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QUANTUM MECHANICAL CALCULATION OF OPTICAL PROPERTIES OF SILICON-OXIDE NANOPARTICLES USING BORN-MAYER POTENTIAL

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Abstract

In this work, the basic postulates of quantum mechanics are applied to calculate the optical properties of silicon oxide nanoparticle using Born-Mayer potential. The Born-Mayer potential was inputted into the time independent Schrödinger equation and the radial wave function was obtained by solving the equation using Runge-Kutta fourth and fifth order method.. The radial wave functions were then used to evaluate the expectation values of the energy of the system. The energies were used in the calculation of the optical properties such as, absorption coefficient extinction coefficient, real and imaginary dielectric constant and optical conductivity of the system. The accuracy of the theoretical model used for calculating the optical properties of silicon oxide nanoparticles was validated by comparing the results with experimental values using the Tauc plot which was used to determine the energy band gap (E_g) of silicon oxide nanoparticles and its optical properties empirically. The results obtained shows an oscillating radial wave function which decays exponentially in amplitude along the direction of propagation due to the core-shell nature of silicon-oxide nanoparticles The curve of the absorption coefficient shows a band gap value of 9.0 eV which is the theoretical band gap value of silicon oxide nanoparticle. The calculated and experimental curves of the absorption, extinction coefficients and the optical conductivity almost ride on each other and also showed good agreement between the theoretical calculation and experimental data.

1. Introduction

Quantum mechanics, also known as quantum physics is a branch of Physics which describes nature at the smallest scales of energy levels of atoms and subatomic particles. Quantum mechanics provides a reliable method to calculate the total energy of an ensemble of electrons and atomic nuclei. One of the postulates of quantum mechanics is that the state of a system can be fully described by the mathematical function $\boldsymbol{\psi(r_1, r_2 \ldots t)}$ where $\boldsymbol{r_1, r_2}$ are the spatial coordinates of particles**1**, **2,** etc. that constitute the system and $\boldsymbol{t}$ is the time. This is known as the wavefunction of the system and can be evaluated by solving a wave-like equation, known as the Schrodinger equation [1]. Schrodinger equation is a linear partial differential equation that describes wave function or state function of quantum mechanical system. The equation has two "form", the time-dependent Schrödinger equation (TDSE) and time-independent Schrödinger equation (TISE). The form of the equation used depends on the physical situation. In quantum mechanics, the wave function is the most complete description that can be given to a physical system like silicon-oxide nanoparticles and according to the principle of quantum mechanics, the wave function of the electrons in the system has the main importance in description of optical, electrical and thermal properties of the system [2, 3]. Solution to Schrödinger's equation describes not only molecular, atomic, and subatomic systems; also macroscopic system, possibly even the whole universe [4]. The equation is central to all applications of quantum mechanics including, quantum field theory which combines special relativity with quantum mechanics. Nayyar, *et al,* [5] presented a theoretical approach to calculate the absorption coefficient of silicon nanostructure. He used quantum mechanical calculation on the interaction of photons with the electrons of the valence band; one model is that, the oscillator strength of the direct optical transition is enhanced by the quantum confinement effect in silicon nanocrystallites. He discovered that the absorption coefficient showed a peak at high photon energy. Similarly, Anande *et al,*[6] calculated the optical absorption coefficient of a silicon nanowire using quantum mechanical

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model and discovered a very good agreement between theory and experimental data at low photon energies and the discrepancy between experimental data and theory at high photon energies probably due to free carrier absorption as well. In this research work, radial Schrodinger equation with interacting Born-Mayer potential is used to calculate the Microscopic optical properties of silicon oxide nanoparticles.

2. Computational Methods

Silicon oxide is a chemical compound with a formula SiO_2 most commonly found in nature as quartz. It is the major constituent of sand and the abundant families of material. The structure of the silicon oxide is similar to other silicon based alloys build-up from tetrahedral entities centered on a silicon atom [7].

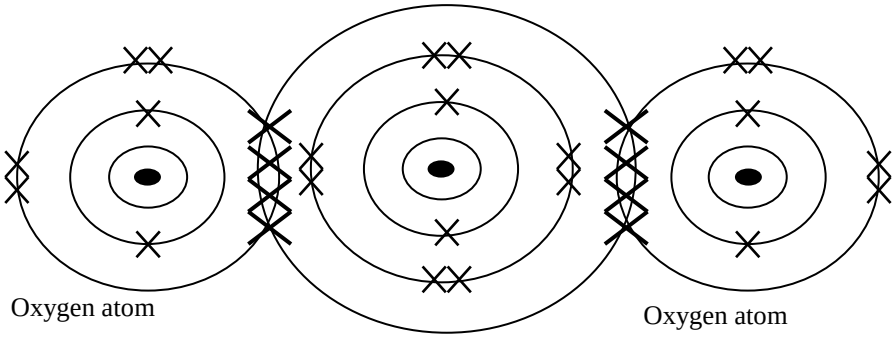

Figure 1: Sketch of Silicon oxide bonding

Silicon oxide nanoparticles are assumed to be spherical in shape; so the spherical polar form of the Schrodinger equation is used to describe the state of the system. Consider the time-independent Schrödinger equation given in equation 1:

