STEFANO CURTAROLO

- MULTIATOMS
- LCAO
- 2 ATOMS
- 4 ATOMS
- DEBYE-HUCKEL

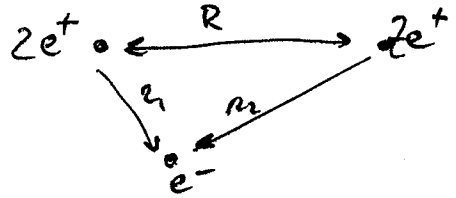
M1 - M16

H1 - H2

MULTIATOMS (MOLECULES)

1 e ⇒ 2 nuclei

LCAO



H_2^+

$$V(r_1, r_2, R) = -e^2\left[\frac{1}{r_1} + \frac{1}{r_2} + \frac{1}{R}\right] \Rightarrow$$

FROZEN IONS
BORN–OPPENHEIMER
R constant ⇒ with C.M. electrons hollow ⇒

$$\hookrightarrow E_{mol} = E_{ee}(R) + \underbrace{\frac{e^2}{R}}_{\text{nuclei}}$$

$$V(r_1, r_2) = e^2\left[-\frac{1}{r_1} - \frac{1}{r_2}\right] \Rightarrow$$

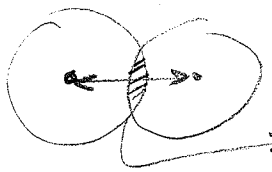
↓ function of R because $\vec{r}_2 = f(\vec{r}_1, \vec{R})$

LCAO : Linear Combination Atomic Orbitals

$a_0 \to \frac{a_0}{Z}$

ϕ_1 = wavefunction of atom 1 ⇒ GS = $\frac{1}{\sqrt{\pi a_0^3}} e^{-r_1/a_0}$ $1s_1$

ϕ_2 = wavefunction of atom 2 ⇒ GS = ↗



→ superposition (R)

R↓, super ↑, R↑, superpos ↓ exponentially

take real for simplicity

$$\psi = c_1\phi_1 + c_2\phi_2 \Rightarrow \text{to normalize}$$

$$\hat{H}\psi = E\psi \qquad H|\psi\rangle = E|\psi\rangle$$

$$\bar{E} = \frac{\int \psi^* \hat{H} \psi \, dV}{\int \psi^* \psi \, dV} = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} =$$

$$= \frac{\int (c_1\phi_1^* + c_2\phi_2^*)\hat{H}(c_1\phi_1 + c_2\phi_2)\, dV}{\int (c_1\phi_1^* + c_2\phi_2^*)(c_1\phi_1 + c_2\phi_2)\, dV} \Rightarrow$$

COULOMB INTEGRALS $H_{ii} \equiv \int \phi_i^* \hat{H} \phi_i \, dV$

BOND INTEGRAL $H_{ij} \equiv \int \phi_i^* H \phi_j \, dV$ } for numerator

(SUPERPOSITION) OVERLAP INTEGRAL $S_{ij} = \int \phi_i^* \phi_j \, dV$ } for DEN

$S_{ii} = 1$ (normalization)

same for symmetry

$$\Rightarrow E = \frac{c_1^2 H_{11} + c_2^2 H_{22} + c_1 c_2 (H_{12} + H_{21})}{c_1^2 + c_2^2 + c_1 c_2 (S_{12} + S_{21})}$$

$H_{12}(R \to \infty) \to 0$

$S_{12}(R \to \infty) \to 0$

$$E_{LCAO} = \frac{c_1^2 H_{11} + c_2^2 H_{22} + 2 c_1 c_2 H_{12}}{c_1^2 + c_2^2 + 2 c_1 c_2 S_{12}}$$

Variational principle: solution of the problem $\left(\frac{\delta E}{\delta \psi} = 0\right) \Rightarrow$ minimize E over all possible choices of ψ (guesses)

$$\Rightarrow \frac{\partial E}{\partial c_1} = \frac{\partial E}{\partial c_2} = 0 \quad \text{, minimize}$$

$$\frac{\partial E}{\partial c_1} = 0 \Rightarrow \frac{1}{D}\frac{\partial N}{\partial c_1} - \frac{N}{D^2}\frac{\partial D}{\partial c_1} = 0 \quad * D^2 \Rightarrow \frac{\partial N}{\partial c_1} - E\frac{\partial D}{\partial c_1} = 0$$

$$\Rightarrow 2c_1 H_{11} + 2c_2 H_{12} - E(2c_1 + 2c_2 S_{12}) = 0$$

$$\begin{cases} c_1(H_{11} - E) + c_2(H_{12} - E S_{12}) = 0 \\ c_1(H_{12} - E S_{12}) + c_2(H_{22} - E) = 0 \end{cases}$$

and $\frac{\partial E}{\partial c_2} = 0$ is?

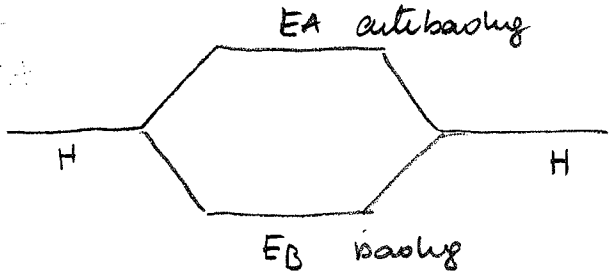
$H = H_{11} + H_{22}$ COULOMB is identical for H_2^+

$$\Rightarrow \begin{bmatrix} (H_{11} - E) & (H_{12} - E S_{12}) \\ (H_{12} - E S_{12}) & (H_{22} - E) \end{bmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = 0$$

$\det(\,) = 0$ secular order equation 2 solutions

$$E_A = H + \left(\frac{H_{12} - H S_{12}}{1 + S_{12}}\right) \uparrow \quad c_1 = -c_2$$

$$E_B = H - \left(\frac{H_{12} - H S_{12}}{1 - S_{12}}\right) \downarrow \quad c_1 = c_2$$

