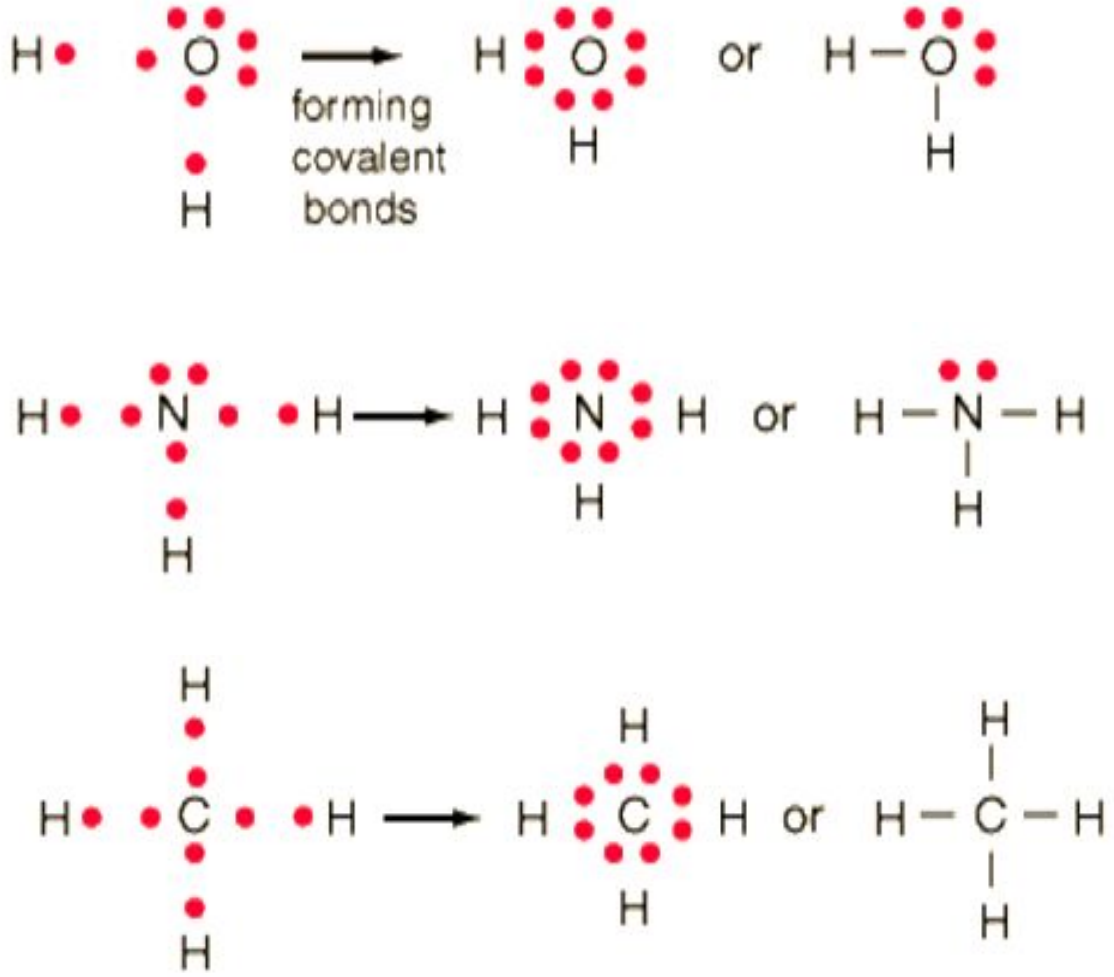
Lewis Theory of Bonding (1916)

Key Points:

- The noble gas electron configurations are most stable.
- Stable octets can be formed through the transfer of electrons from metals to non-metals.

- Stable octets can also form through sharing of electrons between non-metals (covalent bonding).
- Electrons are most stable when they are paired.

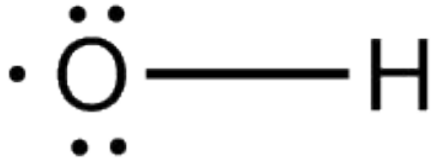
Electron Dot Diagrams & Lewis Structures



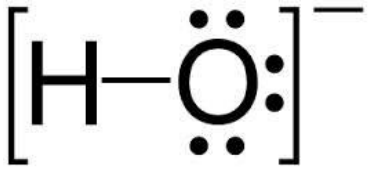
Free Radicals

- Atoms or molecules with unpaired electrons.
- These are very reactive substances.

