

Answer on Question #55173 - Chemistry - General chemistry

Question:

Consider a bonding electron in a diatomic molecule from the molecular orbital point of view. If the probabilities of finding the electron in atomic orbitals Ψ_A and Ψ_B are 0.25 and 0.75, respectively, what is the LCAO wave function for the electron (Neglect overlap).

Answer:

$$\Psi = C_1\Psi_A + C_2\Psi_B.$$

Ψ_A and Ψ_B are orthonormal which means:

$$\frac{1}{4} = \int C_1\Psi_A C_1\Psi_A dV = C_1^2$$

$$C_1 = \pm \frac{1}{2}$$

Likewise:

$$C_2^2 = \frac{3}{4}$$

$$C_2 = \pm \frac{\sqrt{3}}{2}$$

We have two possible answers:

$$\Psi = -\frac{1}{2}\Psi_A + \frac{\sqrt{3}}{2}\Psi_B$$

$$\Psi = \frac{1}{2}\Psi_A - \frac{\sqrt{3}}{2}\Psi_B$$

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