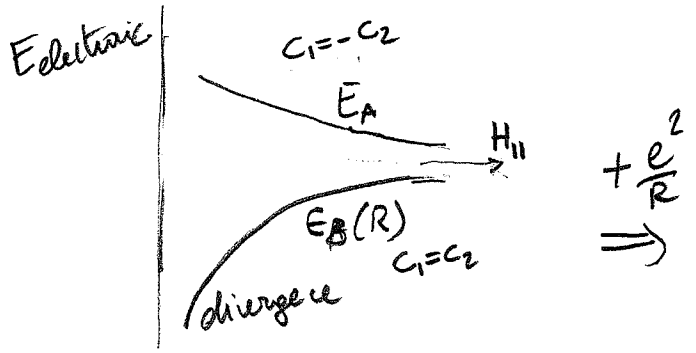


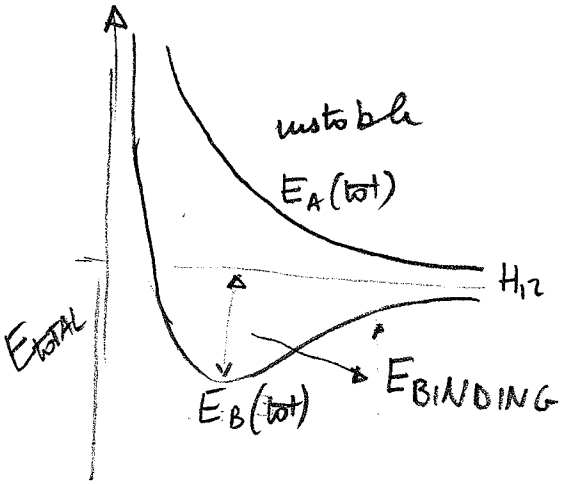
$H_{12}(R\to\infty)\to 0$

$S_{12}(R\to\infty)\to 0$

$S_{12}(R\to 0)\to 1$

$S(R\to 0)\to 1 \Rightarrow$



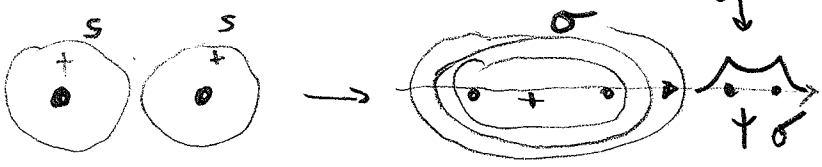


total E = $E_{electronic} + E_{ions}(R)$

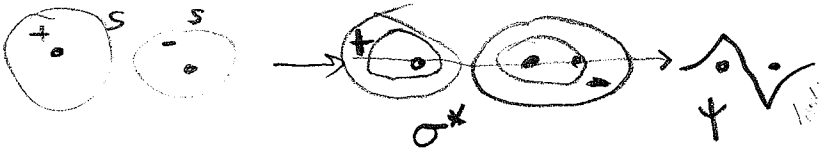
$= \frac{e^2}{R^*}$

stabile

$\psi_B = c_1(\phi_1+\phi_2)$ $\quad \psi^2$



$\psi_A = c_1(\phi_1-\phi_2)$ $\quad \psi^2$

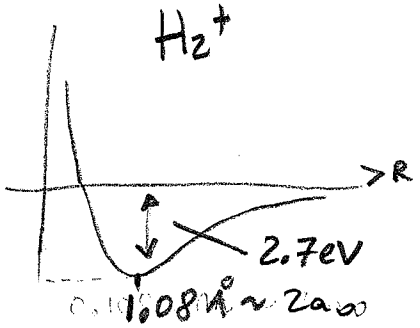


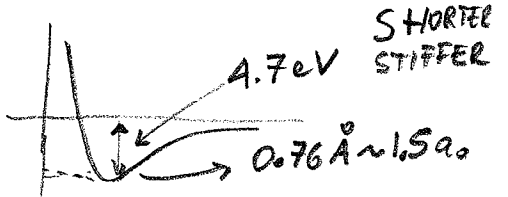
$s + s \to \sigma + \sigma^*$

$p + p \to (\pi + \pi^*)\ \&\ (\sigma + \sigma^*)$

$d + d \to$ troubles in solids (need $e_g + t_{2g}$)

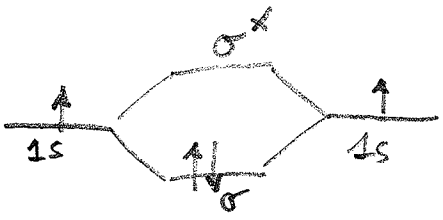
$f + f \to$ more troubles.

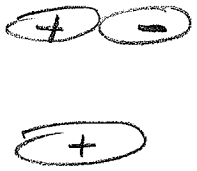




LITHIUM

H_2

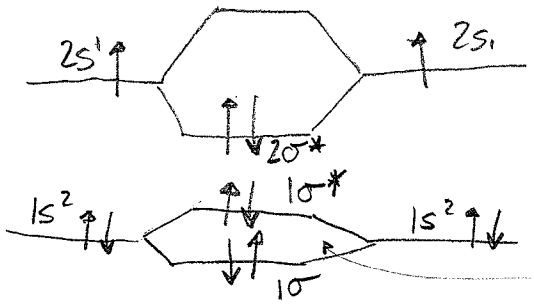




$$E_A = H + \frac{(H_{12} - HS_{12})}{1 + S_{12}}$$

$$E_B = H - \frac{(H_{12} - HS_{12})}{1 - S_{12}}$$

Li_2 $1s^2 2s^1$

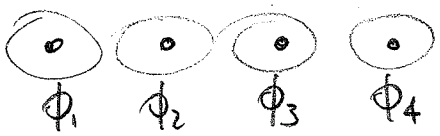


deeper electrons ⇒

$S(1s) < S(2s)$ ⇒

opening is smaller

Li_4 now there are 4 atoms

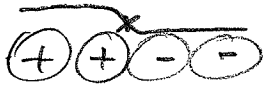


⇒ solution $\psi = \sum c_i \phi_i$

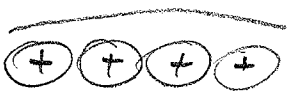
all c > 0 for convention

$\psi_4 = c_{41}\phi_1 - c_{42}\phi_2 + c_{43}\phi_3 - c_{44}\phi_4$ 3 nodes A

$\psi_3 = c_{31}\phi_1 - c_{32}\phi_2 - c_{33}\phi_3 + c_{34}\phi_4$ 2 nodes S

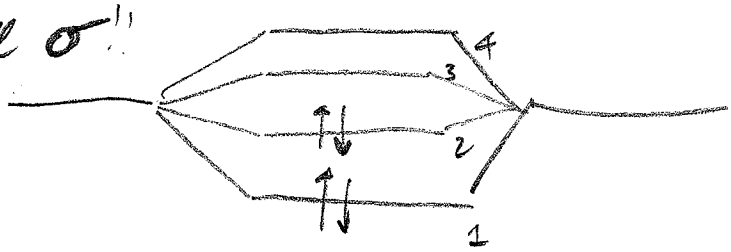


$\psi_2 = c_{21}\phi_1 + c_{22}\phi_2 - c_{23}\phi_3 - c_{24}\phi_4$ 1 node A



$\psi_1 = c_{11}\phi_1 + c_{12}\phi_2 + c_{13}\phi_3 + c_{14}\phi_4$ 0 nodes S

spherical, all σ!!