$$H\psi_{nlm} = E\psi_{nlm} \quad (1)$$

The equation in three dimensional polar coordinates is given as:

$$\left[\frac{-\hbar^2}{2m}\left(\frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{1}{r^2}\left(\frac{1}{sin\,\theta}\frac{\partial}{\partial\theta}sin\,\theta\frac{\partial}{\partial\theta} + \frac{1}{sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)\right) + V_{(r)}\right]\psi_{nlm}(r,\theta,\phi) = E\psi_{nlm}(r,\theta,\phi) \quad (2)$$

Equation (2) can be split into one dimensional second order differential equation in each coordinate following the separation technique defined by:

$$\psi_{nlm}(r,\theta,\phi) = R_{nl}(r)Y_{lm}(\theta,\phi) \quad (3)$$

When substituting equation (2) into (3), the partial derivatives can be expressed as ordinary derivatives. The equation can then be separated in to a radial part and an angular part with a colatitudes equation and an azimuthal equation. The radial part collects all terms that depend on the radial coordinate (r) and sets it equal to a constant which contains the orbital quantum number l given as:

$$\frac{d^2}{dr^2}rR_{nl}^{(r)} + \frac{2m}{\hbar^2}V_{(r)}rR_{nl}^{(r)} + \frac{2m}{\hbar^2}ErR_{nl}^{(r)} = l(l+1)\frac{R_{nl}^{(r)}}{r} \quad (4)$$

With substitution of $R_{(r)} = \frac{U(r)}{r}$ this leads to equation (5):

$$\frac{d^2}{dr^2}U_{nl} + \frac{2m}{\hbar^2}\left[E + V_{(r)} - \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]U_{nl} = 0 \quad (5)$$

The potential $V_{(r)}$ in equation (5) is the sum of the Coulomb potential and Born-Mayer repulsive potential [8,9,10].

Born-Mayer potential is a short range repulsive potential which occurs when the wave function of inner-shell electrons or the nuclei begin to overlap [11].

The Born-Mayer potential is given as:

$$V(r) = B\,exp\left(\frac{-r}{\rho}\right) \quad (6)$$

Where B and ρ are empirical constants and r is the distance between the atoms or electrons. In this research work, the coulomb potential can be obtained in figure 1 by assuming the eight electrons involved in the covalent bonding as the active electrons. The effective potential $V_{(eff)}$ is the sum of the coulomb and the interaction Born-Mayer potential given as:

$$V_{(eff)} = -2\left(\frac{ze^2}{4\pi\varepsilon_0 r_1} + \frac{ze^2}{4\pi\varepsilon_0 r_2} + \frac{ze^2}{4\pi\varepsilon_0 r_3} + \frac{ze^2}{4\pi\varepsilon_0 r_4}\right) \quad (7)$$

The potential can be written in reduced oxygen and silicon nuclei form as:

$$V_{(eff)} = -2\left[4\left(\frac{(ze)_O(ze)_S}{(ze)_O+(ze)_S}\right)e\right] + Be^{-\frac{r}{\rho}} \quad (8)$$

Substituting equation (8) in to (5)

$$\frac{d^2U_{nl}}{dr^2} + \frac{2m}{\hbar^2}\left[E - 2\left[4\left(\frac{(ze)_O(ze)_S}{(ze)_O+(ze)_S}\right)e\right] + Be^{-\frac{r}{\rho}} - \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]U_{nl} = 0 \quad (9)$$

Equation (9), is the Schrödinger equation for the reduced nuclei of oxygen and silicon with Born-Mayer repulsive interaction in the attractive field of the electron-nuclei. The attractive field of the electron-nuclei can either be electron-oxygen nuclear interaction or electron- silicon nuclear interaction.

2.1 Numerical Solution of Radial Schrodinger Equation

The solution of radial Schrodinger equation was obtained using Runge-Kutta fourth order method to implement the shooting method which converts the boundary value problem (BVP) of second order ordinary differential equation into a system of two firsts order initial value problem (IVP) of ordinary differential equation. The ODE45 code in matlab which is based on Runge-Kutta $\mathbf{4^{th}}$and $\mathbf{5^{th}}$method was used to implement Runge-Kutta algorithm in MATLAB [12,13].