- e.g. **reactive** hydroxyl radical (OH)

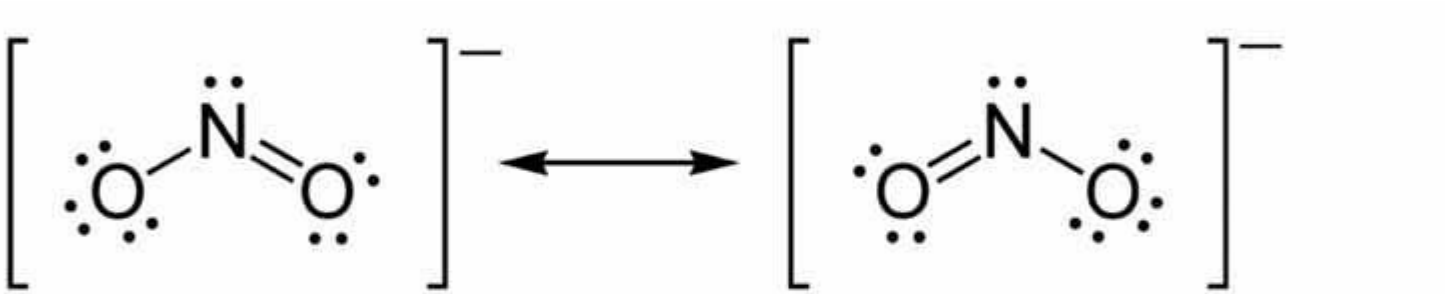


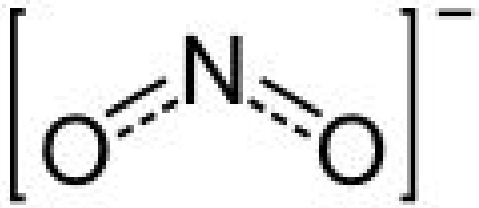
vs. **stable** hydroxide ion (OH^-)



Resonance

- When 2 possible Lewis structures are possible, a hybrid or “resonance” structure is assumed.
- Electrons are assumed to be “delocalized”
- e.g. nitrite ion





Practice:

Draw the Electron Dot and Lewis Structure for these covalently bonded elements, compounds or ions:

a) F_2
b) NF_3
c) N_2F_2
d) N_2
e) PCl_5
f) CN^-
g) NH_4^+
h) OCl
i) BrO_2^-
j) SO_3^{2-}
k) O_3

Write your answers on the board.

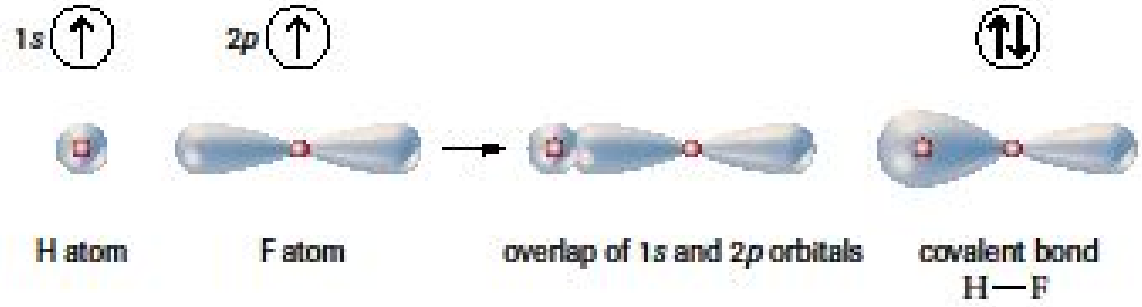
Valence Bond (VB) Theory (1928)

- VB Theory is a quantum mechanical model of bonding.
- Covalent bonds form when a pair of half-filled orbitals overlap to form combined (or bonding) orbitals.
- Bonding orbitals contain 2 electrons with opposite spin.