MORE COMPLICATE STRUCTURES!

LCAO $(H_{ii}, H_{ij}, S_{ij}) \Longrightarrow$ DEBYE HUCKEL MODEL (α, β)

$H_{ii} = \int \phi_i \hat{H} \phi_i \, dV \Longleftrightarrow \alpha$ all identical atoms

COULOMB

$H_{ij} = \int \phi_i \hat{H} \phi_j \, dV \Longrightarrow = \begin{cases} \alpha & |i-j|=0 \quad \text{same} \\ \beta & |i-j|=1 \quad \text{first neighbours} \\ 0 & \text{elsewhen} \end{cases}$

BOND

$S_{ij} = \int \phi_i \phi_j \, dV \Longrightarrow = \begin{cases} 1 & |i-j|=0 \quad \text{normalization} \\ 0 & \text{elsewhere} \end{cases}$

OVERLAP

NO OVERLAP drastic? yes but works

for $H_2 \Rightarrow \begin{vmatrix} H_{11}-E & H_{12}-ES_{12} \\ H_{12}-ES_{12} & H_{22}-E \end{vmatrix} \begin{pmatrix} c_1 \\ c_1 \end{pmatrix} = 0 \Rightarrow \begin{vmatrix} \alpha-E & \beta \\ \beta & \alpha-E \end{vmatrix} \Rightarrow 0$

$(\alpha-E)^2 - \beta = 0$

$\Rightarrow E \quad \cancel{\alpha-\beta} \quad \cancel{\alpha+\beta}$

for $Li_4 \Rightarrow \begin{vmatrix} \alpha-E & \beta & 0 & 0 \\ \beta & \alpha-E & \beta & 0 \\ 0 & \beta & \alpha-E & \beta \\ 0 & 0 & \beta & \alpha-E \end{vmatrix} \Rightarrow \det = 0$

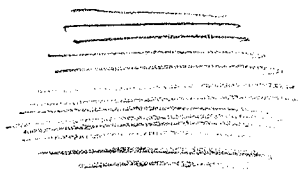
β is negative

$E = \begin{cases} \alpha-1.6\beta \\ \alpha-0.6\beta \\ \alpha+0.6\beta \\ \alpha+1.6\beta \end{cases}$

$\alpha - 2\beta$

$N \to \infty$

E = continuum



E_F

$\alpha + 2\beta$

Solution

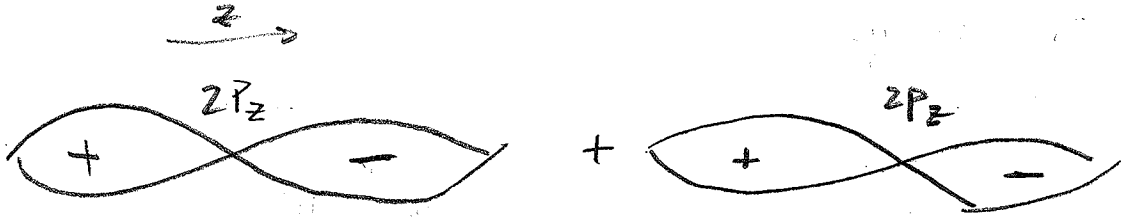
$$\psi_i = \sum_j c_{ij}\phi_j \qquad c_{ij} = \sqrt{\frac{2}{N+1}}\sin\left(\frac{\pi ij}{N+1}\right)$$

$$E_i = \alpha + 2\beta\cos\left(\frac{\pi i}{N+1}\right)$$

DEBYE HUCKEL MODEL.

↳ MORE NODES, WIGGLES ⇒ higher energy

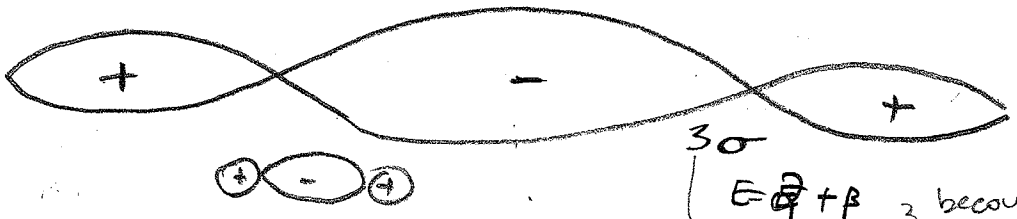
what about if I mix P orbitals?



SIMMETRIC PROBLEM

⇒ 2 SOLUTION SYMM & ANTI

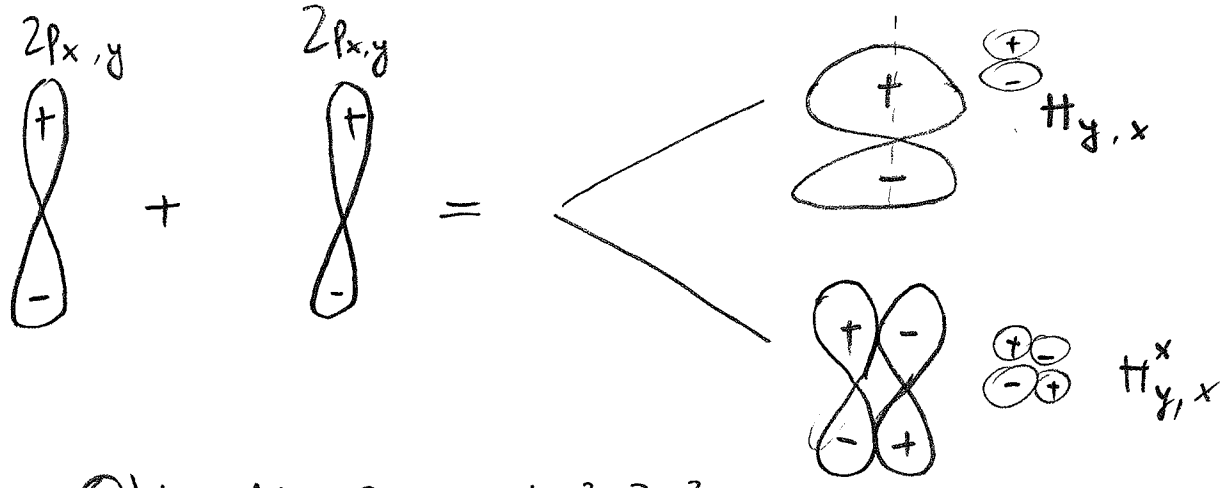
SIMM E_σ lower energy



$E = \alpha + \beta$ 3 because $1s \to 1\sigma$, $2s \to 2\sigma$, $2p \to 3\sigma, \pi$