Consider equation (9) above, and define

$$Q_{(r)} = \frac{d}{dr}U_{nl} \quad (10)$$

This gives:

$$\frac{d}{dr}Q_{(r)} = -\frac{2m}{\hbar^2}\left[E - 2\left[4\left(\frac{(ze)_O(ze)_S}{(ze)_O+(ze)_S}\right)e\right] + Be^{-\frac{r}{\rho}} - \frac{\hbar^2}{2m}\frac{l(l+l}{r^2}\right]U_{nl} \quad (11)$$

Equation (10) and (11) are the two first order coupled system of one dimensional differential equation that were sole using ODE 45 code.

2.2 Evaluation of optical properties of silicon oxide nanoparticles1

2.2.1 Absorption coefficient of silicon oxide nanoparticles

The optical properties of silicon oxide nanoparticles are characterized by the response of the material to incident electromagnetic radiation [14]. In this research work, the optical properties consider include absorption coefficient, extinction coefficient, real dielectric constant, imaginary dielectric constant and optical conductivity. Silicon oxide nanoparticles are known to have a quasi-direct band gap due to the nature, size and geometry of the molecule [15]. The assumption of parabolic band gap behavior has to be taken to make the associated mathematical calculation easy [16]. Consider a photon with energy $\hbar\boldsymbol{\omega}$ incident on the silicon oxide nanoparticle, the electron in the valence band at state $\boldsymbol{o}$ is excited to a state $\boldsymbol{m}$ in the conduction band. Consider a situation where the inter band transitions depend on the momentum matrix element, at any instance of time, the Hamiltonian for an electron in the presence of an electromagnetic field is [17]:

$$H'_{mo} = \frac{e\vec{A}}{2m}(\hat{a}.\vec{p}) \quad (12)$$

Where $\vec{A}$ is vector potential, $\hat{a}$ is unit polarization vector and $\vec{p}$ is canonical momenta

Using the above equation, the reduced transition probability for electron to make transition from state $\boldsymbol{o}$ in the initial (valence) to state $\boldsymbol{m}$ in the final (conduction) is

$$W_{om} = \frac{2\pi}{\hbar}t\left[\left(\frac{eA}{2m}\right)^2(\hat{a}.\vec{p})^2\right]\delta(E_m - E_o - \hbar\omega) \quad (13)$$

Where $\delta(E_m - E_o - \hbar\omega)$ is the Dirac delta function and t is time

This is the transition probability of one primitive cell. To get the total transition probability for quasi-direct band to band transition, the sum of equation (13) over all N values of k, and also over varying wavelength of the incoming photon $\hbar\omega$ [18]. Let us assume that the incoming photon is monochromatic wave, the transition probability for monochromatic wave can be obtained by considering the volume occupied by each value of $\vec{k}$: as

$$\Omega_k = \left(\frac{2\pi}{V}\right)^3 \quad (14)$$

And the Fermi Dirac distribution is also given by:

$$f_o(E,T) = \frac{1}{1+exp^{(E-E_f)/KT}} \quad (15)$$

E is the electron energy, and E_f is the Fermi level in the material under consideration, K is the Boltzmann constant, and T is the temperature of operation[18,19]. The total probability for an electron to transit between states in a quasi-direct band gap material can be calculated by integrating the transition probability (13) over the first Brillion Zone, keeping in mind the

Fermi Distribution. This total probability has to be multiplied by a factor of 2, to incorporate the effects of spin of an electron, during the absorption of photon. Hence, total probability

$$Y_{om} = \frac{2V}{(2\pi)^3}\int W_{om} f_o(1-f_o)d\vec{k} \quad (16)$$

And the transition probability rate $r_{om}(=\frac{Y_{om}}{Vt})$ as

$$r_{om} = \frac{2}{(2\pi)^3}\int \frac{W_{om}}{t} f_o(1-f_o)d\vec{k} \quad (17)$$

Using the transition rate, W_{om} calculated in (13), the transition probability rate r_{om} is written as,

$$r_{om} = \frac{e^2A^2}{8\pi^2\hbar m^2}\int(\hat{a}.\vec{p})^2\delta(E_m - E_o - \hbar\omega)f_o(1-f_o)d\vec{k} \quad (18)$$

From the absorption of parabolic band, we get:

$$E_m - E_o = E_g + \frac{\hbar^2k_m^2}{2m_e} + \frac{\hbar^2k_o^2}{2m_h}$$

Assuming $m \neq o$; then

$$E_m - E_o \approx E_g + \frac{\hbar^2k^2}{2m_r} \quad (19)$$

where the reduced mass, m_r is given by:

$$\frac{1}{m_r} = \frac{1}{m_e} + \frac{1}{m_h} \quad (20)$$

E_g is the energy band gap for the material (silicon oxide nanoparticle), m_e is the mass of the electron with wave vector k_m and m_h is the mass of the hole with wave vector k_o. m_r is the reduced mass for the electron and the hole.

