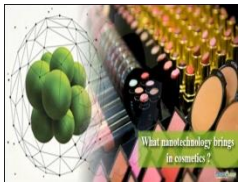
Tutorial On Introduction of nanoscience and nanotechnology-I

By
DR RAKESH KUMAR SINGH
HEAD-Academic , Nanotechnology center, AKU





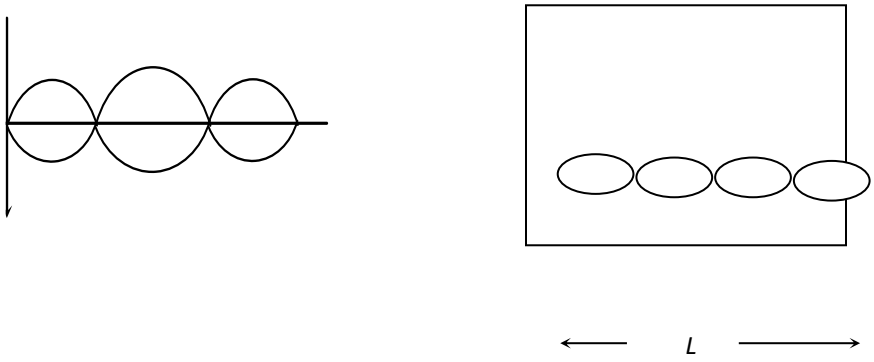


WHY NANO-MATERIALS HAVE DRASTIC CHANGES COMPARED TO BULK SIZE

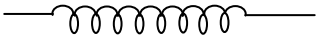
Special emergent behavior at nanoscale is due to following

(1) Quantum confinement and
(2) Surface effect

Quantum science is the study of materials at small level (molecular level, atomic level. While Classical science is the study of objects of big object which can be seen by our eyes. Confinement means motion of an electron in a certain direction. Here we will discuss motion of a particle / electron in box of length of length L.



The motion of electrons in behave like a wave, such can be seen on a Slinkey also.



slinkey

If stationary likes wave formation occurs. Then according to principle of superposition of wave , $\Delta x = n\lambda$ where λ -wavelength of wave , $\Delta x =$ path difference

Or $2L = n\lambda$

According to de broglie

$$\text{Wavelength } \lambda = \frac{h}{p}$$

The energy in terms of momentum of electron is given by

$$E = \frac{p^2}{2m}$$

$$\mathbf{E} = \frac{h^2}{\lambda 2m}$$

Or, $$E_n = \frac{h^2 n^2}{8mL^2}$$

Or, $$E_1 = \frac{h^2}{8mL^2} \qquad E_2 = \frac{4h^2}{8mL^2} \quad E_3 = \frac{9h^2}{8mL^2}$$ for n=1, 2,3

This the expression for quantum confinement**.**

Example- Using a particle in a box model, calculate how much energy in given of in the form of photon emitted, when the electrons in the atom jumps 5^{th} energy state to 4^{th} energy state. What is the wavelength of the emitted radiation, suppose radiaus of the atom is 100 pm.

Ans. According to particle in a box, wall energy of a atom

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

$$= \frac{(6.632)^2 \times 10^{-68}}{8 \times 9.1 \times 10^{-31} \times 10^{-20}}$$

$$= \frac{(6.632)^2\ 10^{-68} \times 10^{31}}{8 \times 9.1}$$

$$= \frac{6.632 \times 6.632 \times 10^{16}}{6 \times 9.1} = 1.5 \times 10^{-19} \times 9$$

$$\Delta E = 1.5 \times 10^{-18}(5^2 - 4^2)$$

$$= 1.5 \times 10^{-18}(25 - 16)$$

$$= 1.5 \times 10^{-18}$$

$$= 13.5 \times 10^{-18} \times 9 \ \text{Joule}$$

Now, wavelength of radiation emitted is

$$\lambda = \frac{hC}{\Delta E} = \frac{1242}{13.5 \times 10^{-8}} = \frac{1242 \times 10^{-19}}{13.5 \times 10^{-18}}$$ =9.2 x10^{-9} m

The emitted radiation belong to ultraviolet radiation. This result show the distribution of electrons are different in orbit, therefore the wavelength, of emitted radiations will be different. They may be in UV range, visible range, I.R range. The visible range of light is in the range of 400nm – 700

nm. Beyond visible range of light is called radiation. The UV radiation is below 400 nm & IR radiation is above 700 nm.