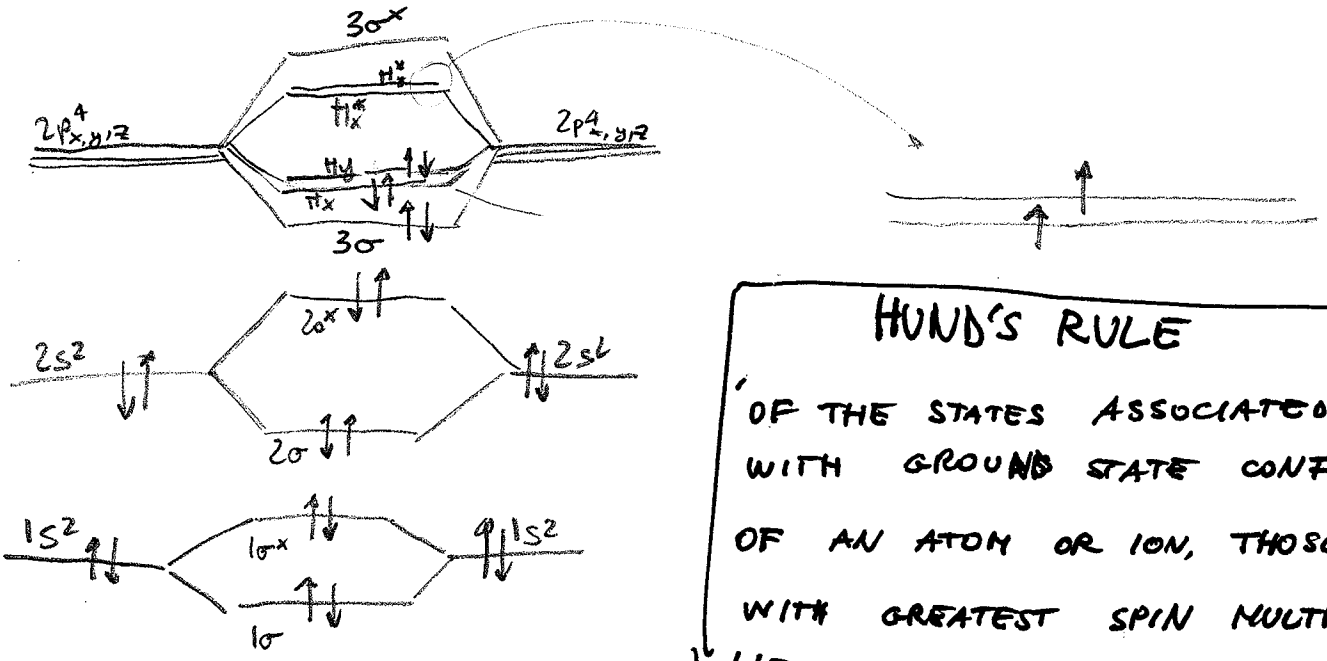
ANTI E_σ Higher energy

$E = \alpha - \beta$



OXIGEN O_2 $1s^2\ 2s^2\ 2p^4$

eigth electron:



HUND'S RULE

OF THE STATES ASSOCIATED WITH GROUND STATE CONFIGURATION OF AN ATOM OR ION, THOSE WITH GREATEST SPIN MULTIPLICITY LIE DEEPEST IN ENERGY

— LIFE ⇒ O_2 gets close to ENHOGLOBINE !

⇒ O_2 is PARAMAGNETIC , S_2 again

N_2 $1s^2\ 2s^2\ 2p^3$ is DIAMAGNETIC ! !

F_2 $1s^2\ 2p^2\ 2p^5$ is DIA ' .

— FOR O_2, F_2 $3\sigma \downarrow$ of π

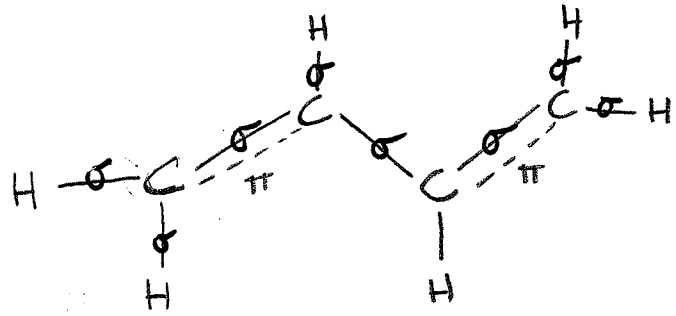
— FOR Li_2 to N_2 $\pi \downarrow$ then 3σ

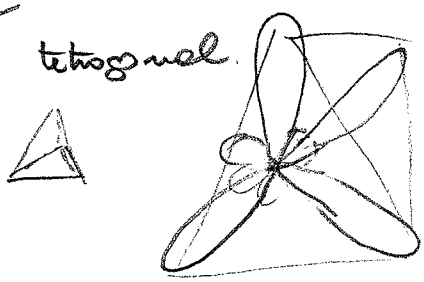
MF

BUTADIENE

$C = 1s^2\ 2s^2\ 2p^2$

sp^3 tetragonal

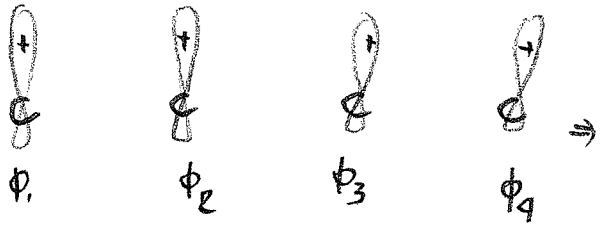




$= \sigma, \sigma^*$

$= \pi, \pi^*$

where are such π? localized?