Substituting equation (19) in to (18) gives

$$r_{om} = \frac{e^2A^2}{8\pi^2\hbar m^2}\int(\hat{a}.\vec{p})^2\delta\left(E_g + \frac{\hbar^2k^2}{2m_r} - \hbar\omega\right)f_o(1-f_o)d\vec{k} \quad (21)$$

Introducing a dimensionless term oscillator strength given as $O_s = \frac{2(\hat{a}.\vec{p})^2}{m\hbar\omega}$ and also $d\vec{k} = 4\pi k^2 dk$ in to equation (21) and taking out those terms that do not vary with the variation of $\boldsymbol{k}$ out of the integral gives [20],

$$r_{om} = \frac{e^2A^2}{8\pi^2\hbar m^2}f_o(1-f_o)\left(\frac{O_s\hbar m\omega}{2}\right)\int\delta(E_g + \frac{\hbar^2k^2}{2m_r} - \hbar\omega)4\pi k^2 dk \quad (22)$$

The delta function has a property, such that

$$\int_{\infty}^{-\infty} f(x)\delta(x-a)dx = f(a)$$

Using the above property in equation (22), the transition probability rate becomes [21,22]:

$$r_{om} = \frac{e^2\sqrt{m}}{8\pi\hbar^3}\left(\frac{2m_r}{m}\right)^{3/2}A^2O_sf_O(1-f_O)\sqrt{\hbar\omega - E_g} \quad (23)$$

Absorption Coefficient is defined as the transition rate per unit quantum flux (quantum flux is defined as the number of incident photons per unit area in unit time)[23]. Quantum flux can be calculated from the average value of poynting vector s per unit wavelength energy.

The various relations are given as:

Quantum flux:

$$(\phi) = \frac{\langle\vec{S}\rangle}{\hbar\omega} \quad (24)$$

The poynting vector is given as:

$$\vec{S} = \vec{E}\times\vec{H} \quad (25)$$

Where Electric field $(E) = A\omega\hat{a}\,sin(\vec{q}.\vec{r} - \omega t)$ and magnet field

$(\mu H) = -A(\vec{q}\times\vec{a})\,sin(\vec{q}.\vec{r} - \omega t)$

Introducing the two terms in equation (25) gives,

Average poynting vector:

$$\langle\vec{S}\rangle = \frac{1}{2}|q|\frac{\omega A^2}{\mu} \quad (26)$$

But the magnitude of the wave vector of a photon is given as $|q| = \frac{\omega\eta}{c}$, hence , equation (26) becomes,

$$\langle S\rangle = \frac{1}{2}\eta\mathcal{E}_o c\omega^2A^2 \quad (27)$$

Substituting (27) in to (24) Quantum flux becomes,

$$\phi = \frac{\frac{1}{2}\eta\mathcal{E}_o c\omega A}{\hbar} \quad (28)$$

Using the above relation, Absorption Coefficient $\alpha\left(=\frac{r_{om}}{\phi}\right)$ becomes [23-24]

$$\alpha(\omega) = \left(\frac{e^2\sqrt{m}}{4\pi\varepsilon_o c\hbar^2}\right)\left(\frac{2m_r}{m}\right)^{3/2}\left(\frac{O_o}{\eta}\right) f_o(1-f_o)\sqrt{\hbar\omega - E_g} \quad (29)$$

3.4.2 Refractive index of the material

The imaginary part of the refractive index $k(\omega)$ (extinction coefficient) can be evaluated from the absorption coefficient by [25]

$$k(\omega) = \frac{\alpha(\omega)c}{2\omega} \quad (30)$$

3.4.3 The real and imaginary Dielectric function

The complex index of refraction is given as

$$N_{complex} = \sqrt{\mu\varepsilon_{complex}} \quad (31)$$

For non-magnetic material, $\mu = 1$,and where $N_{complex}$ is usually written in terms of its real and imaginary parts as

$$N_{complex} = \eta + ik \quad (32)$$

With the definition for $N_{complex}$,the dielectric function was evaluated from the relation

$$\varepsilon_{complex} = \varepsilon_1 + i\varepsilon_2 = (\eta + ik)^2 \quad (33)$$

