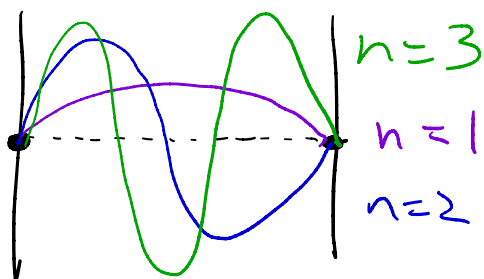May the 4th, 2020

Standing wave — In standing waves, energy is quantized, meaning it can only have specific values.

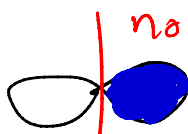n=3
n=1
n=2

The # of nodes total) = n-1
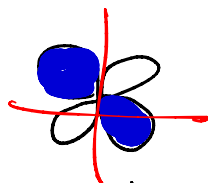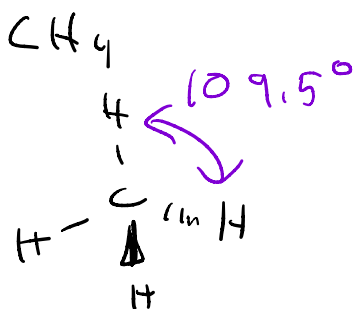
node

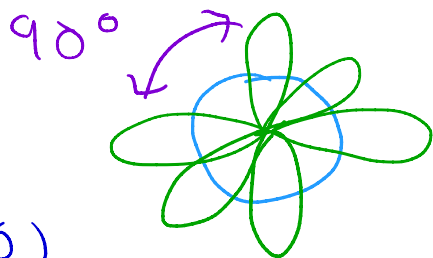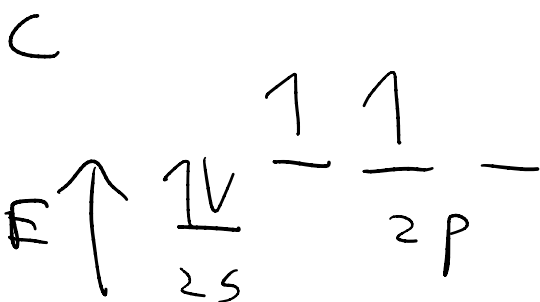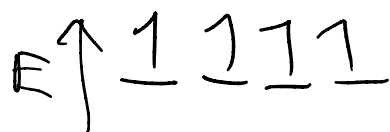1s
$\ell=0$

2p
$\ell=1$

3d
$\ell=2$

$\ell \rightarrow$ orbital angular momentum $\rightarrow$ how "fast" an electron is moving around the nucleus.

The # of spherical nodes = ℓ

The unique shapes of atomic orbitals are due to the fact that there is exactly one nucleus.

CH₄

CH_4

$109.5°$

tetrahedral

E↑ 1 1 1 1

C

E↑ $1\downarrow$ $\underline{1}$ $\underline{1}$ —
       $2s$ $2p$

$90°$

Atomic orbitals (AO)
fail to describe the structure of
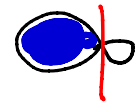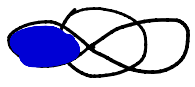molecules because molecules contain
multiple nuclei.

   In methane, all bonds are equal
in energy and the bonds form
tetrahedral geometry (109.5° angles)
even though the valence orbitals of
carbon are unequal in energy and
different in geometry.

   Solution: Create a new set of
hybrid orbitals by combining
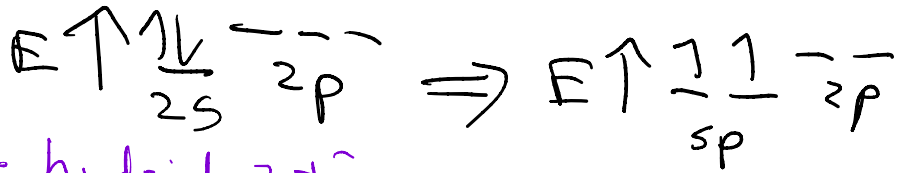   AOs.

How hybridization works → model

H — Be — H

180°

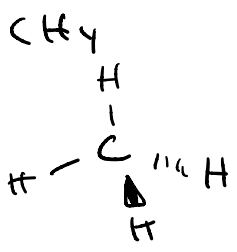Shading in these diagrams represents the sign (+ or −) of Ψ (wavefunction)

overlap

Hybridization creates orbitals with the right geometry and correct energy,

180°

$$E \uparrow \quad \underline{\uparrow\downarrow} \quad \overline{--} \atop 2s \quad 2p \quad \Rightarrow \quad E \uparrow \quad \underline{\uparrow \; \uparrow} \atop sp \quad \overline{--} \atop 2p$$
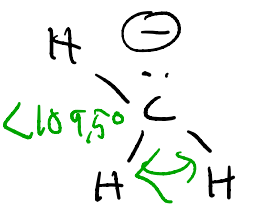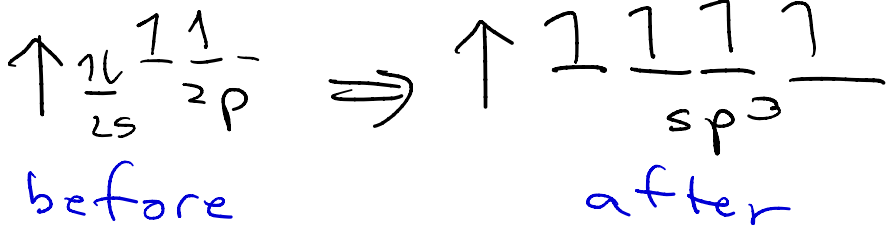
before hybridization