$\phi_1 \quad \phi_2 \quad \phi_3 \quad \phi_4$

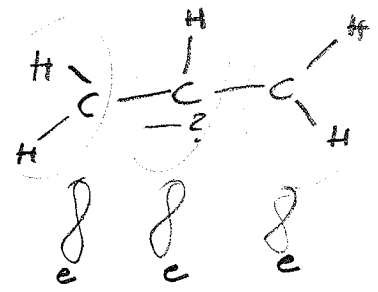
E	NODES			
	3		$\psi = c_1\phi_1 - c_2\phi_2 + c_3\phi_3 - c_4\phi_4$	$\alpha + 1.6\beta$
	2		$\psi = c_1\phi_1 - c_2\phi_2 - c_3\phi_3 + c_4\phi_4$	$\alpha - 0.6\beta$
	1		$\psi = c_1\phi_1 + c_2\phi_2 - c_3\phi_3 - c_4\phi_4$	$\alpha + 0.6\beta$
	0		$\psi_1 = c_1\phi_1 + c_2\phi_2 + c_3\phi_3 + c_4\phi_4$	$\alpha + 1.6\beta$

delocalized

$$\begin{vmatrix} \alpha-E & \beta & 0 & 0 \\ \beta & \alpha-E & \beta & 0 \\ 0 & \beta & \alpha-E & \beta \\ 0 & 0 & \beta & \alpha-E \end{vmatrix} \Rightarrow x = \frac{\alpha-E}{\beta} \quad \begin{vmatrix} x & 1 & 0 & 0 \\ 1 & x & 1 & 0 \\ 0 & 1 & x & 1 \\ 0 & 0 & 1 & x \end{vmatrix}$$

ALLYL

PLANAR



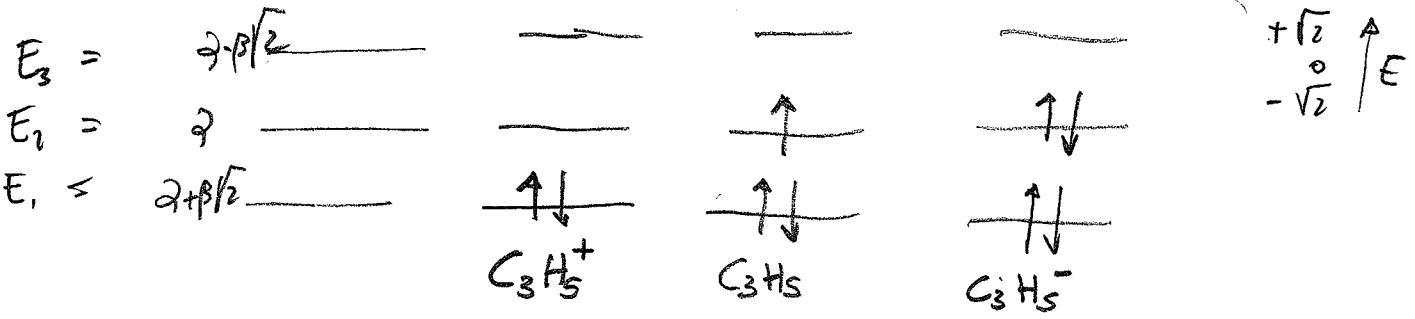
$x \equiv (\alpha - E)/\beta$

$$\begin{vmatrix} x & 1 & 0 \\ 1 & x & 1 \\ 0 & 1 & x \end{vmatrix} \Rightarrow \det = 0$$

$x^3 - 2x = 0 \quad \begin{matrix} x = 0 \\ x = \sqrt{2}, -\sqrt{2} \end{matrix}$

$x = \frac{\alpha - E}{\beta} \qquad E = \alpha - \beta x = \begin{cases} E = \alpha \\ E = \alpha \pm \sqrt{2}\beta \end{cases}$

$\beta < 0$



c? ψ_1

$$\begin{vmatrix} x & 1 & 0 \\ 1 & x & 1 \\ 0 & 1 & x \end{vmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = 0$$

$E_1 (x = -\sqrt{2}) \Rightarrow$

$$\begin{cases} c_1\sqrt{2} + c_2 + 0 = 0 \\ c_1 + c_2\sqrt{2} + c_3 = 0 \\ 0 + c_2 + c_3\sqrt{2} = 0 \end{cases}$$

remember $c_1^2 + c_2^2 + c_3^2 = 1$

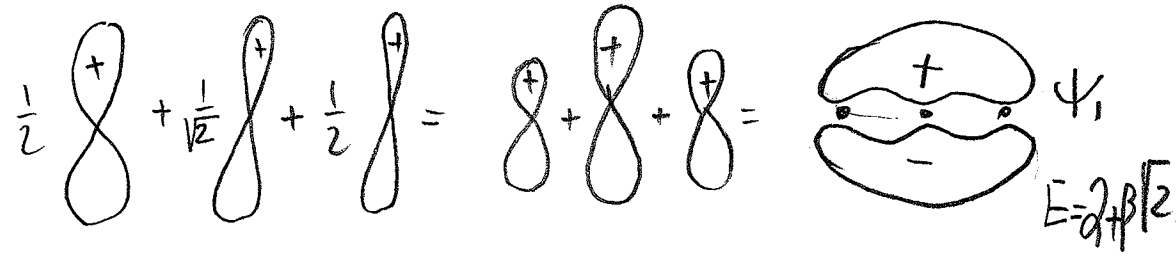
$c_1 = c_3$ from (1)-(3)

$c_2 = c_1\sqrt{2}$ from (2)

$(1, \sqrt{2}, 1) \Rightarrow \left(\frac{1}{2}, \frac{1}{\sqrt{2}}, \frac{1}{2}\right)$

$\sqrt{1 \; 2 \; 1} \Rightarrow 4 = 2$

$$\psi_1 = \frac{1}{2}\phi_1 + \frac{1}{\sqrt{2}}\phi_2 + \frac{1}{2}\phi_3$$

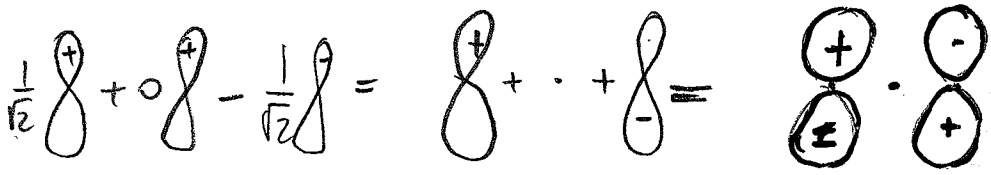


MG

ψ_2 ?

$$\begin{vmatrix} x & 1 & 0 \\ 1 & x & 1 \\ 0 & 1 & x \end{vmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = 0 \quad \overset{x=0}{\Rightarrow} \quad \begin{cases} c_2 = 0 \\ c_1 + c_3 = 0 \\ c_2 = 0 \end{cases} \Rightarrow \quad (1, 0, -1) \Rightarrow \left(\frac{1}{\sqrt{2}}, 0, -\frac{1}{\sqrt{2}}\right)$$