Yielding real and imaginary part of dielectric function as [26],

$$\varepsilon_1 = \eta^2 - k^2 \quad (34)$$

$$\varepsilon_2 = 2\eta k \quad (35)$$

3.4.4 The optical response of a material

The optical response of silicon oxide nanoparticle can be obtained in terms of the optical conductivity $\boldsymbol{\sigma(\omega)}$ which is given by the relation [26],

$$\sigma(\omega) = \frac{\alpha(\omega)\eta c}{4\pi} \quad (36)$$

The Schematic flow chart showing the Evaluation Stages in the Simulation is given in the Figure 2 below:

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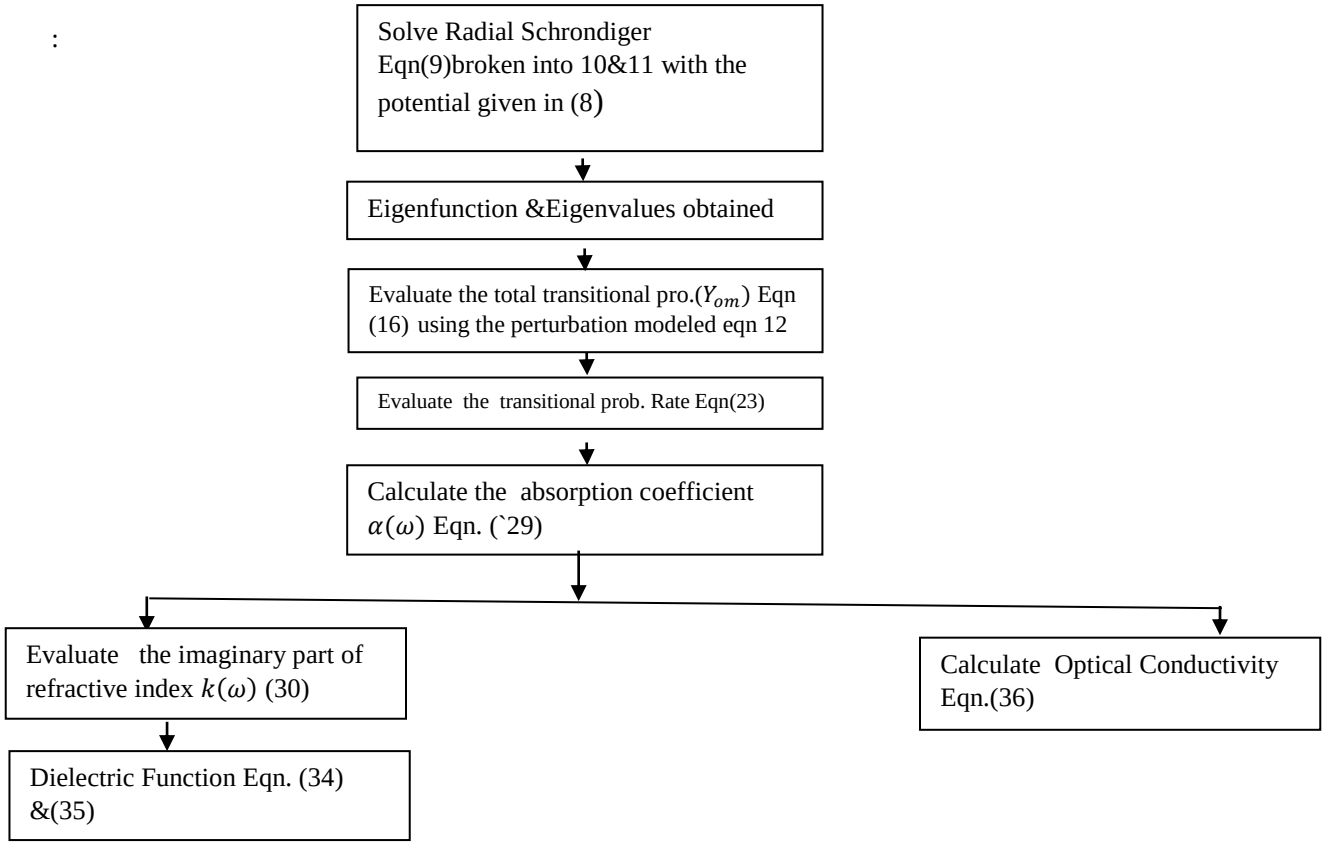

3. Results and Discussions

In this step, the radial wave function for silicon oxide nanoparticle would beobtained considering boundary conditions and physical confinements.

