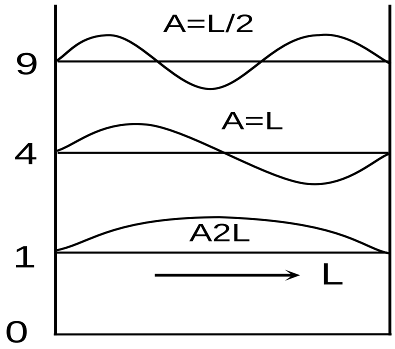
Tutorial On Introduction of nanoscience and nanotechnology-2
By
DR RAKESH KUMAR SINGH
HEAD-Academic , Nanotechnology center, AKU

FERMI ENERGY (E_F)

Fermi energy related to free electrons of a material. The force on electrons in a gas very week. According to Pauli exclusion principle. A electron of mass m confine in a box of length ℓ by infinite potential

$$E = \frac{n^2 h^2}{8mL^2}$$



eign value & eign function the wave function of electron in terms of Schrodinger equation

$$\boxed{H + \varphi = E\psi}$$

Where $\psi \varsigma$ wave function, H = eign function, E = eign values

H = T + V = k.E + P.E

$$= \frac{P^2}{2m} + 0$$

Now, $H\psi = \frac{1^2 h^2 \partial^2 \psi}{2m \partial \pi^2}$

$$H\psi = \frac{h^2 \partial^2}{2mdx^2}$$

$$E = \frac{h^2 \partial^2}{2mdx^2}$$

The wave function of an electron is determine by

$$\psi_n = A\sin\left(\frac{2\pi x}{\lambda_n}\right) \text{ when } L = \frac{n\lambda m}{2}$$

Or $\psi_n = A\sin\left(\frac{n\pi x}{L}\right)$ when A is a con…………

Thus, $E_n = \frac{h^2}{2m}\left(\frac{n\pi}{L}\right)^2$

This is the energy level of from electron of mass m confined to length. Now in a matter these various electrons having with some energy levels. Suppose N is the total no. of electron of represent the total top most field energy level. A/c to phy quantum principal each energy levels with quantum n accommodate 2 electrons with spin up & down in that case

$$E_n = \frac{h^2}{2m}\left(\frac{n\pi}{L}\right)^2$$

For n electron $\varepsilon_P = \frac{h^2}{2m}\left(\frac{N\pi}{L}\right)^2$

This energy is called the fermi energy which was determine by the scientist Fermi This the energy of the top most field level in the ground state of N electron system at room temperature. Maximum Nobel prize given in the field of electron till now. Total energy of nth electrons in the ground state for individual electrons is given by

$$E_0 = 2\sum_{n=1}^{n=n/2} E_n \;=\; 2\sum_{n=1}^{n=n/2} \frac{h^2}{2m}\left(\frac{N^\pi}{L}\right)^2$$

$$E_0 = 2\frac{h^2\pi^2}{2mL^2} \sum_{n}^{n=n/2} n^2$$

$$= 2.\frac{\pi^2 h^2}{2mL^2} \sum 1^2 + 2^2 + 3^2 ....5^2$$

$$= 2.\frac{\pi^2 h^2 N^2}{2mL^2}\left(\frac{N}{2}\right)^3$$

$$= 2.\frac{\pi^2 h^2 N^2}{2mL^2}\frac{N}{8} = \frac{1}{3} NE_F$$

Density of state

$$D = \frac{dn}{d\varepsilon}$$

The density of state is define the no. of electronic state per will energy range. For a free electron the energy level contains two electronic state. Therefore, the density of state.

$$D = \frac{2dn}{dE}$$

$$E_n = \frac{L^2}{2m}\left(\frac{n\pi}{L}\right)^2$$

Differentiating

$$dE_n = \frac{h^2}{2n}\left(\frac{\pi}{L}\right)^2 2ndn$$

$$D = \frac{dn}{dE} = \frac{42}{n}\sqrt{\frac{m}{2E_n}}$$

Density of state Engineering (DOS)

The energy eign values of a particles is defined as

$$E = \frac{n^2 h^2}{8mL^2}$$

$$E \propto \frac{1}{L}$$

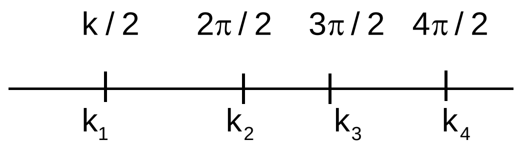
For large value of L, then the energy values may be treated as continuous. But if L is small then energy state may or may not continuous. The no. of energy Eigen state between the energy leves E & E + dE can be asked to below that actual confinement. If the energy Eigen states no. is dN then v = density of state (DOS) = g(E) dE