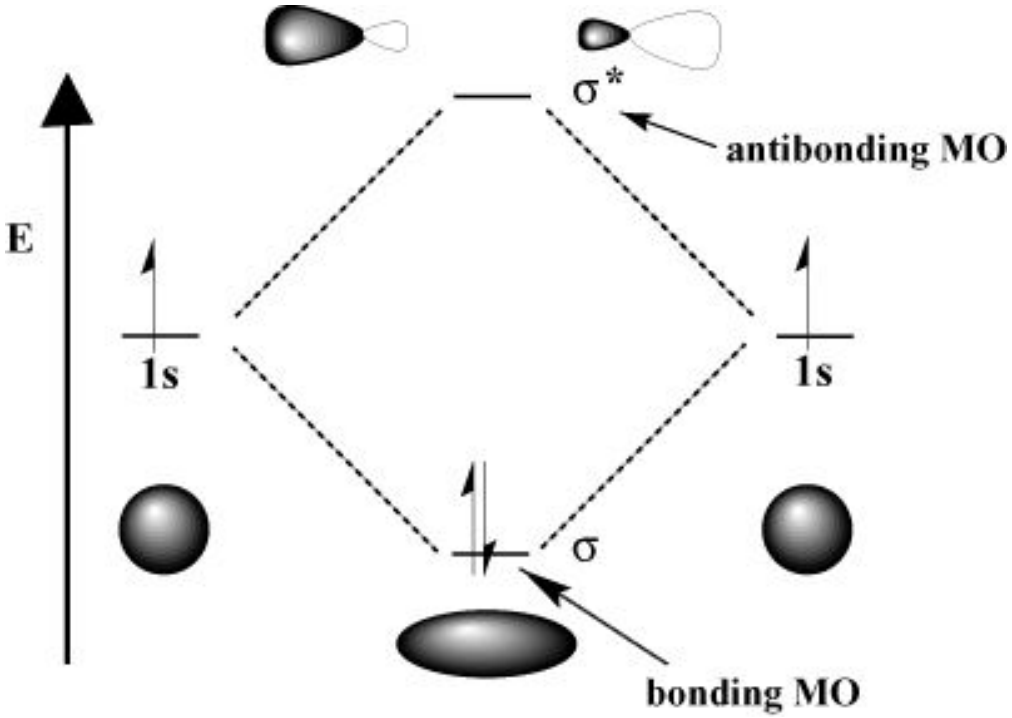
- Electron density is highest between the 2 nuclei.
- Direct overlap of orbitals is called a **sigma (σ) bond**

VB Theory (continued)

- Overlapping orbitals can also form between *s* and *p* orbitals (e.g. HF)



- Combined orbital (**sigma bond)** represents a lower energy state of the two atoms.


E
σ*
antibonding MO
1s
1s
σ
bonding MO

Molecular Orbital (MO) Theory (1933)

- Lewis Theory considers all 4 electrons around carbon to be identical.
- Contradicted by the Wave-Mechanical Model ($1s^2 2s^2 2p^2$)
- Experimental evidence confirmed the Lewis model of carbon bonding in compounds (e.g. CH_4)!
- Carbon does contain 4 identical covalent bonds !?!

- [Complete the Orbital Representation Table Now]

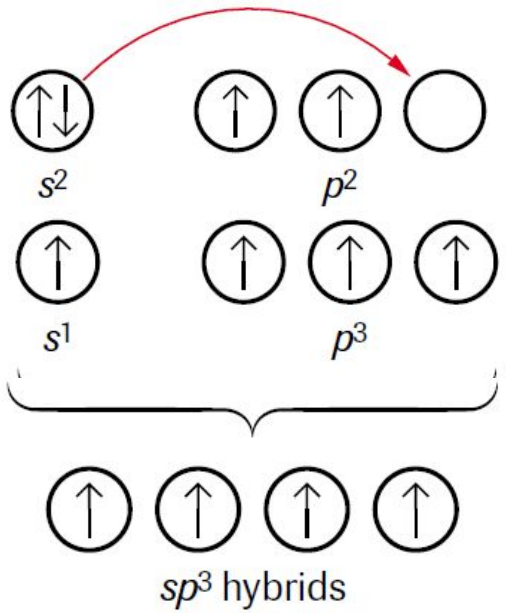
Molecular Orbital Theory

- States that atomic orbitals can combine to form molecular orbitals (MO)
- MO are combinations of Schrodinger's equations containing multiple nuclei.

