

## Normalised VB wave function and MO wave function for H<sub>2</sub> molecules:

H<sub>2</sub> molecules contains two electrons labelled 1 and 2 and two Hydrogen nuclei labelled A and B. The pairing of electrons leads to the formation of a covalent bond.

In the VB approach, if electron 1 is on nucleus A then electron 2 would be on nucleus B and vice-versa. Since however the two electrons are indistinguishable, therefore the VB wave function for H<sub>2</sub> molecule can be written as,

$$\psi_{VB} = \left(\frac{1}{\sqrt{2}}\right) [\phi_A(1) \phi_B(2) + \phi_A(2) \phi_B(1)] \quad \text{--- (1)}$$

where  $\frac{1}{\sqrt{2}}$  is the normalization constant obtained by normalizing  $\psi_{VB}$ .

In MO theory, the MO wave function for H<sub>2</sub> molecule is given by

$$\psi_{MO} = \psi_1 \psi_2 \quad \text{--- (2)}$$

where  $\psi_1$  and  $\psi_2$  are the normalized wave functions for MO's of H<sub>2</sub> given by

$$\psi_1 = \left(\frac{1}{\sqrt{2}}\right) [\phi_A(1) + \phi_B(1)] \quad \text{--- (3)}$$

$$\psi_2 = \left(\frac{1}{\sqrt{2}}\right) [\phi_A(2) + \phi_B(2)] \quad \text{--- (4)}$$

Multiplying  $\psi_1$  and  $\psi_2$  we get  $\psi_{MO}$  as

$$\psi_{MO} = \frac{1}{2} [\phi_A(1) + \phi_B(1)] [\phi_A(2) + \phi_B(2)] \quad \text{--- (5)}$$

$$= \frac{1}{2} [\phi_A(1) \phi_A(2) + \phi_B(1) \phi_B(2)] + \frac{1}{2} [\phi_A(1) \phi_B(2) + \phi_B(1) \phi_A(2)] \quad \text{--- (6)}$$

In eq<sup>n</sup> (6) the first two terms represent the probability of finding both the electrons on the same atom at the same time.

In other words, these terms represent the ionic structure of H<sub>2</sub> molecule which may be written as  $H_A^- H_B^+$  and  $H_A^+ H_B^-$ .

The last two terms represents the covalent structure of H<sub>2</sub> molecule

Comparing  $\psi_{VB}$  and  $\psi_{MO}$ . We observe that while the wavefunction in VBT does not give any weightage to ionic structures, the MOT gives equal weightage to covalent and ionic structure.