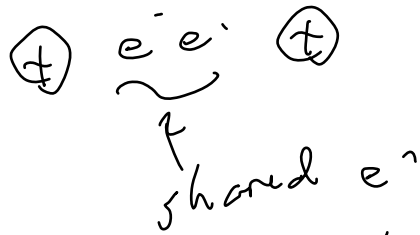


# Ch. 4 Valence bond theory

- applies to covalent bond/cpd

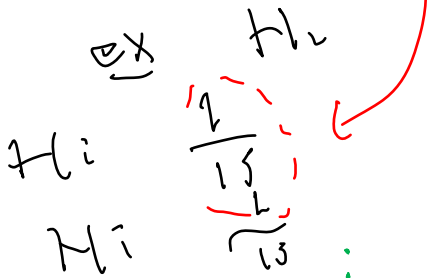
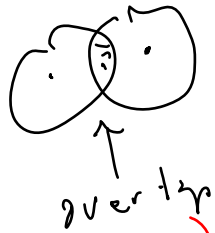
↑  
- overlap of AO

- share  $e^-$  ↑  
 overlap of  
 - sAO & sAO  
 - pAO & pAO  
 - pAO & sAO

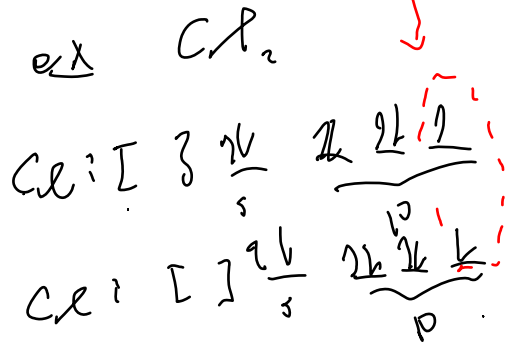


basis of covalent bond  
 mutual attraction of shared  $e^-$  by the  
 nuclei of the atoms in the bond

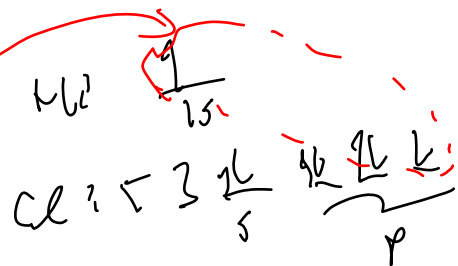
overlap of sAO



overlap of pAO



overlap of sAO & pAO



# Ch. 9.5 hybrid orbitals (HO)

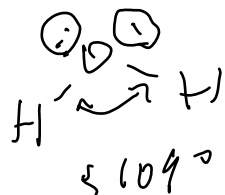
- its a "combination of AO"
- needed to "explain" some covalent cpd bonding
- modify valence bond theory

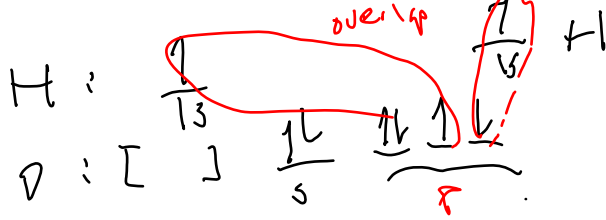
overlap of AO  $\rightarrow$  overlap of AO  $\neq$  for hybrid orbital

<u>HO</u>	<u>Contains</u>	<u>bond angles</u>	<u><math>\Sigma</math> exponents on stuff</u>	<u># on central atom</u>
			<u># bond + nonbond pairs</u>	
$sp$	1 s-AO 1 p-AO	$180^\circ$	2	2
$sp^2$	1 s-AO 2 p-AO	$120^\circ$	3	3
$sp^3$	1 s-AO 3 p-AO	$109^\circ$	4	4
$sp^3d$	1 s-AO 3 p-AO 1 d-AO	$120^\circ$ $90^\circ$	5	5
$sp^3d^2$	1 s-AO 3 p-AO 2 d-AO	$90^\circ$	6	6