- Formation of a MO involves electron promotion & orbital hybridization.

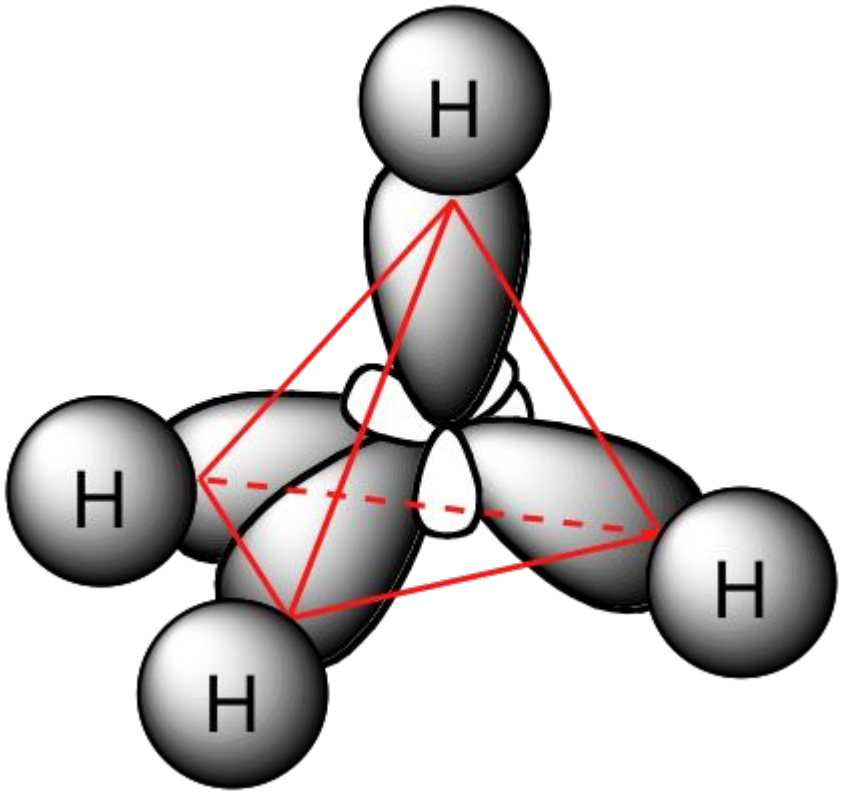
MO Formation in Carbon

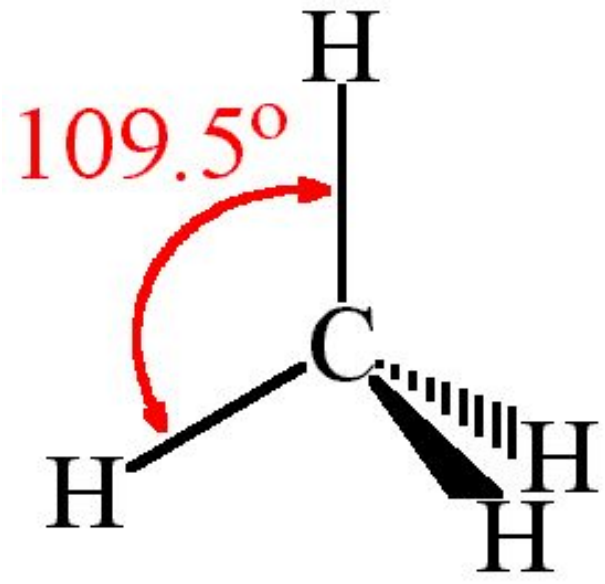
1) A 2s electron is “promoted” into the empty p orbitals.
2) The $2s^1 2p^3$ atomic orbitals undergo hybridization to form 4 half-filled sp^3 bonding orbitals.
3) Each identical sp^3 orbital can form a **sigma bond** with another half-filled orbital.



sp^3 Hybridization and Shape

- Electron repulsion moves the 4 bonding orbitals as far apart as possible, forming the tetrahedral shape.