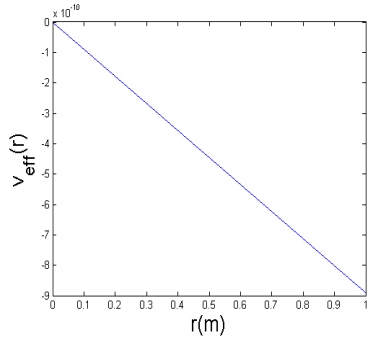

Figure 3: Sketch of effective potential

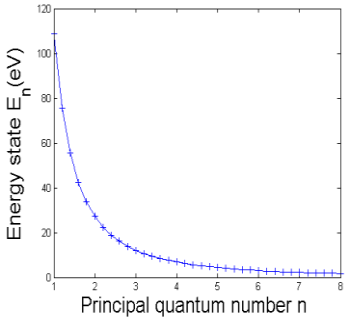

Figure 4:State $E_n(eV)$ versus n

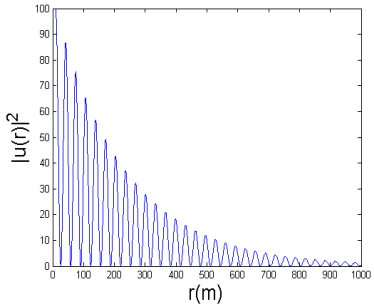

Figure 5 E_1=108.8eV, n=1, h=0.5, L=1000

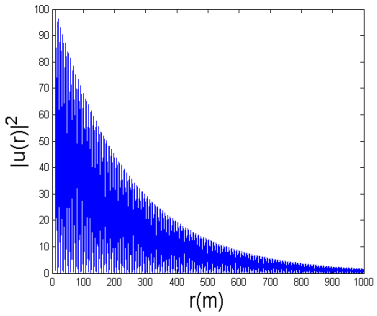

Figure 6:E_2=27.2eV, n=2,h=0.5, L=1000

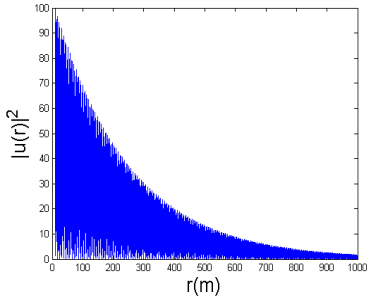

Figure 7:E_3 =12.09eV, n=3,h=0.5,L=1000

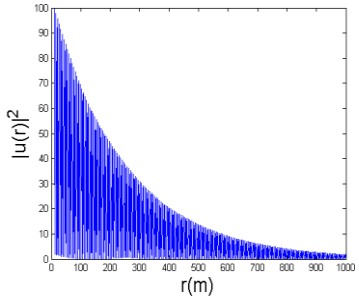

Figure 8: E_4=6.8eV, n=4,h=0.5, L=1000

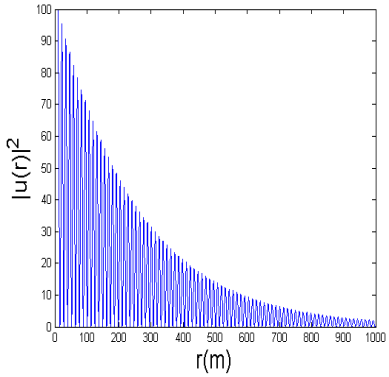

Figure 9: $\mathrm{E}_6 = 4.352\mathrm{eV}, \mathrm{n} = 6, \mathrm{h} = 0.5, \mathrm{L} = 1000$

