

Today:

- VSEPR and Molecular Geometry
- Orbitals and Phasing
- Bonding
- Hybridization

Last week:

- Lewis structure
- Octet Rule
- Formal charge

Lewis structures → show bonding/ connectivity between atoms

BUT

we don't know how atoms are arranged in 3D space

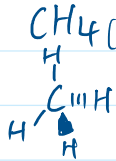
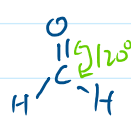
↳ Need something else to understand molecular geometry

VSEPR model: Valence Shell Electron Pair Repulsion

↳ predicts molecular geometry

↳ place all "group" (bonds, lone pairs) as far apart as possible

↳ single/double/triple bonds all are one region of e<sup>-</sup> density

<u>Example</u>	<u># of regions of e<sup>-</sup> densities around a central atom</u>	<u>[VSEPR] Predicted Geometry</u>	<u>Predicted Bond angle</u>
$\text{CH}_4$ ( $\text{H}_2\text{O}$ , $\text{NH}_3$ ) 	4	Tetrahedral	109.5°
	3	Trigonal planar	120°

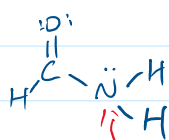


2

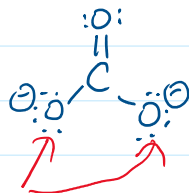
Linear

 $180^\circ$ 

This table and VSEPR breaks down for some molecules:



NOT Tetrahedral  
(not sp<sup>3</sup>) as VSEPR  
predicts



Time  
Capsule

VSEPR will accurately predict structures when we consider all valid resonance contributing structures

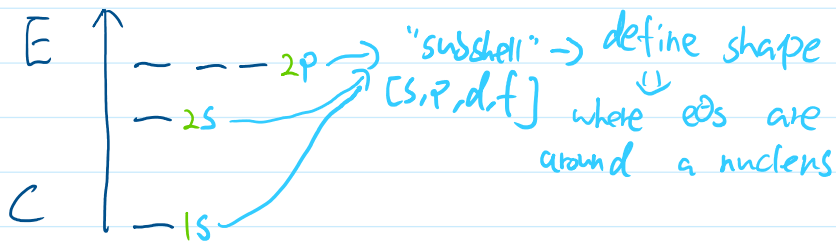
"where are the electrons?"

↳ surrounded nuclei, but in specific region

e<sup>-</sup>s exist in "orbitals" → 3D locations around nuclei where e<sup>-</sup>s are  
→ have specific energies

orbitals have defined energies, shapes (described by multiple quantum numbers)

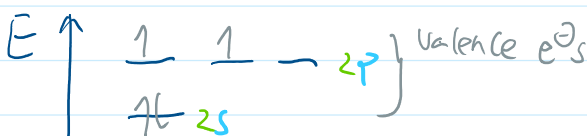
e<sup>-</sup> configuration  
↳ the energy diagram  
that shows distribution of  
e<sup>-</sup> in atoms



"shell" → row of periodic table  
[1, 2, 3, ...] determines valence shell  
dictates bonding  
C is in row 2,  
valence e<sup>-</sup>s are in  
2nd shell

Carbon

recall  ${}^6\text{C} \rightarrow 6e^-$   
group 4 → 4 valence e<sup>-</sup>



C can make 4  
covalent bonds to fill  
its valence shell

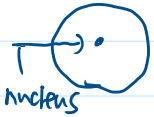
dark line

$C \mid \uparrow \downarrow \mid 1s$   
 each line represents an atomic orbital

covalent bonds to fill its valence shell

## Orbital shape

S-orbitals → held closer to the nucleus



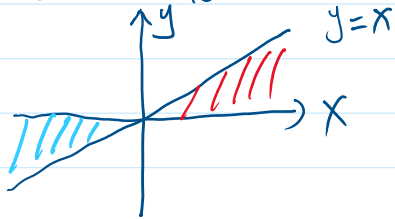
↓  
lower in E. than P orbitals

P-orbitals → have +/- phasing  
Dumbbell shape



↓  
e<sup>-</sup> density is equal in +/- lobes

Phasing: +/- answers to math solutions of math equations that describe orbitals



The "area" is the same, the "sign" is different

+/- does not directly mean constructive/destructive addition

+ and + ⇒ constructive addition

+ and - ⇒ destructive addition

Let's look at bonding of H<sub>2</sub>

↳ To covalent bond → share 2e<sup>-</sup>, between 2 H atoms to fill valence (shared e<sup>-</sup>s)

Hydrogen = H → 1e<sup>-</sup> → need 2nd e<sup>-</sup> to fill the valence shell

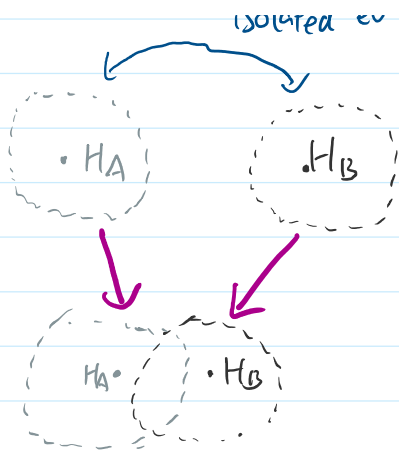
↳ can do this by sharing the 2nd e<sup>-</sup> w/ a second H-atom

E ↑

H | 1s

isolated e<sup>-</sup> cloud of H- atoms





Bring  $H_A$  and  $H_B$  together in space and overlap orbitals to set a bond to form!