Example 2- It was found recently by research group of nano technology centre AKU & NIT Patna that rare earth element (Eu) doped in Nickle ferrite ($N_iFe_2O_4$) magnetic electronics materials. They found the energy bond gap was found 1.765 eV, 1.778 eV, 1.782 eV and 1.7440 evV. For molar ratio of Eu = 0.00 mole, 0.02 mole , 0.04 mole, 0.06 mole. (Reference, R. K Singh et al, J. material Chem and Phy 241 (2020) 122383)

The such changes in energy bond gap is due to quantization effect. This shows as the crystalline size changes the energy gap also found change. Such energy bond gap can be calculated using UV – visible NIR spectrometer. The crystalline size of a material determine using X-ray diffectometer (XRD) and Electron microscope.

SURFACE EFFECT

When the size of the material is reduces to small level, the more & more surface creates. The reaction probability increases because the probability of maximum reactivity is possible at the surface.

$$\frac{\text{Surface}}{\text{Volume}} = \frac{4\pi r^2}{\frac{4}{3}\pi r^2} \propto . \frac{1}{r}$$

This result shows as the size of the material reduces (R) the surface upon volume ratio increases

sides = 3
surface = 3^2 x 6 = 54
volume = 3^3 = 27

surface/volume = 2

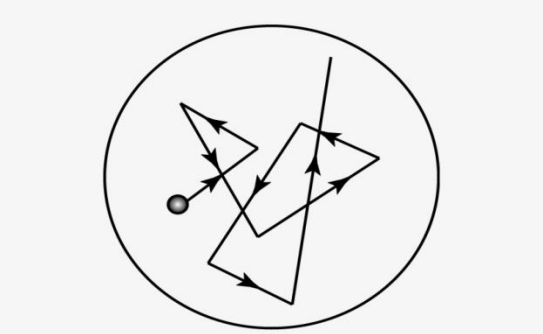
sides = 2
surface = 2^2 x 6 = 24
volume = 2^3 = 3

surface/volume = 3

sides = 1
surface = 1^2 x 6 = 6
volume = 1^3 = 1

surface/volume = 6

BROWNIAN MOTION



Brownian Movement

Brownian motion is the random motion of particles suspended in a fluid (a liquid or a gas) resulting from their collision with the fast-moving molecules in the fluid. Einstein observed the motion of a particle in the fluid (collidial particles). The size of the collide particle is in nanometer range but motion of these particles depends on the coefficient of viscosity of fluid and the diameter of the particles. Generally all medicines are nano crystalline materials. For better action on human bodies the particle size shall be uniform.

