Hybridization: The Shape Of Things To Come

A. Intro
**B. Electron Counting**

**In Atoms**

<table>
<thead>
<tr>
<th>Element</th>
<th>Electron Configuration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Neon</td>
<td>1s² 2s² 2p⁶</td>
</tr>
<tr>
<td>Potassium</td>
<td>1s² 2s² 2p⁶ 3s² 3p⁶ 4s¹</td>
</tr>
<tr>
<td>Silicon</td>
<td>1s² 2s² 2p⁶ 3s² 3p²</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>1s² 2s² 2p³</td>
</tr>
<tr>
<td>Carbon</td>
<td>1s² 2s² 2p²</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>1s¹</td>
</tr>
<tr>
<td>Fluorine</td>
<td>1s² 2s² 2p⁵</td>
</tr>
<tr>
<td>Bromine</td>
<td>[Ar] 3d¹⁰ 4s² 4p⁵</td>
</tr>
<tr>
<td>Chlorine</td>
<td>1s² 2s² 2p⁶ 3s² 3p⁵</td>
</tr>
<tr>
<td>Oxygen</td>
<td>1s² 2s² 2p⁴</td>
</tr>
<tr>
<td>Sulfur</td>
<td>1s² 2s² 2p⁶ 3s² 3p⁴</td>
</tr>
<tr>
<td>Boron</td>
<td>1s² 2s² 2p¹</td>
</tr>
</tbody>
</table>
In Molecules, and Valency

2 electrons in the first shell,
8 in the second,
16 in the third.

*share* completely donate or receive electrons.

each hydrogen atom has 2 first shell electrons
One bond containing 2 electrons is formed in this sharing process
*valency* of hydrogen in \( \text{H}_2 \) is 1

\( \text{He} \)

\[
\begin{array}{cccccccc}
\text{C} & 4 & \text{N} & 3 & \text{O} & 2 & \text{F} & 1 & \text{Cl} & 1 & \text{Br} & 1 & \text{S} & 2 \\
\end{array}
\]

may only bring 1
common molecules is 1.

\[
\begin{array}{cccccccc}
\text{C} & \text{CH}_4 & \text{N} & \text{NH}_3 & \text{O} & \text{H}_2\text{O} & \text{F} & \text{HF} & \text{Cl} & \text{HCl} & \text{Br} & \text{HBr} & \text{S} & \text{H}_2\text{S} \\
\end{array}
\]

\( \text{N} 2s^22p^32p^12p^11s^11s^1 \text{ H}_3 \)

The blue and red electrons are shared in bonds, two per bond, so ammonia has two electrons that are not in bonds, *ie* a lone pair.


Favored electron count for that is 8

electrons is lost

C. Mixing Atomic Orbitals To Maximize Overlap In Molecules

Combining s- and p-Orbitals
called atomic orbitals.
have different shapes as atomic orbitals.
hybridized to make them.  
2 molecular orbitals, of three gives 3, and of n gives n.

denoted as \( sp \), whereas \( sp^2 \) surfaces are formed if two \( p \)-orbitals are mixed with one \( s \)-
a \( sp^3 \) hybrid.

**Geometric Shapes**

- \( s- \)
- \( d- \)
- \( d- \)
- \( p- \)

the boy *in the middle*.
girl-boy-girl angle is 180° 
ideal bond angle.

middle of a *triangle* with 
then 120°.

a *tetrahedron*, 
109°.
Shapes Of Molecules Based On Geometric Shapes

2 sp-hybrid orbitals.
3 hybrid orbitals, and
4 arise from.

**Bold** lines mean
**dashed** lines

A tetrahedron of sp$^3$ hybrids
if 4 bonds
sp hybrid orbitals.

0 lone pairs
it is tetrahedral.

3 lone pairs.

4 entities
hydrogen fluoride is approximately tetrahedral.

Water
4 objects
tetrahedral

hydrogen chloride, 4
Cl is tetrahedral
ammonia, 4
tetrahedral

hydrogen sulfide, 4
tetrahedral arrangement; and,

borane, 3
triangular arrangement.

C in methane is tetrahedral with a dihedral angle of 109°

O in water is tetrahedral with a dihedral angle of 109°

Br in hydrogen bromide is tetrahedral with a dihedral angle of 109°

N in ammonia is tetrahedral with a dihedral angle of 109°

S in H₂S is tetrahedral with a dihedral angle of 109°

B in BH₃ is trigonal with a dihedral angle of 120°
an $sp$ hybrid consisting of 2 MOs in a linear arrangement with a dihedral angle of $180^\circ$.

3 $sp^2$ MOs, and these arrange in a trigonal arrangement with a dihedral angle of $120^\circ$.

4 $sp^3$ MOs, and these arrange in a tetrahedral arrangement with a dihedral angle of $109^\circ$.

Examples:

- Water ($H_2O$)
- Hydrogen fluoride ($HF$)
- Methane ($CH_4$)
- Hydrogen bromide ($HBr$)
- Borane ($BH_3$)
- Hydrogen sulfide ($H_2S$)
- Phosphine ($PH_3$)
- Silane ($SiH_4$)
- Carbon tetrachloride ($CCl_4$)
D. Multiple Bonds

8 electrons in its second shell
7 electrons in its second shell; this is not a relatively reactive.

$sp^3$ hybridized
σ-bonded \( sp \) hybridized C-atoms

\[ \text{ethene before mixing p-orbitals} \]

\[ \text{ethene after mixing p-orbitals} \]

are called \textit{sigma}.

\( \pi \) bond.
Maximal overlap \textit{is} achieved
Perpendicular \( p \)-orbitals \textit{do} interact.

of a \( \pi \) bond.
1 line(s), and \( \pi \)-bonds are represented by adding 2 parallel line(s).

\begin{align*}
\text{isoprene} & \quad \text{pyruvic acid} & \quad \text{an imine} & \quad \text{lactic acid} & \quad \text{benzene} & \quad \text{β-pinene} \\
\text{# 2} & \quad \text{# 2} & \quad \text{# 1} & \quad \text{# 1} & \quad \text{# 3} & \quad \text{# 1} \\
\end{align*}

because they \textit{would not} contribute to the binding interaction.
Atoms in molecules \textit{can} selectively
Carbene, CH₂, has 6 shared electrons in the C-second shell. This is called the singlet state.

Alternatively, carbenes can be sp²-hybridized with one electron in each of the hybrid lobes that does not point to a hydrogen; this is a triplet state.

\[ \text{singlet} \]
\[ \text{triplet} \]
\[ \text{unstable triplet} \]

\[ \text{σ-bonded sp hybridized C-atoms} \]

\[ \text{ethyne before mixing p-orbitals} \]
\[ \text{ethyne after mixing p-orbitals} \]
two $\pi$ bonds surrounding the $\sigma$ bond called a **triple** bond.

It does not matter if they are $sp$ hybridized, three $sp^2$, and four $sp^3$. 
acetic acid

cis-1-hydroxy-2-butene

naproxen

alendronate

aspirin

zidovudine (AZT)