Bonding orbital (bond)

$\sigma$ -Bond  
sigma

Both  $e^-$ s are shared between  $H_A$  and  $H_B$

Formation of Covalent Bond between  $H_A$  and  $H_B$

molecular orbital

restrap @ 5:05 pm 😊

To understand bonding in carbon containing molecules, recall:

Quantum mechanics: when we add X numbers of orbitals together, we get out X new orbitals

↳ start w/ 4 orbitals  $\rightarrow$  get out 4 new orbitals

Two accepted theories for bonding:
 

- Valence Bond Theory (VBT)  $\rightarrow$  help us understand ( $\sigma$ )
- molecular orbital theory  $\rightarrow$  ( $\pi$ ) (MOT)

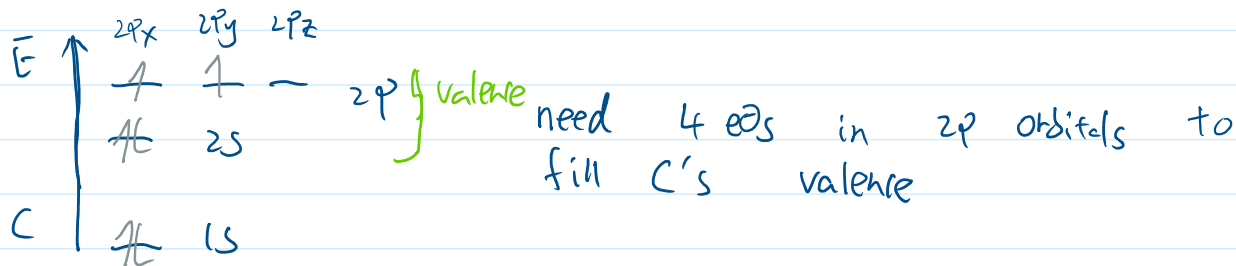
we use VBT to understand  $\sigma$ -bonds  $\rightarrow$  come from the overlap of hybridized orbitals  
 recall the Hot Dog/Diet Coke  $\downarrow$  meat

we use MOT to understand  $\pi$ -bonds = double/triple bonds

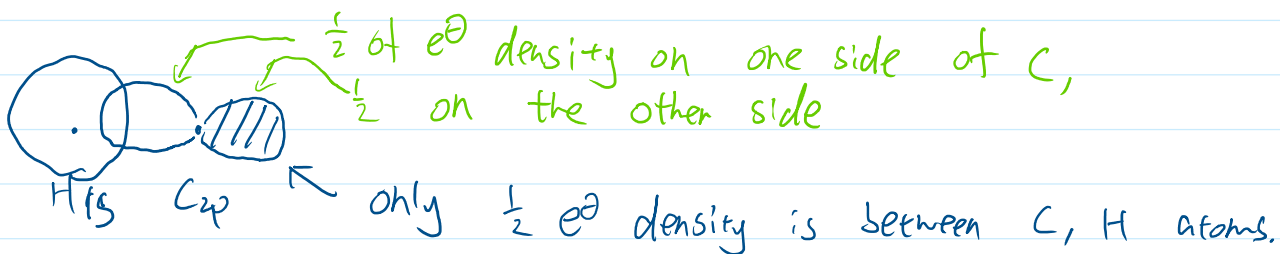
we use MOT to understand  $\pi$ -bonds = double/triple bonds

comes from the overlap of 2p atomic orbitals  
 ↓  
 think about Diet Coke!

RECALL  $e^-$  configuration for Carbon:



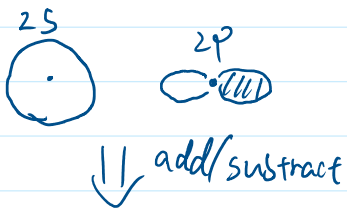
if: C-H bond w/ C 2p orbitals



Can't form a bond w/ H 1s  $\Rightarrow$  because not enough orbital overlap for a bond (sharing  $e^-$ s between atoms)

Orbitals are waves, they have shapes  
 waves can add

VBT = math combination on one 2s<sup>atomic</sup> orbital and one 2p atomic orbital produces 2 equivalent sp-hybridized orbitals

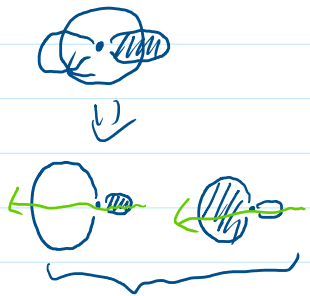


"Hybrid" = made of 2 components

Prins = Gas + Electric



"hybridized orbitals" = made of s and p  
 atomic orbitals

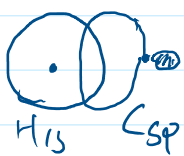


"hybridized orbitals" = made of s and p atomic orbitals  
 (sp, sp<sup>2</sup>, sp<sup>3</sup>)  
 how many 2p atomic orbitals are "used" in hybridization

two sp-hybridized orbitals

Have directionality - we can make bonds w/ Hybridized orbitals

C-H w/ H<sub>1s</sub> and Csp



σ-Bond between C and H formed w/ hybridized orbitals

σ<sub>H1s-Csp</sub>

example	(C) Atom Hybridization	Types and # of hybridized orbitals		Types and # of pure atomic orbitals	
		Types	#	Types	#
H-C≡C-H	sp-hybridized (s <sup>1</sup> p <sup>1</sup> =sp) ↑	sp	2	2p	two
$\begin{array}{c} \text{O} \\    \\ \text{H}-\text{C}-\text{H} \\ \uparrow \end{array}$	sp <sup>2</sup> -hybridized	sp <sup>2</sup>	3	2p	one
$\begin{array}{c} \text{H} \\   \\ \text{H}-\text{C}-\text{H} \\ \uparrow \\ \text{H} \end{array}$	sp <sup>3</sup> -hybridized	sp <sup>3</sup>	4 make σ bonds	NO 2p orbitals! Can make π bonds!	