FUNDAMENTAL FORCES IN NATURE

Fundamental Force Particles

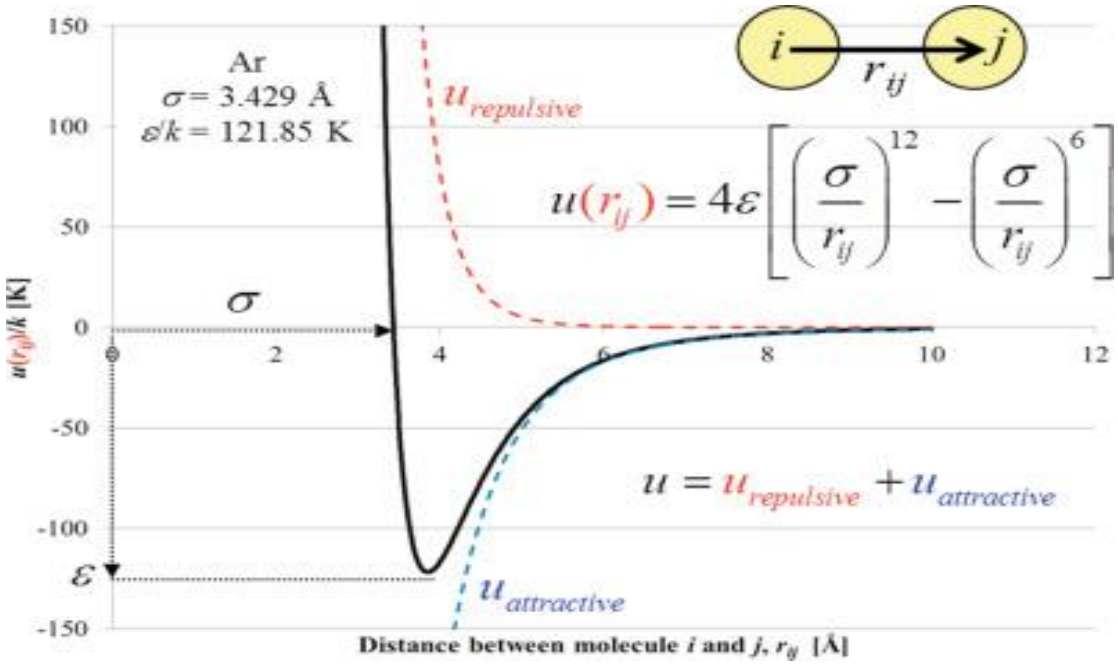
Force	Particles Experiencing	Force Carrier Particle	Range	Relative Strength*
Gravity acts between objects with mass	all particles with mass	graviton (not yet observed)	infinity	much weaker ↓
Weak Force governs particle decay	quarks and leptons	W^+, W^-, Z^0 (W and Z)	short range	
Electromagnetism acts between electrically charged particles	electrically charged	γ (photon)	infinity	
Strong Force** binds quarks together	quarks and gluons	g (gluon)	short range	much stronger

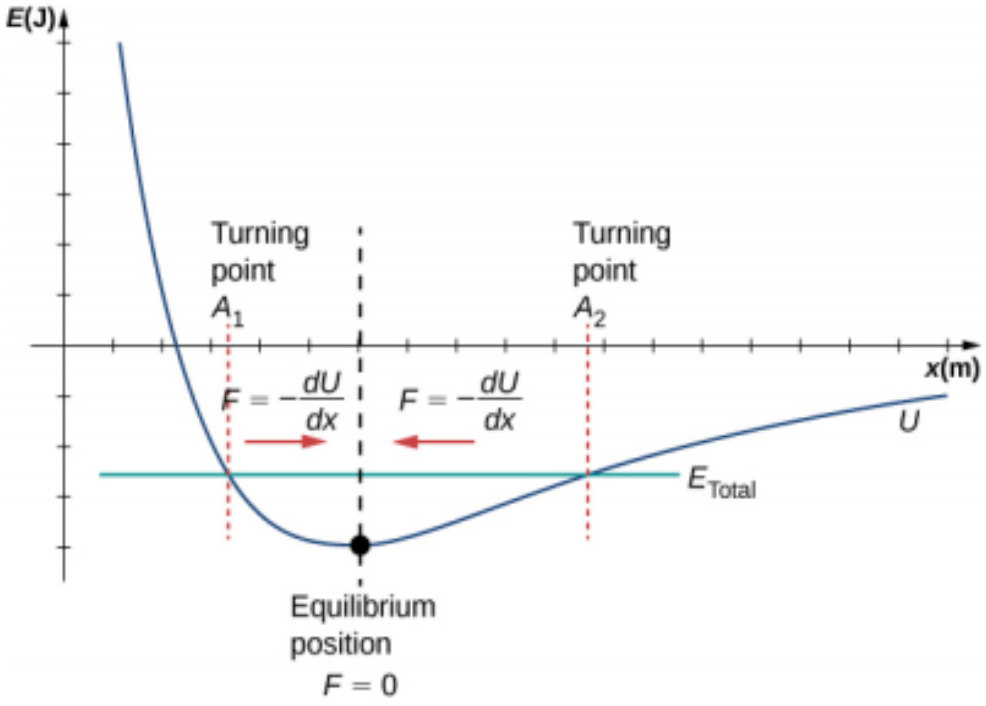
At nano scale the masses are very small, therefore gravitational force is negligible, but electromagnetic force is very large. The frictional forces, spring force, viscous force are

examples of electromagnetic forces. Motion of lizard on vertical wall, The lizard never fall from a wall, this is due to the nanoscales interaction between the wall & leg for of a lizard.

Que: Gravitational force and Electromagnetic force and Nanotechnology ?