ex 1

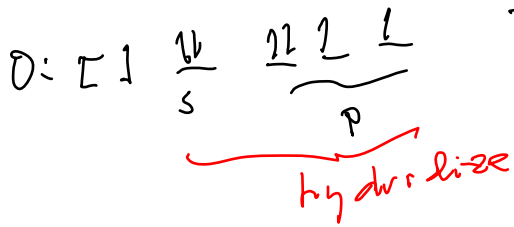
$H_2O$



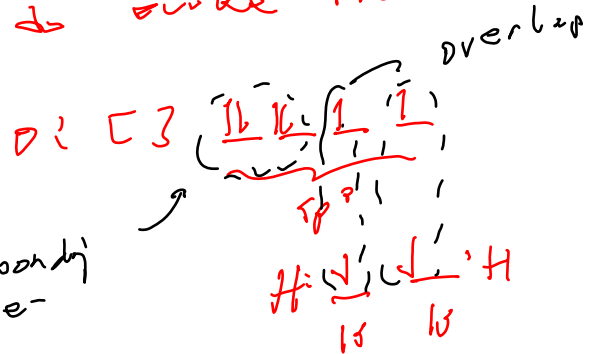


overlap of sAO with  $\neq$   
 predicts bond angle =  $90^\circ$   
 but VSEPR predicts bond angle  $\sim 107^\circ$

$\therefore$  conflict  
 overlap of AO is invalid  
 $\therefore$  need to make HD



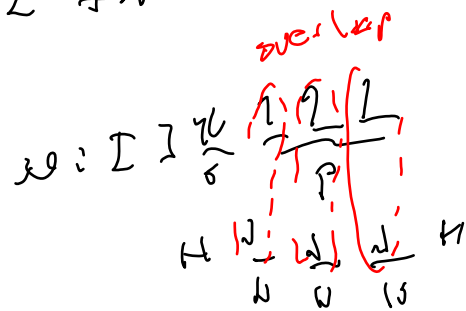
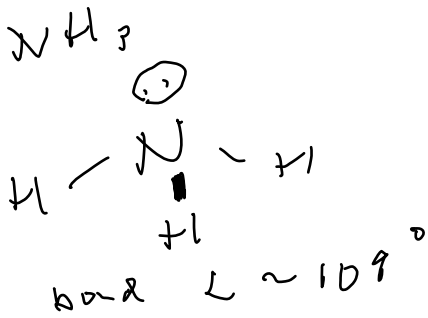
hybridize



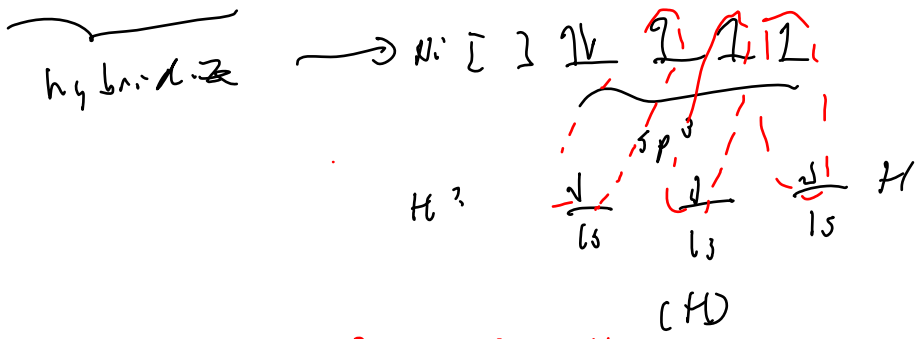
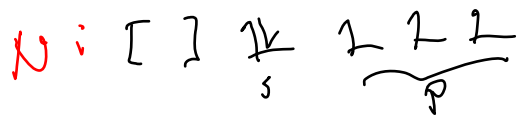
overlap of  $sp^3$  HD in O  $\neq$  sAO with

note: know need  $sp^3$  HD in O  $2x$   
 b/c from VSEPR, know bond  $\angle \sim 109^\circ$   
 $sp^3$  HD generates/allow/form  $\sim 109^\circ$   
 i.e. to identify the type of hybrid orbital,  
 "match" bond  $\angle$  from VSEPR

ex

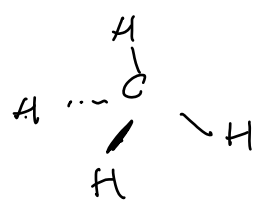
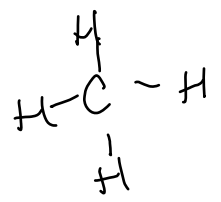


but product bond  $\angle \sim 107^\circ$   
 VSEPR bond  $\angle \sim 109^\circ$   
 $\therefore$  need HD