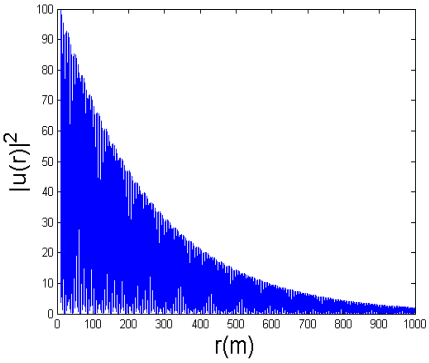

Figure 10:E_6=3.022eV n=6, h=0.5,L=1000

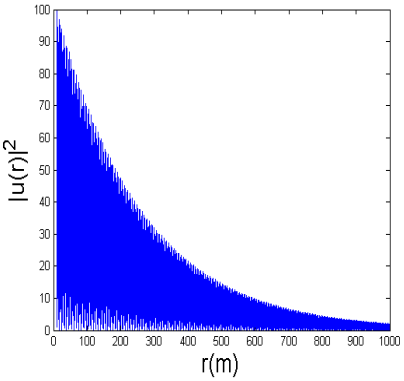

Figure 11: E_7=2.22eV, n=7, h=0.5, L=1000

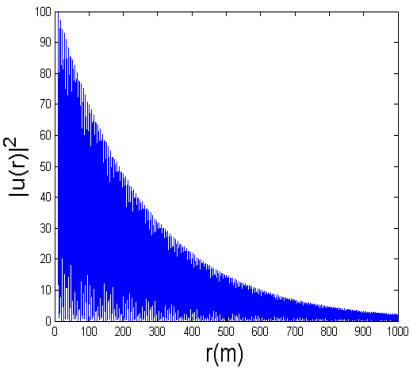

Figure 12: E_8=1.70eV, n=8, h=0.5, L=1000.

In quantum mechanics, a quantum mechanical system or particle that is bound or confined partially can only take on certain discrete values of energy called energy eigenvalue denoted as E_n . The subscript n called the principal quantum number which determines the overall energy of each orbital or wave function of the system [27]. In this research, the energy state relation to the principal quantum number is represented by the equation

$$E_n = \frac{-E_0}{n^2} \tag{37}$$

where $E_0 = -108.8\, eV$ (the negative sign in the equation indicates that work has to be done to remove an electron from the atom).

The energy state for this system (silicon oxide nanoparticle) is considered based on the hydrogen atom model. Figure 3 shows a sketch of the effective potential$V(r)$ as a function of the linear coordinate $r(m)$ for silicon oxide nanoparticles. Figure 4 shows that as the principal quantum number (n) increases the absolute value of energy state decreases. This means an electron with the lowest value of "n" has more energy and is located on the orbital or wave function closer to the nucleus. As the value of "n" increases the atomic size increases and more orbital or wave functions are formed. At $n = 1$ and $E_1 = 108.8\, eV$ (figure 5) a sinusoidal wave of one wavelength (λ) is observed. The periodic nature is that, the amplitude of the wave decay all through along the direction of propagation, this is due to the effect of core-shell nature of silicon oxide nanoparticles and this creates a perturbation in the wave that results to the decay of the wave as it propagates. In figure 6, at $n = 2$ and $E_2 = 27.2\, eV$ there is partial formation of the wave packet which is due to high frequency that arises as the wave travel and it makes the line of propagation of the wave to become compactable and the amplitude decay throughout the direction of propagation.

The wave packet that over crowds at the middle is observed at energy of $E_3 = 12.09\, eV$,$n = 3$ (figure7). This core region (over crowd) of wave packet is due to the core region of the silicon oxide nanoparticle and the shell region (less crowd) of the wave packet indicates the shell region of the silicon oxide nanoparticle [28]. Although, at $E_4 = 6.8\, eV, n = 4$ (figure 8) the wave packet nature of the probability distribution disappeared but high oscillation is observed due to high frequency and the wave became more compacted while the amplitude die down along the direction of propagation.

At higher states $E_5 = 4.352\, eV, n = 5$ (figure 9) some oscillations are lost as the value of n increases making the waves to be in phase as it travels. Figure 10, at an energy of $E_6 = 3.022\, eV$ and $n = 6$ shows a combination of many waves having a distribution of frequencies which reinforced along the direction of propagation. The reinforcement is more pronounced in figure 11, at energy of $E_7 = 2.22\, eV$ and $n = 7$, this is due to various components sinusoidal waves of different phases and amplitudes which interfere constructively only over a small region of space. Hence, the constructive interference became more in the core region of the silicon oxide nanoparticle as indicated by figure 12 at energy $E_8 = 1.70\, eV$ and $n = 8$. The interference may be due to the repulsion created by the Born-Mayer potential when the wave function of the inner-shell electrons or nuclei begins to overlap.

In [28] the literature revealed that the energy and the probability distribution near the core centre increase as the quantum integer numbers n *and* l are enhance. Hence, the wave distortions are sensible in the core where the wave number is larger than the shell, because of the semiconductor behavior of the shell; the wave function is a damping wave. The result in this

research work is in good agreement with the literature because a sinusoidal wave whose amplitude drops exponentially with the radial distance is observed and this is due to the semiconductor nature of silicon oxide nanoparticle. Also, the formation of the wave packet at the core region of silicon oxide nanoparticle is due to constructive interference of the sinusoidal waves.

3.1 Optical Properties of Silicon Oxide Nanoparticle

In quantum mechanics, to relate a quantum mechanical calculation to a physical system (silicon oxide nanoparticle), the "expectation value" of the measurable parameter is calculated [29]. The expectation value of the energy was evaluated using equation (38) and the result was used in the calculation of optical properties of silicon oxide nanoparticle

$$< E >= \frac{\int_{-\infty}^{\infty} U_{(r)}^{*} H U_{(r)} dr}{\int_{-\infty}^{\infty} U_{(r)}^{*} U_{(r)} dr} \qquad (38)$$

The value of the expectation energy was substituted in equation (15) as the ground state electron distribution function energy which was used in the calculation of the absorption coefficient.