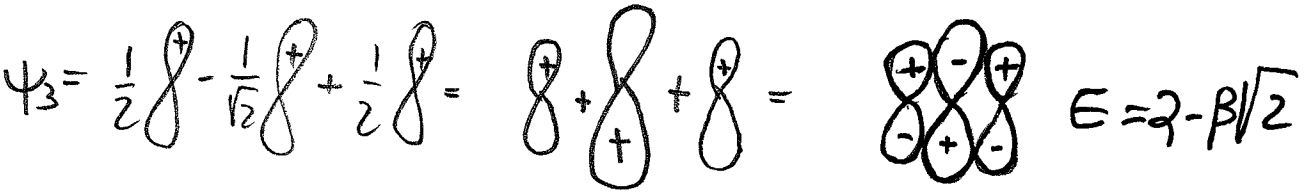
$$\Rightarrow \psi_2 = \frac{1}{\sqrt{2}}\phi_1 + 0\phi_2 - \frac{1}{\sqrt{2}}\phi_3 \Rightarrow$$



$E = \alpha$

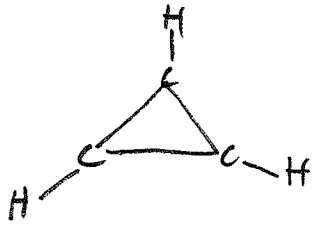
ψ_3

$$\begin{vmatrix} x & 1 & 0 \\ 1 & x & 1 \\ 0 & 1 & x \end{vmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = 0 \quad x = \sqrt{2} \quad \begin{cases} c_1\sqrt{2} + c_2 = 0 \\ c_1 + \sqrt{2}c_2 + c_3 = 0 \\ c_2 + \sqrt{2}c_3 = 0 \end{cases} \Rightarrow \left(\frac{1}{2}, -\frac{1}{\sqrt{2}}, \frac{1}{2}\right)$$



$E = \alpha - \beta\sqrt{2}$

CYCLO PROPENIL



$$\begin{vmatrix} x & 1 & 1 \\ 1 & x & 1 \\ 1 & 1 & x \end{vmatrix} \xrightarrow{\det} 0 \qquad x^3 - 3x + 2 = 0 \qquad x = -2, +1, +1$$

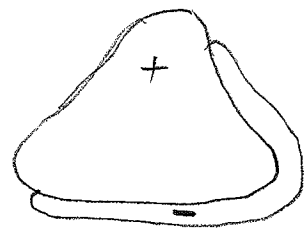
+1 is double

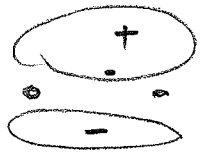
$$E = \alpha - \beta x$$

$$E_1 = \alpha + 2\beta$$

$x = -2$ $\qquad \begin{vmatrix} -2 & 1 & 1 \\ 1 & -2 & 1 \\ 1 & 1 & -2 \end{vmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = 0 \qquad \left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right)$

$\psi_1 =$ $\frac{1}{\sqrt{3}}$ (+ −) $\frac{1}{\sqrt{3}}$ (+ −) $\frac{1}{\sqrt{3}}$ (+ −) $=$





$$E_2 = E_3 = \alpha + \beta$$

$$\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \text{↓ double}$$

$c_1 + c_2 + c_3 = 0$ ⇐ plane in $(c_1 c_2 c_3)$

$c_1^2 + c_2^2 + c_3^2 = 1$ (norm)

~~get~~

get 2 vectors in the plane $v_1 = (1, -1, 0)$ and orthogonal

$v_2 = (1, 0, -1)$

⇒

M11.

$|V_1| = 1$ $\qquad$ $|V_2| = 1$

$V_1 = \left(\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}, 0\right)$ $\qquad$ $V_2 = \left(\frac{1}{\sqrt{2}}, 0, -\frac{1}{\sqrt{2}}\right)$

$V_1 \cdot V_2 = \frac{1}{2} \Rightarrow$ not orthogonal $\Rightarrow$

$V_2^* \equiv V_2 - \underbrace{(V_1 \cdot V_2)}_{\frac{1}{2}} V_1$ $\qquad$ GRAM-SCHMIDT

$V_2^* \cdot V_1 = V_2 \cdot V_1 - (V_1 \cdot V_2)(V_1 \cdot V_1) = 0$

$V_2^* = \left(\frac{1}{\sqrt{2}}, 0, -\frac{1}{\sqrt{2}}\right) + \left(-\frac{1}{2\sqrt{2}}, +\frac{1}{2\sqrt{2}}, 0\right)$

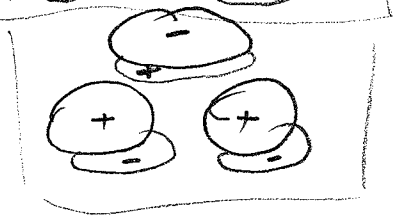
$= \frac{1}{2\sqrt{2}}(1, 1, -2)$ $\qquad$ $|V_2^*| = \sqrt{\frac{6}{4 \cdot 2}} = \sqrt{\frac{3}{4}} = \frac{\sqrt{3}}{2}$

$\Rightarrow$

$$V_2 = \frac{1}{\sqrt{6}}(1, 1, -2)$$

$$V_1 = \left(\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}, 0\right)$$

$\psi_2 =$ 

$\psi_3 =$ 

and all linear combinations!

$\Rightarrow E$

$\alpha-\beta$ $\qquad$ $\alpha-\beta$ or ?

$\alpha+2\beta$ $\uparrow\downarrow$

M12

CYCLIC DEBYE HUCKEL

Linear chain N (open)

$$\begin{vmatrix} x & 1 & 0 & & \\ 1 & x & 1 & & \\ & 1 & x & 1 & \\ & & 1 & \ddots & 1 \\ 0 & & & 1 & x \end{vmatrix} \Rightarrow$$

$$x_i = -2\cos\left[\frac{i\pi}{N+1}\right] \Rightarrow c_{ij} = \sqrt{\frac{2}{N+1}}\sin\left(\frac{\pi ij}{N+1}\right)$$

i = ORBITAL INDEX $i=[1,\dots N]$

$j=[1,N]$ ATOM INDEX

$$E_i = \alpha - x_i\beta$$

Cyclic polyene

$$\begin{vmatrix} x & 1 & & & 1 \\ 1 & x & 1 & & \\ & 1 & x & 1 & \\ & & 1 & \ddots & 1 \\ 1 & & & 1 & x \end{vmatrix} \Rightarrow$$

$$x_i = -2\cos\left(\frac{2\pi i}{N}\right)$$

~~$c_{ij} = \sqrt{\frac{1}{N}}\, e^{i\left(\frac{2\pi ij}{N}\right)}$~~

- Real = unique
- complex $\Rightarrow$ degenerate, one has to take linear combination to have real coefficients