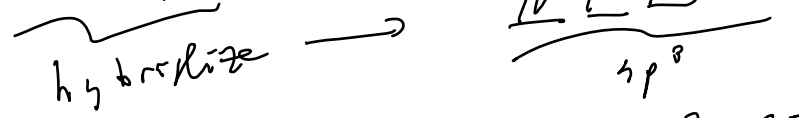
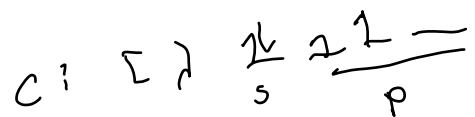


overlap of  $sp^3$  HD in C  
& s.AO in H; 3x

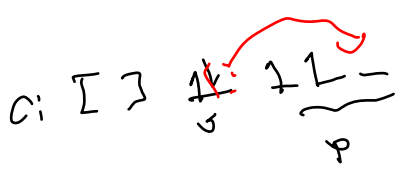
ex 3 CH<sub>4</sub>



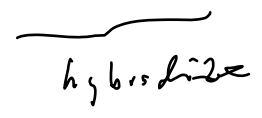
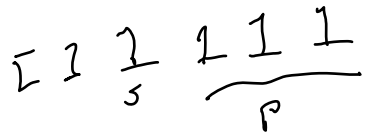
bond  $\angle \sim 109^\circ$



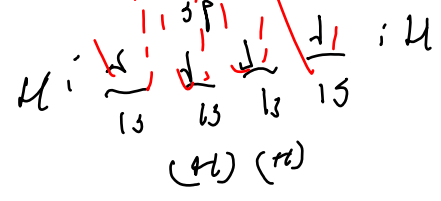
one orbit form only 2 covalent bond  
... something is "wrong"



"excite"



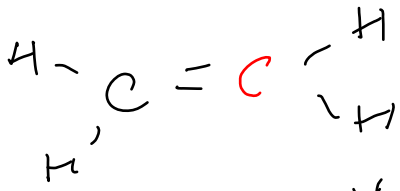
overlap of  $sp^3$  HD in C  
& s.AO in H  
etc



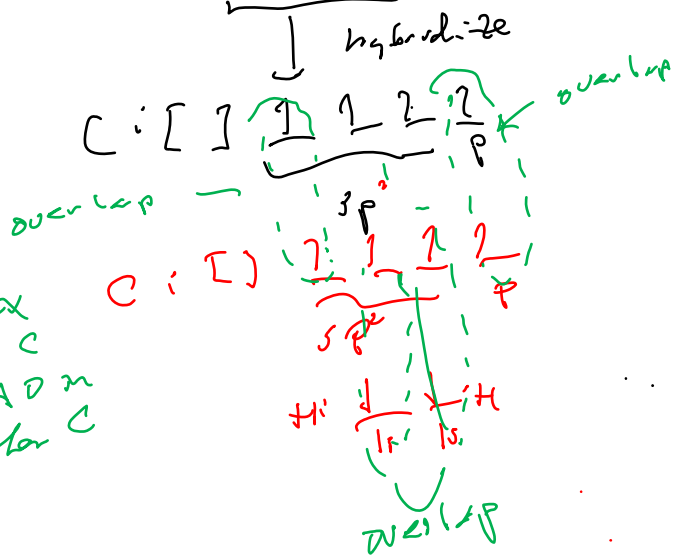
ex 5  $PF_5 \rightsquigarrow sp^3d$   
ex 6  $NF_5 \rightsquigarrow$  can't be formed b/c ...

ch 9.6  
ex 7

multiple bond: double or triple bond



bond angle  $\sim 120^\circ$



overlap of  
 $C-H$   $sp^3$  AO in C &  $s$  AO in H; ex  
 $C-C$   $sp^2$  AO in C & other  $sp^2$  AO in C  
 double bond: overlap of  $p$  AO in C &  $p$  AO in the other C

inter nuclear axis

a line/axis that connects the nuclei of adjacent atoms in a covalent bond

sigma bond: overlap of

AO &/or HO on the inter nuclear axis

pi bond

- overlap of AO &/or HO not on  
 - involve  $p$  AO