STRUCTURE AND BONDING MODELS

QUANTUM MECHANICS : The term “QUANTUM MECHANICS”is made up of two words QUANTUM+MECHANICS. The term “MECHANICS” refers to science of motion of the body. The other word is “QUANTUM” which is Latin word for “Amount” and in modern conventions is used to represent smallest possible discrete unit of any physical properity.

FUNDAMENTALS OF QUANTUM MECHANICS : The dual behaviour of matter and uncertainity principle give birth to Quantum Mechanics. These ideas inspired Schrodinger and Heisenberg and they independently formulated Quantum Mechanics in 1925,to study the behaviour of microscopic matter. At first sight, the two approaches appeared different but, later Dirac and Newman showed that in essence the two formulations are mathematically equivalent. Here, we will be discussing the basis of the schrodinger quantum theory

SCHRODINGER WAVE EQUATION [**TIME INDEPENDENT**]:

Schrodinger proposed Quantum theory to explain the behaviour of microscopic particles taking into account the wave nature of particles as suggested by Debroglie. The Schrodinger quantum theory revolves around a partial differential equation now popularly known as the schrodinger equation which describes the behaviour oif microscopic particles by means of a function called the Wave function “$\boldsymbol{\Psi}$”.

There are two forms of schrodinger equation:

1. Time dependent
2. Time independent

The wave function is a function of particles position and time , $\boldsymbol{\Psi}$(x,y,z,t), in the time dependent schrodinger equation, whereas it is a function of position only, $\boldsymbol{\Psi}$(x,y,z) in the time independent equation. The discussions are restricted to schrodinger time independent Quantum Mechanics.

Derivation of Schrodinger wave equation:

$$\boldsymbol{\Psi}=A sin\frac{2\Pi x}{\lambda} \longrightarrow 1$$

Differentiating eqn 1 partially wrt x on both sides

$$\frac{\partial\psi}{\partial x} = A\frac{2\Pi}{\lambda}\cos\frac{2\Pi}{\lambda}x \longrightarrow 2$$

Differentiating again eqn 2 partially wrt x on both sides

$$\frac{\partial^2\psi}{\partial x^2} = -A\frac{4\Pi^2}{\lambda^2}\sin\frac{2\Pi}{\lambda}x \longrightarrow 3$$

$$\frac{\partial^2\psi}{\partial x^2} = -\frac{4\Pi^2}{\lambda^2}\boldsymbol{\Psi} \longrightarrow 4$$

From de Broglies wave equation $\lambda = \frac{h}{mv}$ $\longrightarrow$ 5

Substituting eqn 5 in eqn 4

$$\frac{\partial^2\psi}{\partial x^2} = -\frac{4\Pi^2}{h^2}(m^2v^2)\psi \longrightarrow 6$$

We know that E=K.E+P.E

E=1/2mv^2+V

E-V =1/2mv^2

V^2 =2(E-V)/m $\longrightarrow$ 7

Substituting eqn 7 in eqn 6

$$\frac{\partial^2\psi}{\partial x^2} = \frac{-8\Pi^2 m}{h^2}[E-v]\psi$$

$$\frac{\partial^2\psi}{\partial x^2} + \frac{8\pi^2 m}{h^2}[E-v]\psi=0$$

This is one dimensional schrodinger wave equation

Three Dimensional Schrodinger wave equation:

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} + \frac{8\pi^2 m}{h^2}(E-V)\psi = 0$$

It is a 2nd degree differential equation

Where $\boldsymbol{\Psi}$ =wave function of electrons wave

E= Total energy of electron

V= potential energy of electron

h= plank's constant

M= mass of electron

x,y,z = cartesian coordinates

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

Where ∇^2 =Laplacian operator

$$\nabla^2\Psi + \frac{8\Pi^2 m}{h^2}(E-V)\psi$$

$$\nabla^2\Psi = -\frac{8\Pi^2 m}{h^2}(E-V)\psi$$

$$\frac{\nabla^2\psi h^2}{8\Pi^2 m} = -(E-V)\,\psi$$

$$\frac{\nabla^2\psi h^2}{8\Pi^2 m} = -\mathrm{E}\,\psi + V\,\psi$$

$$\frac{-\nabla^2\psi h^2}{8\Pi^2 m} + v\psi = E\psi$$

$$\left(\frac{-\nabla^2 h^2}{8\Pi^2 m} + V\right)\psi = E\psi$$

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

This is the reduced form of schrodinger wave equation

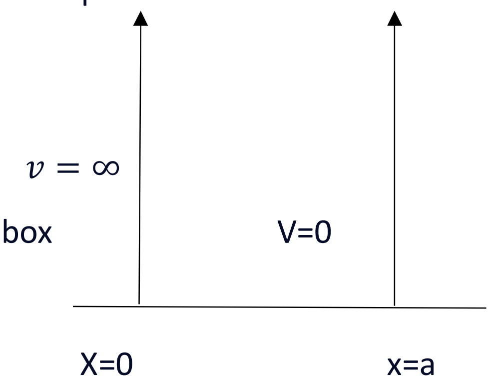
Where $\hat{H}$ =Hamiltonian operator

Wave function ψ is the store house of information . The heart of schrodinger equation is wave function which contains all the information about the system it describes.

