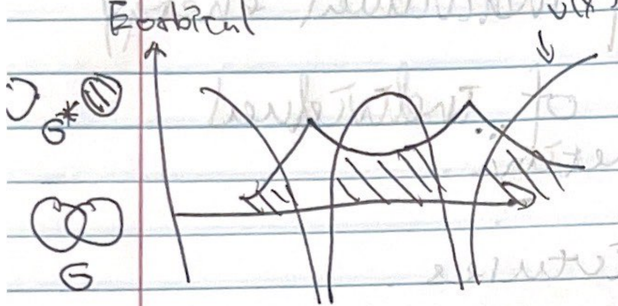
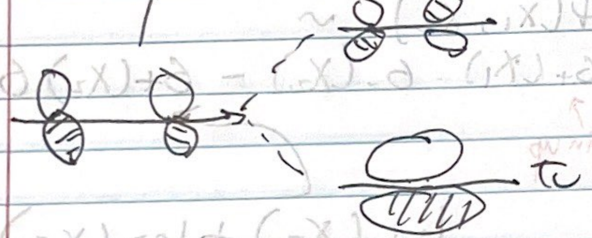
Last Time: bond and antibonding

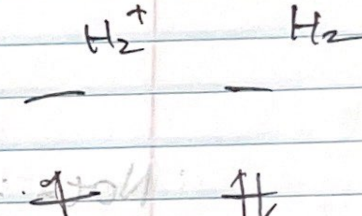


e⁻, in order to bond, is in - superposition state
- in forbidden region

similarly with P orbital



π bonds are weaker. Form σ bonds between. They are not quite putting the e⁻ between the molecules



Today: multi. e⁻ molecules

Let's talk about 2 electrons, which counts the general principle
Let e⁻ #1 satisfy $H_1\psi_1(x_1) = E_1 \psi_1(x_1)$, and e⁻ #2 satisfy $H_2\psi_2(x_2) = E\psi_2(x_2)$. If the e⁻ do not interact strongly.

What does $\psi_{total} = \psi(x_1, x_2)$ look like? E_{total}

A: By energy conservation $E_{total} = E_1 + E_2$

A: Try $\psi_{total} = \psi_1(x_1)\cdot\psi_2(x_2)$.

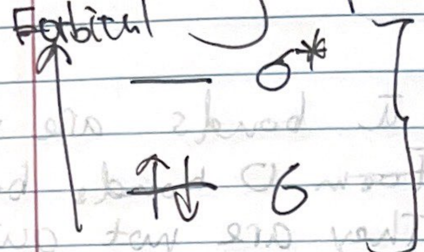
constant   constant

$$H\psi = H\psi_1(x_1)\psi_2(x_2)$$
$$= H_1\psi_1(x_1)\psi_2(x_2) + H_2\psi_1(x_1)\psi_2(x_2)$$
$$= (E_1 + E_2)\psi_1(x_1)\psi_2(x_2).$$

total E = sum of individual energy

total Ψ = product of individual wavefunction.

Meaning of our pictures.



$\Psi(x_1, x_2) \sim$

$\sigma_+(x_1) \cdot \sigma_-(x_2) - \sigma_+(x_2)\,\sigma_-(x_1)$

spin up

$1s_A(x_2) + 1s_B(x_2)$

$\sim e^{-|x_2|/a_0}$.

+

Note: need to make sure the wavefunction is antisymmetric

$$\Psi(x_1, x_2) = -\Psi(x_2, x_1)$$

Hartree-Fock wavefunction.