HATW 9. 5. 24

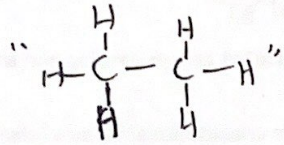
Topics: VSEPR and molecular geometry

Orbitals and phasing

Bonding

Hybridization

Recall: Lewis structures → show bonding/connectivity between atoms.



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

⇓

Need something else to understand molecular geometry

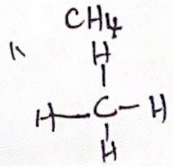
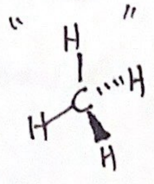
VSEPR model: valence shell electron pair repulsion.

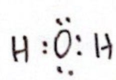
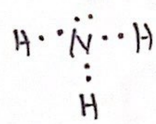
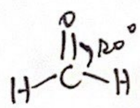
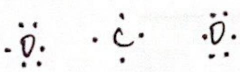
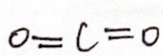
↳ predicts molecular geometry

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

↳ single/double/triple bonds, all are <u>one</u> region of $e^{\ominus}$ density.

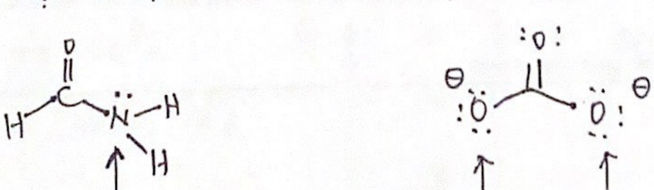
Ex:

	# of regions of $e^{\ominus}$ density around a central atom		VSEPR predicted geometry	predicted Bond angle
CH_4 	4		tetrahedral	109.5°

	# of regions of $e^{\ominus}$ density around a centra atom	VSEPR predicted geometry	predicted bond angle
Ex. H_2O  	4	tetrahedral	109.5°
NH_3 	4	tetrahedral	109.5°
	3	trigonal planar	120°
CO_2  	2	linear	180°

This table and VSEPR breaks down for some molecules:

Ex:



Not tetrahedral (not sp^3 hybridized) as VSEPR predicts.

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

(we'll get back to this after hybridization)

"where are the electrons?"

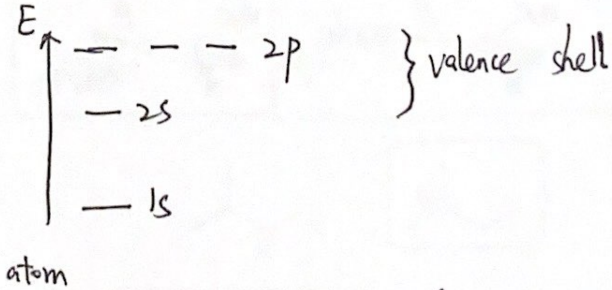
↳ surrounded nuclei, but in specific region.

$e^{\ominus}$ exist in "orbitals" → 3D locations around nuclei where $e^{\ominus}$ are

→ have specific energies.

orbitals have defined energies, shapes

$e^{\ominus}$ configuration diagram shows distribution of $e^{\ominus}$s in atoms



"[1, 2, 3 . . .]" Determines valence shell:

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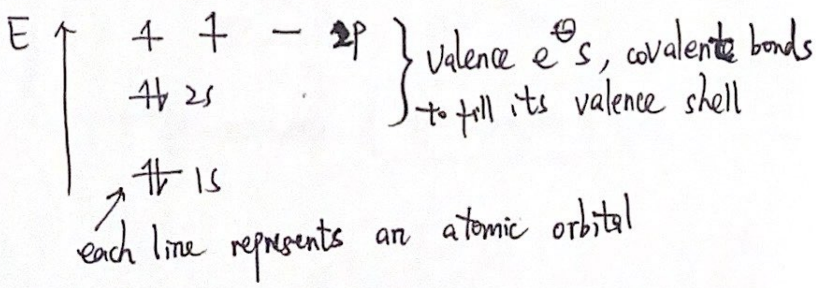
"shell"

"C" is in row 2, valence $e^{\ominus}$s are in 2nd shell.

$_6C$ → 6$e^{\ominus}$s

4 valence $e^{\ominus}$s



orbital shape

s-orbitals → held closer to the nuclei

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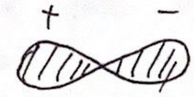
lower in energy than p orbitals

3D speres

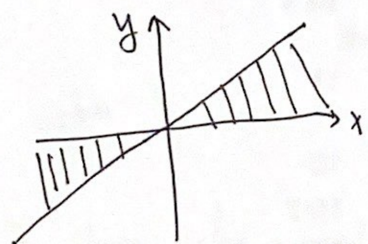
p-orbitals → have +/- phasing

⇓

$e^{\ominus}$ density is equal in +/- lobes



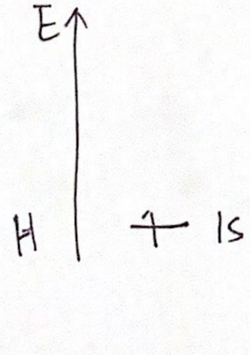
phasing: +/- answers to math solutions that describle orbitals.