As low know energy is equal to

$$E = \frac{n^2 k^2}{2m}$$

$$K = \frac{n\pi}{L} = \text{wave number}$$

$$E = \frac{h^2 n\pi}{2mL}$$



For each value of k there is a each energy state

$$K = \sqrt{\frac{2mE}{h^2}}$$

$$dk = \sqrt{\frac{m}{2h^2}}\, E^{-1/2}\, dE$$

$$g(\in)\, dE = \frac{dN}{dE}$$

The no. of state between the energy level $E \,\&\, E + dE$ is $\frac{dk}{(\pi/2)}$, this is because the move no.K + dk in the given state is Equivalent to E + dE. Therefore the no. of states in the energy level E to E + dE will los same as the k & k- dt

$$dN = \frac{dk}{\pi / L} = \sqrt{\frac{m}{2h^2}}\; E^{1/2}\, dE$$

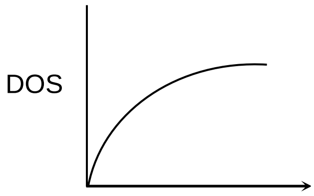
$$\Rightarrow \quad \frac{1}{L}\frac{dN}{de} = \sqrt{\frac{m}{2h^2}}\; E^{-1/2}$$

This result shows the density of state decreases as we suppose higher & higher energy. According to quantum confinement energy is proportional to h^2. The higher volume of n.

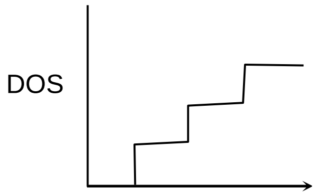
$$(n+1)^2 - n^2 = 2n + 1$$

Kips on increasing so that spacing between energy eign volume increases. Similar way, the density of state for two dimensional box is independent of energy.

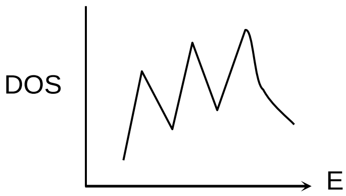
$$\frac{1}{L}\frac{dN}{dE} = \frac{m}{2h^2\pi}$$



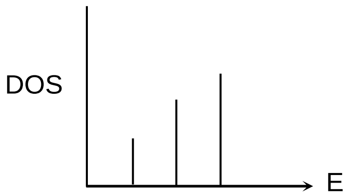
Energy for
Bask



Quantum well



Quantum wire



Quantum det

Quantum wire is a size of material in which electron is allowed to move in one direction, two dimensional is called quantum well, The quantum dot is a electronic structure in which electron are completely confined in there direction of space that can be electrostatics. The size of the quantum dot wavelength of electron. Such material have very individual application in electronic computes sciences bio-technology

<u>The size of quantum dot.</u>

As we know that energy level of quantum dot.

$$\Delta E = E_2 - E_1 = \frac{(2n+1)\,h^2}{2\,mL^2}$$

$$\Delta E = \text{minimum} \;\; n = 0 \;\; \Delta E = \frac{h^2}{8mL^2}$$

$$h = 1 \quad C = \frac{3h^2}{8mL^2}$$

This energy is much greater than thermal energy of room temperature

$$\frac{3h^2}{8mL^2} > kT$$

$$8mL^2 kT < 3h^2$$

$$L < \sqrt{\frac{3h^2}{8mkT}}$$

$$L \propto \frac{1}{\sqrt{T}}$$

SIZE MATTERS IN BIOLOGY

Generally all biological actions are operate in nanos scale. The size of a DNA molecules are nanometer scale . The surface reactivity is defined as

$$\frac{S}{V} \propto \frac{4\pi r^2}{\frac{4}{3}\pi r^3} \propto \frac{1}{r}$$

Metabolism or heat generation in biological sciences is dependent on number of cells or volume (m^3). The heat loss to the environment is proportional to the surface are, (L^2). The surface by volume ratio is proportion to $\frac{L_2}{L_3} \propto \frac{1}{2}$. For smaller organism, heat generation and heat loss proportional to ½. Among eminence of electromagnetic force quantum confinement, surface reactivity the random (prawning) motion of surfaces Plasmon resonance (SPR).

NANOCLUSTER & NANOMATERIALS

The nanomaterials are molecular structure whose sizes are is in between 1nm – 100 nm and These can be visualize using electron microscope. Generally any nano-object consent of 10^8 atoms or molecules less .While the object consent of up to 10^3 atoms /molecular are called cluster & them size should be less than 10 nm. These cluster may be connected with magic number (Hore the magic number should the structure of nanomaterials).The shape of the atom is assumed to be spherical Å then properties depend upon significant influence of the surface reactivity. Suppose, the number of surface atoms spherical m shape consent of 'N' atoms where Na = Avogadro's Number

The volume of such cluster is given by

$$\left(v = \frac{4}{3}\pi R^3\right) N = v_0 N$$

Where r = radius of atoms where v_0 =volume of individual atoms having radius (a)

$$v_0 = \frac{4}{3}\pi a^3$$

In that case the size cluster & radius of individual atoms are related as

$$R = aN^{1/3}$$

The average radius of the atom radius of the atom is 0.1nm, then according to the formula

$R = aN^{1/3}$, the cluster containing of 10^3 atoms, R = 10a = 10 × 0.1 nm = 1 nm. For such cluster, the line is significantly longer. The surface area of cluster

$$A = 4\pi a^2 \ N^{2/3} = So \quad A = 4\pi R^2$$

If the number of atoms on the surfaced of centre is N/s, then s = total surface area

$$S = NS_0 \ = \ 4\pi a^2 \ Ns$$

$$= \ 4\pi a^2 \ \ Ns$$

The ratio of number of atoms on the surface of a to the number of total no. of atom.