Ans. The gravitational force is the force by gravity on object having mass. Mass are responsible for gravitational force it is defined as forces F = mg where g is the acceleration due to gravity. While electromagnetic force are force acting between charge particle, which deals at molecular or atomic level that is at nanoscale. At nano scales, the masses are very small therefore gravitational forces is negligible but electromagnetic forces is very large. Frictional force, spring force are examples of electromagnetic force.





According to the honorable scientist Lennard's Jones, if a two atoms separated by a distances r. then the potential energy

$$U = \frac{A}{r^{12}} = \frac{B}{r^{r}} \quad \text{.....(i)}$$

Where A & B are Vander wall constant & this is called Vander wall interaction forces the equation (i) is written in modified form.

$$U(r) = \varepsilon\left[\left(\frac{2x_{vnd}}{r}\right)^{12} - 2\left(\frac{2x_{vnd}}{r}\right)^{6}\right]$$

Where x_{vnd} is the Vander wall radius $\bar{\varepsilon}$ is well depth, r = inter atomic separation. The relation between force & energy is given by the force between two atom will be maximum when,

$$F_{max} = -\frac{dU}{dr} = 0 \qquad \text{at } r = r_0$$

$$U = \frac{A}{r^{12}} = \frac{B}{r^{r}} \quad \text{.....(i)}$$

Solving this equation, We get , r_0 = 0.27 nm

Putting these values in the equation of force between the two atoms we get

$$F_{atoms} = -1.6 \times 10^{-12} \text{ N}$$

In terms of force of gravity the forces on an H- atom, if Mass of hydrogen =1.6 X 10^{-27} kg.

Therefore the forces of gravitation

$$F = mg$$

$$= 1.6 \times 10^{-27} \times 10$$

$$= 1.6 \times 10^{-26} \text{ N}$$

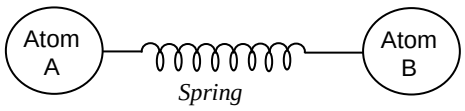
The magnitude of gravitational force is very small as compared to the electromagnetic forces.

The forces between the two atoms:

$$F = 12\varepsilon\left[\frac{(2x_{vnd})^{12}}{r^{12}} - \frac{(2x_{vnd})^{6}}{x^{7}}\right]$$

Due to this forces the spider climb on the wall or celling. Such creatures have a nano scale hairs on on their feet, the more surface area by contact to the surface.

Zero point energy.



Spring forces = - Kx

Spring Potential Energy = $\frac{1}{2}kx^2$

Que. Suppose the grain of pollen having some mass at the tip of a eyelash, the mass of a pollen object is 100 ng & eyelash has a estimated spring constant 0.1N/m. The pollen lands on the eyelash & deflects and starting oscillate. What is the value of number of oscillation for this system.

Ans.

The force excreted by pollen is F = mg

$= 100 \times 10^{-9}$ x 10^{-3} kg × $10 m/s^2$

$= 10^{-9}$ N

This force causes a deflection can be given by

X = F / K

Or, $x = \frac{F}{k} = \frac{10^{-9}\ N}{0.1 N/m} = 10^{-8}\ m$

The potential energy of the spring system $= \frac{1}{2} kx^2 = \frac{1}{2} \times 0.1 \times (10^{-8})^2\ J$. This energy represents the total energy of system to in order to oscillate.

The natural frequency of the oscillation

$= \frac{1}{2\pi}\sqrt{\frac{K}{m}}$ (air resistance any kinds of during is negligible)

$= \frac{1}{2\pi}\sqrt{\frac{0.1}{100 \times 10^{-9}}}$

$= \frac{1}{2\pi}\sqrt{\frac{1}{100 \times 10^{-9}}} = \frac{1}{2\pi}\sqrt{\frac{1}{10^{-6}}} = 5000\ Hz$

But according to quantum sciences the zero point energy is not possible even at T=0

$$E = \left(\frac{n+1}{2}\right) hv$$

$$E = nhv + \frac{hv}{2}$$

$$nhv = E - \frac{hv}{2}$$

$$n = \frac{E}{hv} - \frac{hv}{hv} = \frac{E}{hv} = \frac{1}{2}$$

$$= \frac{4.8 \times 10^{12}}{6.632 \times 5000} = \frac{1}{2} = 10^{12}$$

Que. Why plant & fruits have different colours?