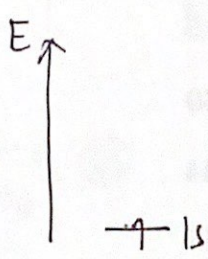


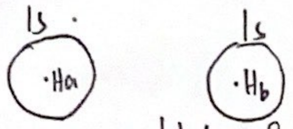
The area is the same, the sign is different.

Let's look at bonding of H_2

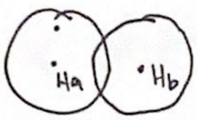
H: $1 e^{\ominus}$ $\xrightarrow[\text{valence shell}]{\text{to fill}}$ need 2nd $e^{\ominus}$



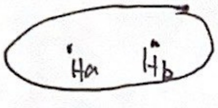




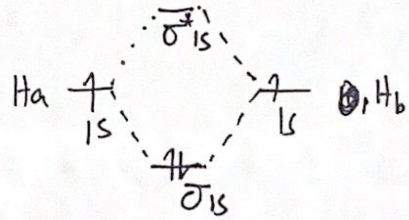
isolated, e$^{\ominus}$ clouds of H atoms



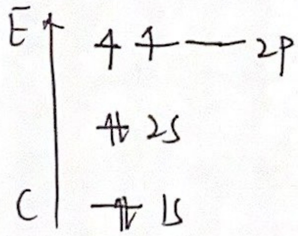
bring Ha and Hb together in space and overlap orbitals to get a bond to form.



← bonding orbital. , σ-bond. , "molecular orbitals."

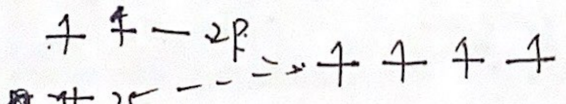


e$^{\ominus}$ configuration for carbon:

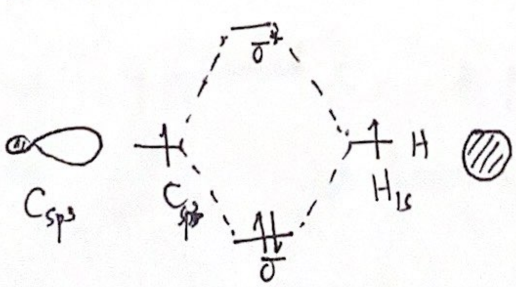


valence shell, need 4 e$^{\ominus}$ in these orbitals to fill C's valence.

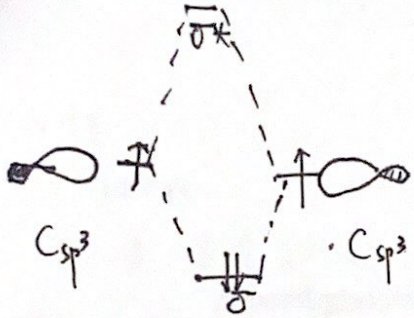
CH4



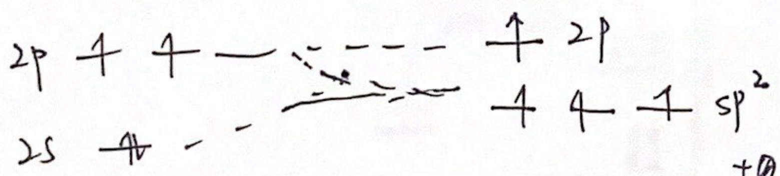
sp^3 hybridization, will e$^{\ominus}$ population for carbon.