Need another explanation?

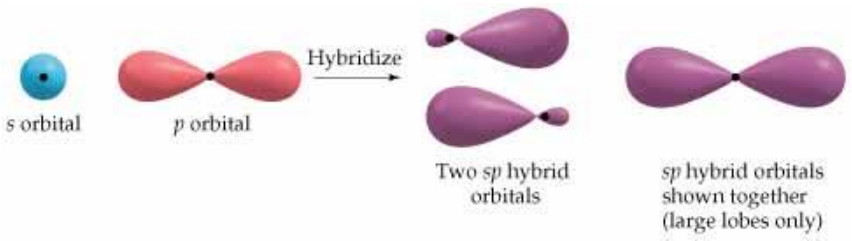
1) Review the extra readings online
2) Watch these clips:

   Hybridization

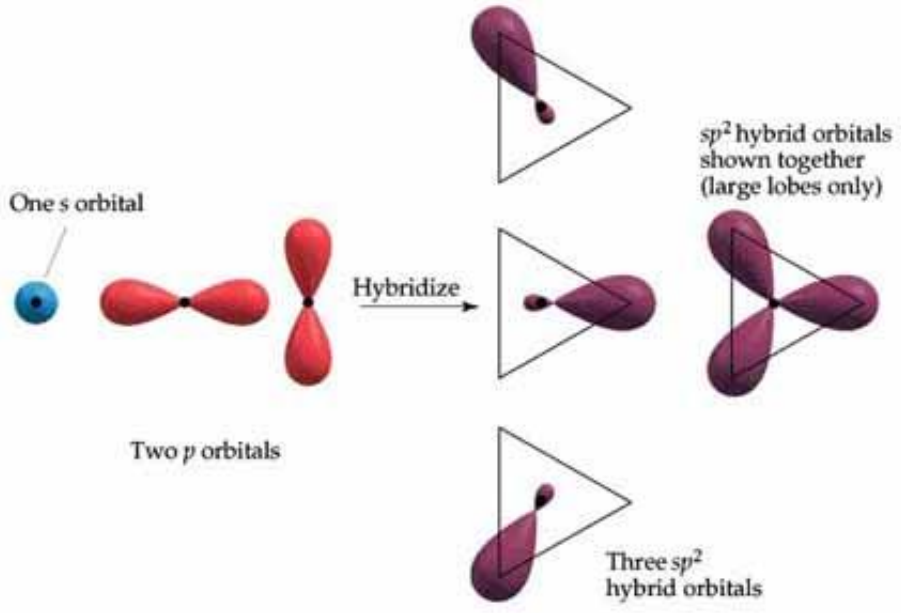
   Molecular Shape and Orbital Hybridization