$$\frac{Ns}{N} = \frac{S_0 V_0}{S_0 V} \ = \ \frac{4\pi a^2 N^{2/3} \times 4\pi a^3}{}$$

$$\frac{Ns}{N} = \frac{S V_0}{S_0 V} \ = \ \frac{NS_0 \ V_0}{S_0 \ V} \ = \ \frac{N.\frac{4}{3}\pi a^3}{\frac{4}{3}\pi r^3}$$

$$\frac{Ns}{N} = \frac{Na^3}{(aN^{1/3})} = \frac{Na^3}{a^3 N}$$

$$\frac{Ns}{N} = \frac{1}{N^{1/3}} \qquad\qquad Ns = \frac{N}{N^{1/3}}$$

This equations shows the proportion of atoms on the surface of a Centre decreases with increasing Centre size provided the size of Centre is ten then 100 nm. In such cases the bond routine reactivity can be explained by using quantum science. This can be justify when the size of a region of electron motion is comparable to the deforming wave length of electron.

Examples

An electron is confined in a cubical box, size $\ell \ = \ 1\mu m \ = \ 10^{-6} m$. Then find the distance between the energy length $E_{113} \ \& \ E_{122}$. Compare this energy with thermal energy at mom temperature. As we know, according to thermodynamics the average thermal energy of electron at mom temp.

$$F_{th} = \frac{3}{2}kT = 38.4\,\text{MeV}$$

According quantum science, the energy of an electron.

$$E_{113} = \frac{n^2 h^2}{8mL^2}\,(nx^2 + ny^2 + nz^2)$$

$$= \frac{n^2 h^2}{8mL^2}\,(1^2 + 1^2 + 3^2)$$

Similarly the magnitude of energy in quantum state (122) E_{122}

$$E_{122} = \frac{n^2 h^2}{8mL^2}\,(1^2 + 2^2 + 2^2)$$

$$E_{113} - E_{122} = \frac{n^2 h^2}{8mL^2} \times 2 = 8.73 \times 10^{-4}\,\text{Mev}$$

This is the energy of a electrons in a cubical box & dimension $(1\mu m \times 1\mu m \times 1\mu m)$

Wave nature of electron, Electron microscopy & Nano technology.

According to de-Broglie, electron become line a wave & wavelength is given by $\lambda = \frac{h}{P}$. The total energy of electrons , E = kinetic energy + Potential energy

$$Eu = \frac{P^2}{2m}$$

$$\frac{P^2}{2m} = \frac{1}{2}mv^2$$

In free particles, then is no inter atomic force

$$\frac{P^2}{2m} = \frac{1}{2}mv^2$$

$$\frac{h^2}{\lambda^2 2m} = \frac{1}{2}mv^2$$

$$\lambda = \frac{h}{\sqrt{2mfu}} = \frac{h}{\sqrt{2mF}} \quad (E = uE + 0)$$

$\Rightarrow$ Two thermal energy of due at room temperature is given by

$$\lambda = \frac{h}{\sqrt{2m\frac{3}{2}uT}} = \frac{h}{\sqrt{3muT}}$$

$\lambda \approx 6\,mm$ at 300 K

The condition for diffraction is that the size of obstacle should be comparable to the wavelength to the of incident radiation or electron.

FREE ENERGY THEORY

The mean free path of green gas, metal is $\lambda = \frac{1}{\sqrt{2}\,na^2}$. Generally MFP should be full same as the lattice Constant spacing a cubical lattice. If wavelength is greater than (d) $\lambda > d$ then electron are Said to be degenerate gas & classical science fairs & quantum same is applicable & such cases generally parameter is defined

$$\varepsilon = \left(\frac{\lambda}{d}\right)^3 > 1 \quad d = \text{Mean free path}$$

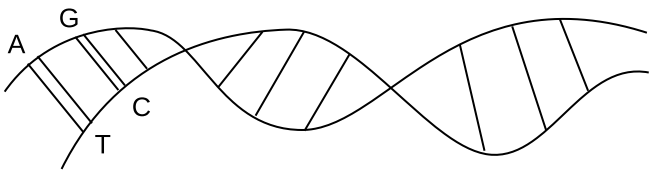
If $\in < 1$ the classical science is applicable. Two optical microscope is based on line visible light .The resolving power & optical microscope.

$$Rp = \frac{1.22\,D}{\lambda}.$$

These electron microscope and being used in medical sciences ,biomedical sciences engineering science NT & same others fields.

Q .It is very difficult to absences, the undivided atoms in the molecules of materials because the image of a double helical DNA molecules on a surface can be seen, this S.T.M is a percussion of atomic force microscope was invented on 1980, Binasal & Rohr on Novel price was given for the work.

DNA = very long molecules heavy 100 bounded to each other by a series & G-bond, looms into double helix.



Every living cell, has a nucleus, is store of genetic material, called DNA, the DNA could helix structure compost of all the genes of living organs One after another genome.