$\Leftarrow$ $c_{ij} = \sqrt{\frac{1}{N}}\, e^{i\left(\frac{2\pi i(j-1)}{N}\right)}$

i = ORBITAL $[1\dots N]$

$j=[1\dots N]$ ATOM

$\sqrt{-1}$

GRAPHICAL

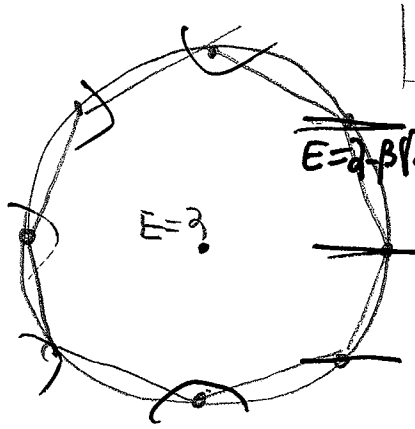
For linear : NO OUT OF DIAGONAL & "FIRST OUT DIAGONAL" elements ⇒ NO degenerate levels

N system

draw circle, centered at $E = \alpha$, radius $2|\beta|$

inscribe polyhedra with $(2n+2)$ corbons from the bottom

Allyl $n=3 \Rightarrow 2n+2 = 8$



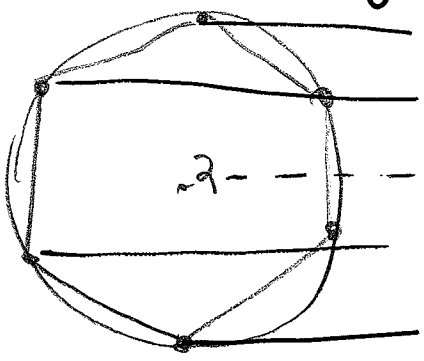
$E = \alpha + \beta\sqrt{2}$ forget, bottom and up, and degeneracies

$E = \alpha$

$E = \alpha + \beta\sqrt{2}$ ⇒ energies

FOR cyclic : inscribe polygon with N corbons

get degeneracies



$E_6 = \alpha - 2\beta$

$E_4, E_5 = \alpha - \beta$

no at $E = \alpha$ need odd number of N.

$E_2, E_3 = \alpha + \beta$

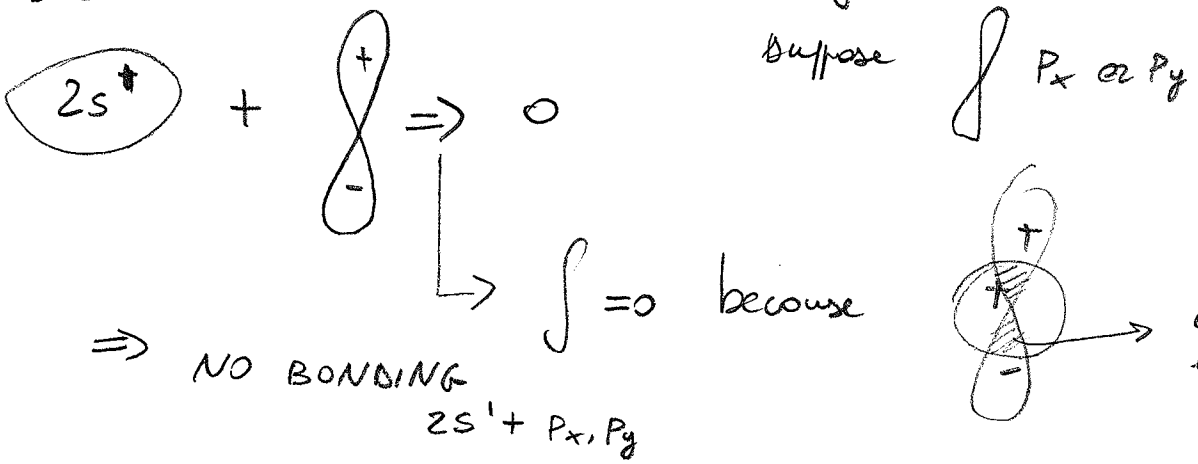
$E_1 = \alpha + 2\beta$

and fill up

BONDING OF ATOMS WITH DIFFERENT OVERLAP

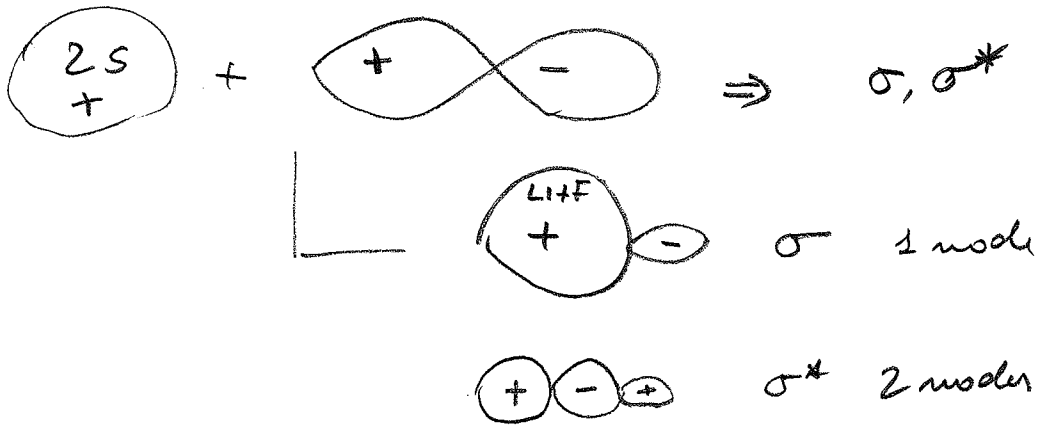
LiF Lithium Fluorine

Li $1s^2 2s$ $\quad$ F $= 1s^2 2s^2 2p^5 \Rightarrow$ only 1 e available

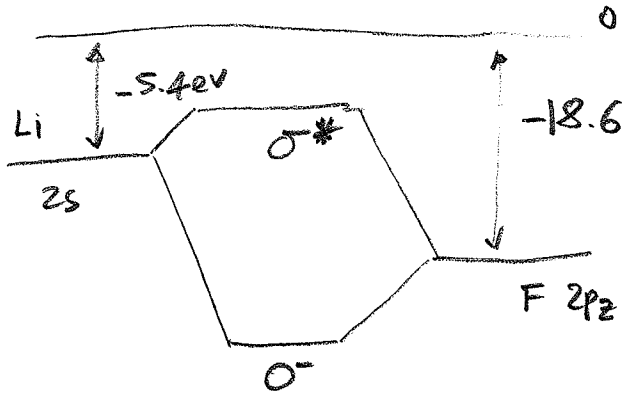


$\Rightarrow$ NO BONDING

$2s^1 + p_x, p_y$



$\Rightarrow$



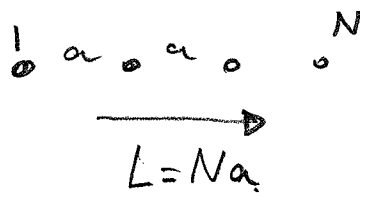
$\psi = C_{Li}\phi_{Li} + C_F\phi_F$

$\psi_{\sigma^*} \Rightarrow C_{Li} >> C_F$

$\psi_\sigma \Rightarrow C_{Li} << C_F$

M95

GENERALIZATION OF D-H for large N



$N \gg 1 \Rightarrow \sim$ periodic
expect results like periodic!