Hybrid Orbitals

s + *p* ⟶ *sp hybrid* *Linear molecule*

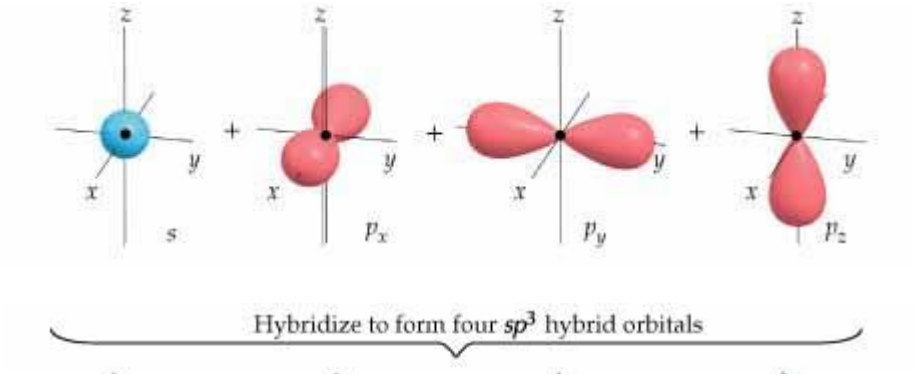


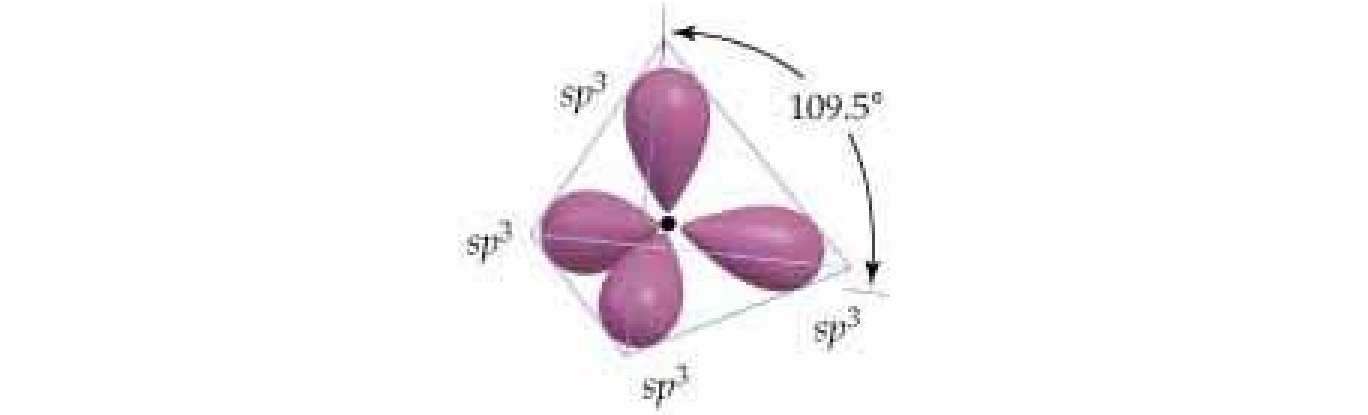
s + *2p* ⟶ *sp*^{2} *hybrid* *Trigonal planar*



Hybrid Orbitals

s + *3p* ⟶ sp^3 *Tetrahedral*

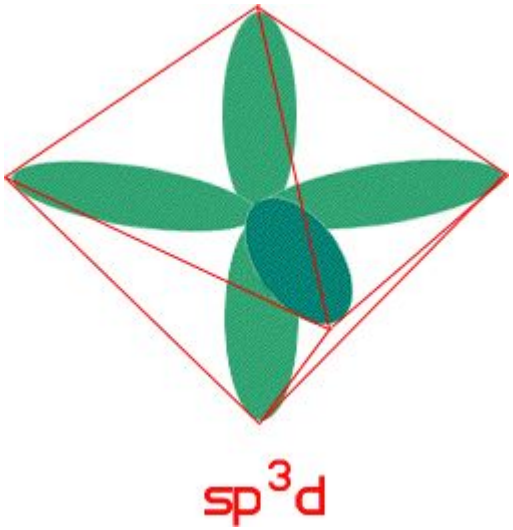




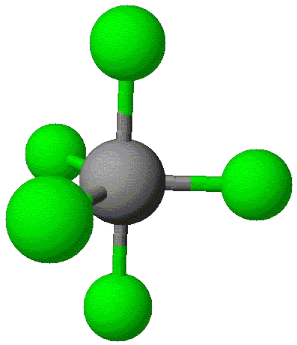
Other hybrids…

- Exceptions to the “octet rule” involve unusual hybrids

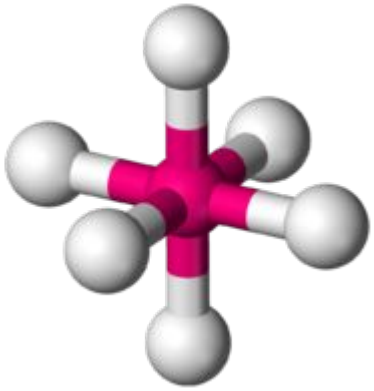
s + *3p* + *d* ⟶ *sp^3d hybridization*



- 5 identical bonding orbitals
- Trigonal bipyramidal shape (e.g. PCl_5)



- *s* + *3p* + *2d* ⟶ sp^3d^2 *hybridization*



- 6 identical bonding orbitals
- Octahedral shape
  (e.g. SF_6)

THINKING EXERCISE

Explain the weird valences of the following central atoms:

- Br in BrF_5
- S in SO_4^{2-}
- N in NO_3^-
- Xe in XeF_4