Linear combination of atomic orbitals (LCAO)
 − Atomic orbitals are added and subtracted to create a new set of hybrid orbitals,
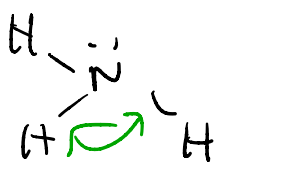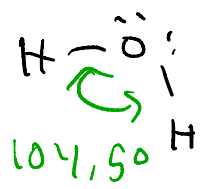
$$\Psi_C = a\Psi_A + b\Psi_B$$

CH_4

H—C with H, H, H bonds (methane structure)

methane

4 equivalent bonds →
4 equivalent hybrids →
4 AOs needed

↑ $\underset{2s}{\text{⇅}}$ $\underset{2p}{\text{↑ ↑ —}}$ ⟹ ↑ $\underset{sp^3}{\text{↑ ↑ ↑ ↑}}$

before   after

H $\ominus$ C, H, H (methyl anion)
< 109.5°

methyl
anion

H—N—H with H (ammonia)
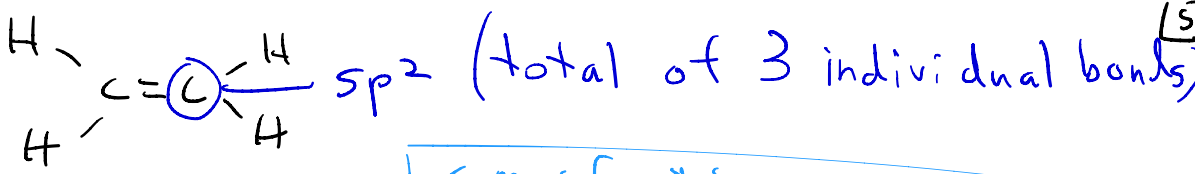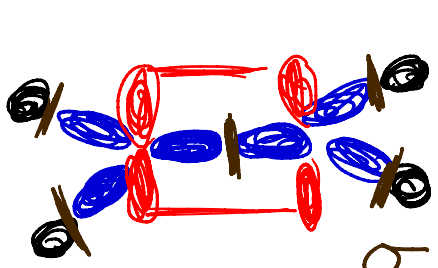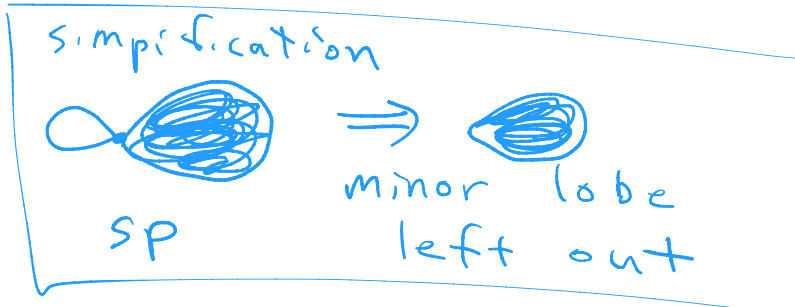107°

ammonia

H—Ö—H (water)
104.5°

water

All of these shapes are almost equal
to tetrahedral geometry → electron pair
geometry. Therefore, they are all
best described by sp^3 hybrids.

# of hybrid orbitals =
    # of bonds and lone pairs

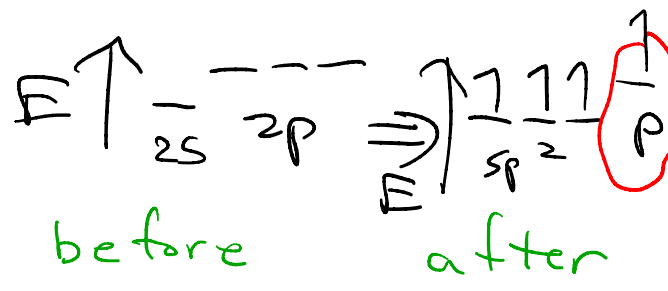single, double, and triple bonds
    are all counted once

H   C=C H   sp² (total of 3 individual bonds)
H   ⊙ H
H

ethene
(ethylene)

simplification

sp   ⟹   minor lobe
            left out

● S
● sp²
● P

σ (sigma) bond

π (pi) bond

one set of
3 sp² orbitals

E↑ = ‾‾‾   ⟹ ↑ ↑ ↑ ↑
     2s 2p   E sp² P
before   after

Shading in this diagram represents
orbital type, not mathematical sign.