$$GS \Rightarrow \psi = \sum_j c_j \phi_j \qquad c_j = \sqrt{\frac{2}{N+1}} \sin\left(\frac{\pi j}{N+1}\right) \quad i=1$$

$$E = \alpha + 2\beta \cos\left(\frac{\pi}{N+1}\right) \quad i=1$$

$N+1 \sim N \qquad \frac{N}{j} \to \frac{Na}{ja} = \frac{L}{ja} \Rightarrow$

$$k = \frac{\pi j}{L} \Rightarrow$$

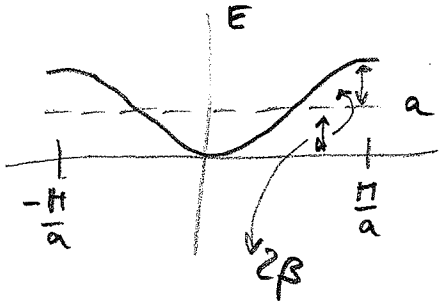
$$c_j \sim \sqrt{\frac{2}{N}} \sin\left(\frac{\pi j a}{L}\right) \simeq \sqrt{\frac{2}{N}} \sin(ka)$$

$j = 1, N \Rightarrow ka = 0, \pi$

Remember $a^* =$ fourier cycle $= \frac{2\pi}{a} \Rightarrow BZ = \left[-\frac{\pi}{a}, \frac{\pi}{a}\right]$?

$\sin(0,\pi) =$ ⌒

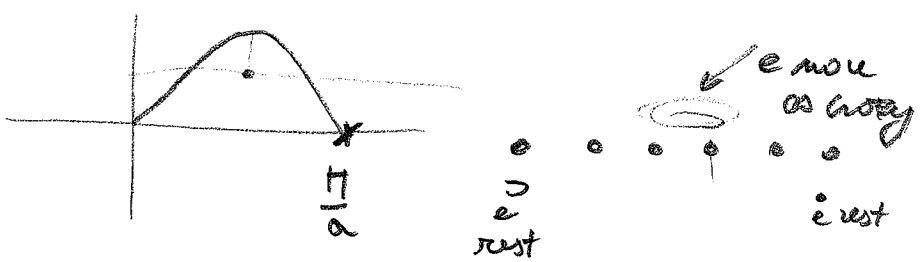
$\cos(0,\pi) \Rightarrow 1, -1$



$$E = \alpha + 2\beta \cos(ka)$$

$$k = \left[0, \frac{\pi}{a}\right]$$

$$V_{group} = \frac{1}{\hbar}\frac{\partial E}{\partial k} = -\frac{2a\beta}{\hbar}\sin(ka)$$



M16

SOLUTION OF SCF

$E_n = -\frac{13.6\, Z^2}{n^2}$ valid only for Hydrogenoid

with more electrons compute numerically

and get. $E(n, \ell)$

: 1s 2s 2p 3s 3p 4s 3d 4p 5s 4d 5p 6s 5d 4f ....

+ Fill up with HUND (level are splitted in m since L·S coupling ⇒ Zeeman)

but some orbitals have very close energy

2s & 2p ⇒ HYBRIDRATION

HYBRIDIZATION of 2s & 2p

need of least 2s, 2p but not too much : 1, 2, 3, 4, 6 symetries possible No 5

Sum of $2s^{\#} + 2p^{\#} < 5$

Max $\left[\#(2s) + \#(2p)\right] = 6 \Rightarrow$ filled no HYB

or $\left[\#(2s) + \#(2p)\right] = 5 \Rightarrow$ no possible

$\left[\#(2s) + \#(2p)\right] = 4 \Rightarrow 4e \underset{\text{Carbon}}{\Rightarrow} s^2p^2 \Rightarrow sp^3 \Rightarrow SP^3_{HYB}$

$\left[\#(2s) + \#(2p)\right] = 3 \Rightarrow 3e \underset{\text{Bozon}}{\Rightarrow} s^2p^1 \Rightarrow sp^2 \Rightarrow SP^2_{HYP}$

$\left[\#(2s) + \#(2p)\right] = 2 \Rightarrow 2e \underset{\text{Berellin}}{\Rightarrow} s^2p^0 \Rightarrow sp^1 = SP_{HYB}$

$\left[\#(2s) + \#(2p)\right] = 1 \Rightarrow$ no HYB electrons stays in 2s

H1

HYBRIDIZATION

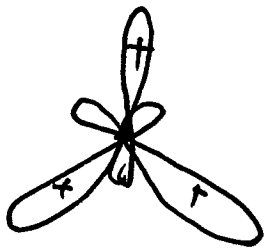
sp^1

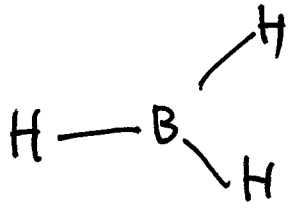
Be (or C in sp)

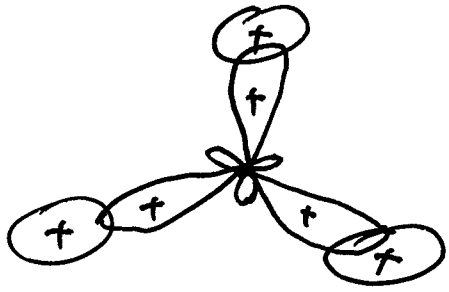
H — Be — H

sp^2

B (or C in sp^2)
trigonale

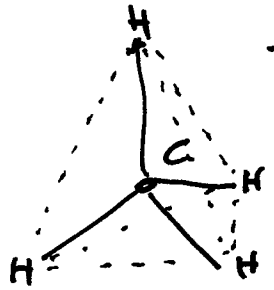






sp^3

C (diamond)



tetrahedron