Quantum Mechanical Study for Particle in a One Dimensional Box :

Let us suppose that a particle in a one dimensional box (so that we know its position lies within the boundary of the box). Let's say along x-axis and is restricted to move in a region of space from x=0 to x=a and that its potential energy (P.E) within box is constant and taken as equal to zero for the sake of convenience

A Particle in a one dimensional box



A Particle in a one dimensional box with P.E=0 insidethe box and P.E =∞ on the walls of the box an outside the box

The Potentail energy inside the one dimensional box can be represented as

V=0 for $0 \leq x \leq a$

V=∞ for $0 > x > a$

Schrodinger equation $\frac{\partial^2 \psi}{\partial x^2} + \frac{8\Pi^2 m}{h^2}(E - v)\psi = 0$ ———— 1

Inside the potential V=0

Then $\frac{\partial^2 \psi}{\partial x^2} + \frac{8\Pi^2 m}{h^2}(E - 0)\psi = 0$

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{8\Pi^2 m}{h^2} E\psi = 0$$

$\frac{\partial^2 \psi}{\partial x^2} + k^2 \psi = 0$ ———— 2

Where $k^2 = \frac{8\Pi^2 m}{h^2} E$ ———— 2(a)

This is the second order partial differential equation which has the General solution of the form

ψ(x)=Acoskx+Bsinkx ———— 3 (A,B,K are constants)

The wave function $\psi(x)$ should be zero everywhere outside the box since the probability of finding the particle outside the box is zero.

Similarly the wave function $\psi(x)$ must also be zero at walls of the box because the probability density ($\psi(x))^2$ must be continuous.

Thus the boundary conditions for this problem are

1. $\psi(x)$ =0 for x=0 ——— 4
2. $\psi(x)$ =0 for x=a ——— 5

Applying the boundary conditions in eqn 3

0=Acosk(0)+Bsink(0)

0=A(1)+B(0)

A=0 ——— 6

Substituting A=0 in eqn 3

$\psi(x)$ =0 *coskx+Bsinkx

$\psi(x)$ = Bsinkx ——— 7

Now applying second boundary condition in eqn 7

$\psi(x)$ =0 for x=a

0=Bsink(a)

This equation will satisfy only for certain values of k, since B cannot be taken zero. B$\neq 0$

Bsinka=0

ka =nΠ

k=$\frac{n\Pi}{a}$ $\longrightarrow$ 8

Substituting k value in eqn 7

We get $\psi(x)$ =Bsin$\frac{n\Pi}{a}(x)$ $\longrightarrow$ 9

By applying normalization condition we can findout the values of B

The Normalization equation is

$\int_0^a |\psi(x)|^2 \, dx = 1$ $\longrightarrow$ 10

Substituting eqn9 in eqn 10

$$\int_0^a B^2 \sin^2\left(\frac{n\Pi}{a}\right) dx = 1$$

$$B^2 \int_0^a \frac{1}{2}\left[1 - \cos\left(\frac{2n\Pi x}{a}\right)\right] dx = 1$$

$$\frac{B^2}{2}\left[x - \sin\left(\frac{\frac{2n\Pi x}{a}}{\frac{2n}{a}}\right)\right]_0^a = 1$$

$$\frac{B^2}{2}[(a-0)-(0-0)] = 1$$

$$\frac{B^2}{2} a = 1$$

$$B = \sqrt{\frac{2}{a}} \longrightarrow 11$$

Substituting eqn 11 in eqn 9 we get

$$\psi(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\Pi x}{a}\right) \longrightarrow 12$$

This is a wave function value (Eigen function) of the particle in one dimensional box

After calculating “Eigen values”(Energy values)

From equations 2(a) and eqn 5

$$k^2 = \frac{8\Pi^2 m}{h^2} E \qquad k^2 = \frac{n^2\Pi^2}{a^2}$$

$$\frac{8\Pi^2 m}{h^2} E = \frac{n^2\Pi^2}{a^2}$$

$$E = \frac{n^2 h^2}{8ma^2} \longrightarrow 13$$

Equations 12 and 13 are the eigen function & eigen values of the particle which is moving in one dimensional box

CASE 1 : For n=1 $\psi(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\Pi x}{a}\right)$

(Wave function)

For n=2 $\psi(x)=\sqrt{\frac{2}{a}}\,sin\left(\frac{2\Pi x}{a}\right)$

For n=3 $\psi(x)=\sqrt{\frac{2}{a}}\,sin\left(\frac{3\Pi x}{a}\right)$

CASE 2: For n=1 $E1=\frac{h^2}{8ma^2}$

(Eigen values)

For n=2 $E2=\frac{4h^2}{8ma^2}$=4E1

For n=3 $E3=\frac{9h^2}{8ma^2}$=9E1

Significance of ψ and ψ^2 :

1. The values of ψ is called wave function (or)Eigen function of the schrodinger equation
2. The wave function $\boldsymbol{\psi}$, contains all the information we want to know about a system
3. All the property of a system can be calculated from its wave function
4. The wave function $\boldsymbol{\psi}$ in the schrodinger equation represents the amplitude of the electron wave
5. The Probability of finding an electron at a given point in the 3D space is proportional to $\boldsymbol{\psi^2}$
6. Hence $\boldsymbol{\psi^2}$ gives the probability of finding an electron with energy ina given region around the nucleus
7. Those places around the nucleus can be detected where the probability of finding the electron is highest.
   Probability $=\int_a^b (\psi)^2\, dV$ = 1

$\psi(psi)$ is a wave function represented in the schrodinger wave equation which represents state of the electron.

$$\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}+\frac{8\pi^2 m}{h^2}(E-V)\psi=0$$

Where ψ^2 gives the probability density of finding the electron ina particular region in space