

In this week, I learned about the Valence bond theory of homonuclear diatomic, Valence Bond, and Molecular Orbital Approaches. VBT cannot describe excited states. I understood the difference between the Hamiltonian of H_2^+ ion and H_2 molecule. In Born-Oppenheimer approximation I learn Nuclei are STATIONARY with respect to electrons. Albeit difficult, can be solved using elliptical polar co-ordinate but for H_2 cannot be solved because r_{12} is not a constant in the expression of Hamiltonian of H_2 . For all the molecules except the simplest molecule H_2^+ , the Schrodinger equation cannot be solved. We get Heitler and London's equation ($\Psi = c_1\psi_1 + c_2\psi_2$) and $H_{12} = -S^2 + K$ where S = Overlap Integral ($\langle \psi_i / H \psi_i \rangle = H_{ii}$, $\langle \psi_i / H \psi_j \rangle = H_{ij}$) and K = Exchange integral we get $E_{\pm} = (J \pm K) / (1 \pm S^2)$ where J = Coulomb Integral. After normalization, we get wavefunction for H_2 is

$$\Psi = \frac{1}{\sqrt{2 \pm 2S^2}} (\psi_{A(1)}\psi_{B(2)} \pm \psi_{A(2)}\psi_{B(1)})$$

Then I learned about hybridization. Linear combination of atomic orbitals **within an atom** leads to more effective bonding. **Square** of a coefficient = **contribution** of that AO in the hybrid orbital.

Hybrid orbitals are **ortho-normal** to each other. **Equivalent** hybrid orbitals (same s-contribution, same p-contribution in each hybrid orbital) have the *same energies*. For *SP hybridization* s and p orbital both have 0.5 contributions each.