CHM102
05|02|2018

Hydrogen atom:

$\hat{H}\psi = E\psi$

$\psi_{n\ell m} = N R_{n\ell}(r)\, \Phi_{\ell m}\left(\frac{x}{r}\frac{y}{r}\frac{z}{r}\right)$

$\psi_{n\ell m} = R_{n\ell}(r)\, Y_\ell^m(\theta,\phi)$

The Hydrogen atom is in it's ground state
i.e $T \to 0K$; $n=1$, $\ell=0$, $m=0$

$\psi_{n=1} = \underbrace{R_{n\ell}(r)}_{\text{Radial part}} \underbrace{Y_\ell^m(\theta,\phi)}_{\text{angular}}$ [for $1\bar{e}$]

ψ_{1s}

$= 2e^{-r}$ $\sqrt{\frac{1}{4\pi}}$

$n=2$; $\ell=0, m=0$ $\psi_{2s} = \frac{1}{2\sqrt{2}}(r-2)\, e^{-r/2}$ $\frac{1}{\sqrt{4\pi}}$

$n=2$, $\ell=1, m=1$ $\psi_{2p_z} = \frac{1}{2\sqrt{6}}\, r e^{-r/2}$ $\frac{\sqrt{3}}{r}\sqrt{\frac{1}{4\pi}} = \frac{\sqrt{3}\,(z/r)}{2\sqrt{\pi}}$

ψ_{1s} = Atomic orbital

$f(x) = \psi_{1s} = AO = \phi$

$|\psi_{1s}|^2$

Hydrogen, H_2 molecule : $H_a - H_b$

Hydrogenic-(like) function

ϕ_1 WF of H_a & ϕ_2 WF of H_b in H_2 molecule

$\psi_1 = c_1\phi_1 + c_2\phi_2$; $\psi_2 = c_1\phi_1 - c_2\phi_2$

linearly combining $\to$ two new WF; called molecular orbitals

LCAO–MO

$\int_{-\infty}^{+\infty} |\psi_1|^2 = 1$

$\int |c_1\phi_1 + c_2\phi_2|^2 = 1$

$c_1 = c_2 = c$

$\Rightarrow c^2 \int (\phi_1 + \phi_2)^2 = 1$

$$c^2 \int (\phi_1+\phi_2)^2 \, d\tau = 1$$

$$c^2 \underbrace{\int \phi_1^2 \, d\tau}_{=1=} + \underbrace{\int \phi_2^2 \, d\tau}_{=1=} + \int 2\,\underbrace{\phi_1\phi_2}_{\text{overlap integral} = S} \, d\tau = 1$$

$$c^2 \left[1 + 1 + 2S \right] = 1$$

$$c = \pm \frac{1}{\sqrt{2}} \; ; \Rightarrow \; c = \frac{1}{\sqrt{2}}$$

$$\psi_1 = \frac{1}{\sqrt{2}}\left[\phi_1 + \phi_2\right] \quad \checkmark$$ bonding MO

$$\psi_2 = \frac{1}{\sqrt{2}}\left[\phi_1 - \phi_2\right] \quad \checkmark$$ Anti-bonding MO

$$\hat{H}\psi = E\psi$$

$$\int \psi H \psi \, d\tau = \int \psi E \psi$$

$$\int \psi \hat{H} \psi \, d\tau = E \underbrace{\int \psi \psi \, d\tau}_{=1=}$$

$$E = \int \psi \hat{H} \psi \, d\tau$$

$$E = \int \frac{1}{\sqrt{2}}\left[\phi_1 + \phi_2\right] \hat{H} \frac{1}{\sqrt{2}}\left[\phi_1 + \phi_2\right] d\tau$$

$$E = \underbrace{\int \frac{1}{\sqrt{2}} \phi_1 \hat{H} \phi_1 \, d\tau}_{q} + \int \frac{1}{\sqrt{2}} \phi_1 \hat{H} \phi_2 \, d\tau + \underbrace{\int \frac{1}{\sqrt{2}} \phi_2 \hat{H} \phi_1 \, d\tau}_{\beta} + \int \frac{1}{\sqrt{2}} \phi_2 \hat{H} \phi_2 \, d\tau$$

Coulombic integral (I.P)

Resonance integrals

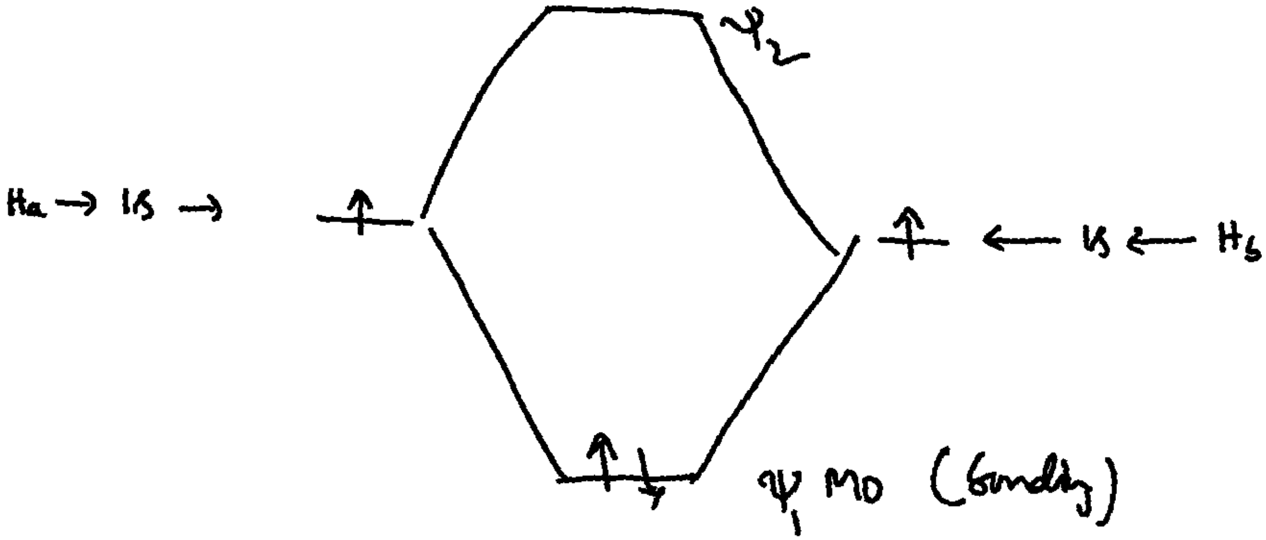
Exchange integral

$$E_1 = q + \beta$$

$$E_2 = q - \beta$$

——— E_2

——— E_1



visit http://winter.group.shef.ac.uk/orbitron/AOs/1s/index.html for orbital shapes.