Ans- The colours of a material is determine through the absorption of light of a given wavelength.

The vitamin A molecules has a linear chain of 10 carbon atoms

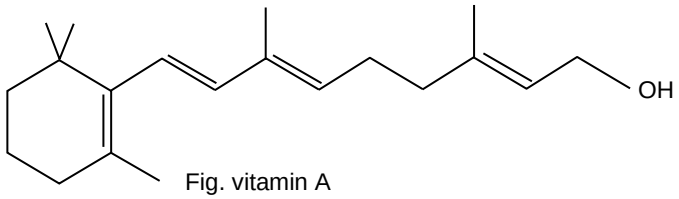


Fig. vitamin A

Each carbon atom have one π electrons of average bond length of C-C is 0.14 nm.

According to quantum confinement relation

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

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

The absorption takes place when electron jumps from lower to high energy state.

$$\Delta E = E_{n+1} = E_n = (2n+1)h^2 \quad = 8mL^2$$

$$\lambda = \frac{hC}{\Delta E} = \frac{hC}{(2n+1)h^2} \times 6mL^2 \; = \; \frac{8mL^2C}{(2n+1)h}$$

n = 10

m= 9.1x 10^{-38} kg

L = 0.14m

$h = 1242$

$$\lambda \; = \; \frac{6 \times 9.1 \times 10^{-31} \times 0.14 \times 3 \times 10^8 \, cm \times 9.1 \times 10}{(2 \times 10 + 1)\, 1242}$$

$$\approx \; 478 \, nm$$

This absorption of wavelength mean to the green colour. Therefore the given material looks like a green. The π electrons in a linear chain molecules can be behave like a free electron in a deep rectangular 1 dimensional potential wall, where ℓ the length of the molecules. For a large value of π electrons the wavelength is proportional to the number of π electrons. This shows the longer molecules has absorption at longer wavelength. In case of pumpkin & carrots approximately about $23\,\pi$ electrons are present & absorption wavelength found at 497 nm. The square well in three-

Dimension in this case the particle of mass m which is restricted to move in a book which sides are a b and c (say) respectively the general equation of confinement.

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

Four = three dimensional spaces

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

The ground state energy value on be obtained when nx = ny = nz = 1
In that case

$$E_{III} = \frac{3h^2}{8mL^2}$$

In this case particle are confined in a cubical region. This is the set of quantum numbers that gives these energy state & set to be non-de generate. In Absorption spectroscopy,there are three possibility for the final existed state.

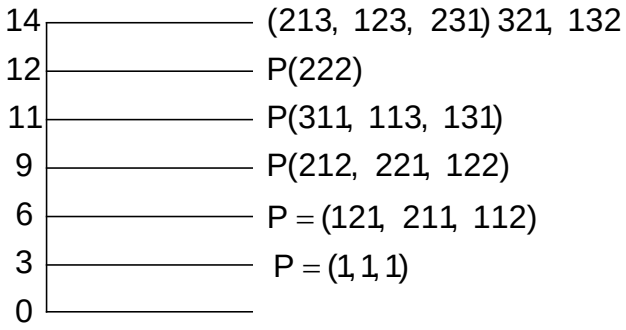
(1) nx = 2 ny = nz = 01
(2) ny = 2 nz = nz = 1
(3) nz = 2 nx = ny = 1

$$E_{2III} = \frac{h^2(2^2 + 1^2 + 1^2)}{8mL^2} = \frac{6h^2}{8mL^2} = \frac{3h^2}{4mL^2}$$

$$E_{121} = \frac{h^2(1^2 + 2^2 + 1^2)}{8mL^2} = \frac{6h^2}{8mL^2} = \frac{3h^2}{4mL}$$

$$E_{112} = \frac{h^2(1^2 + 1^2 + 2^2)}{8mL^2} = \frac{6h^2}{8mL^2} = \frac{3h^2}{4mL}$$

Thus different quantum state possess same energy, this properties is the de- generative. The energy of the particles of deep particles of deep well may as continuous & discrete. The particles has different bound state inside the well.



This figure shows the degrees of degenerate energy level, quantum number of molecules.