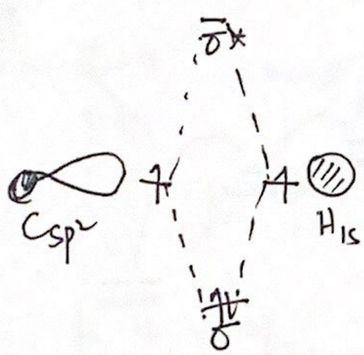


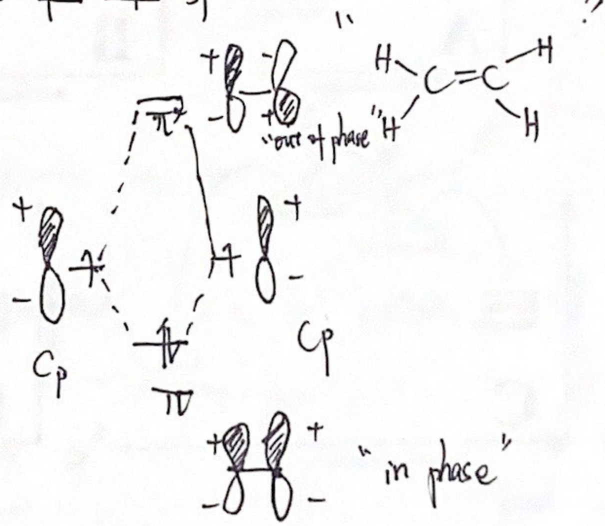
H_3C-CH_3

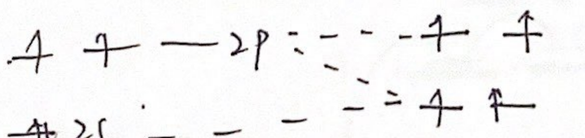


sp^2 hybridization



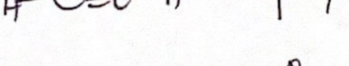




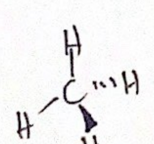


2p orbitals, 2 "π" bonds can form

H−C≡C−H sp hybridized C, 2 p orbitals, 2 sp orbitals



sp^2 hybridized C, sp^2 orbitals × 3, p orbital × 1

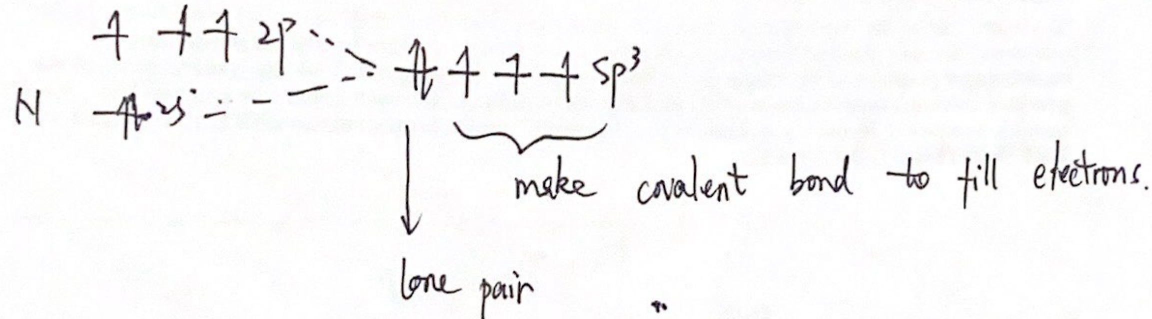


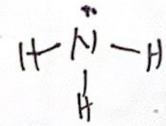
sp^3 hybridized C, sp^3 orbitals × 4, no p orbitals

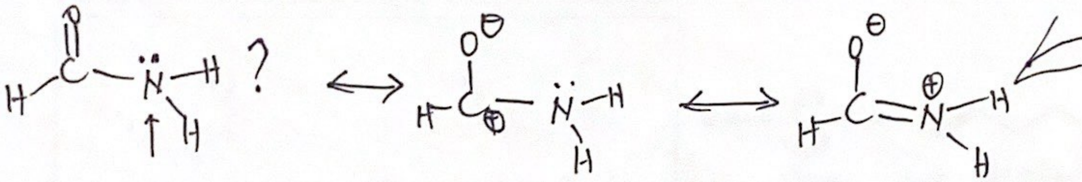
⇓

can't make π bonds!

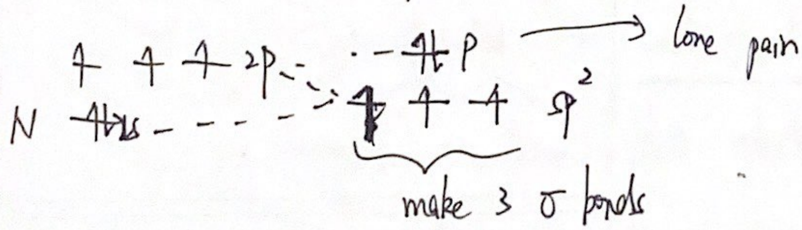
NH3







N is sp² hybridized, 3 × sp² orbitals, 1 p orbital.



⇓ to form "π" bond in the minor contributing structure.

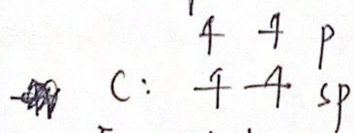
HCN

H−C≡N: 2 π bonds

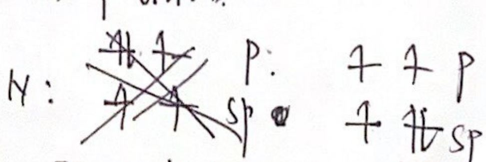
C: sp hybridized: 2 × sp orbitals, 2 × p orbitals

N: sp hybridized 2 × sp orbitals, 2 × p orbitals

2.



[2 σ bonds, 2 π bonds]



[1 σ bond, 2 π bonds]