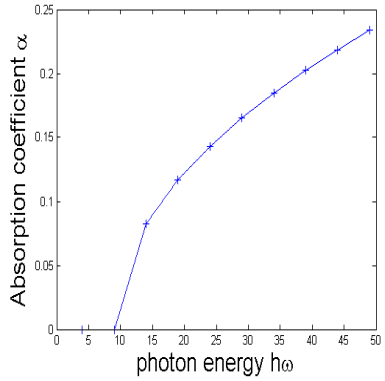

Figure:13 Absorption coeff.vs Photon energy

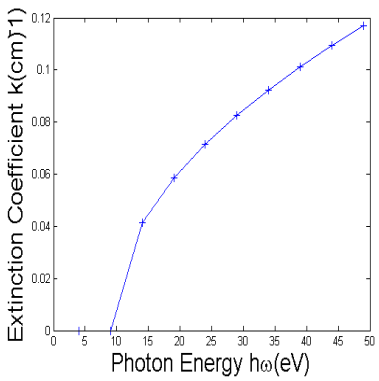

Figure 14:Extinction coeff. vs Photon energy

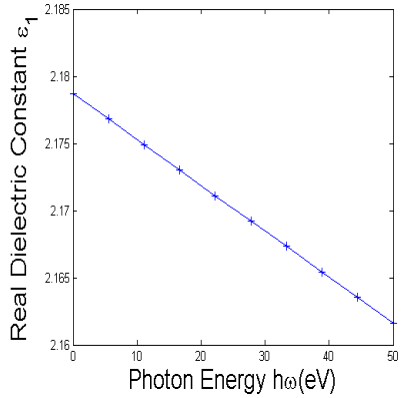

Figure 15: Real Dielectric Constant Vs Photon energy

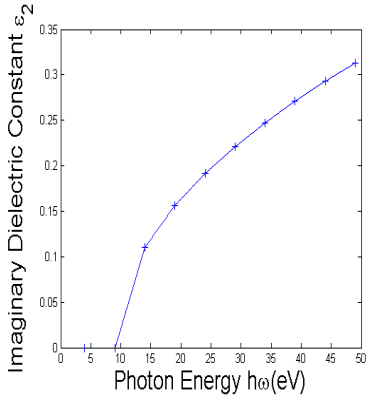

Figure 16:Imaginary Dielectric Constant Vs Photon Energy

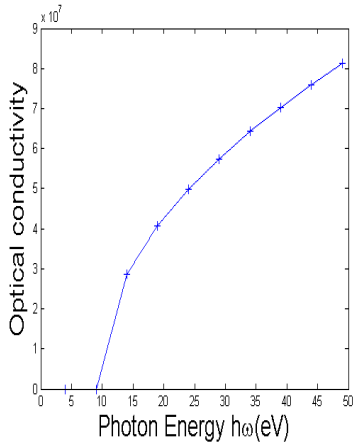

Figure 17:Optical Conductivity Vs Photon energy

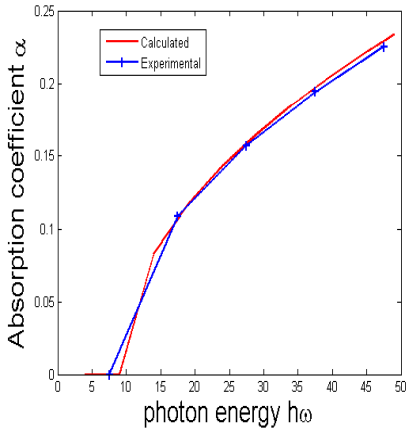

Figure 18: Calculated and Experimental Absorption Coeff.Vs Photon energy.

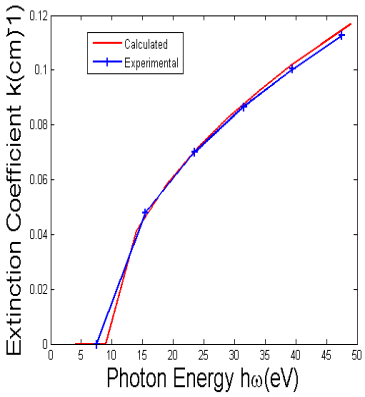

Figure 19: Calculated and Experimental Extinction Coeff. Vs Photon energy

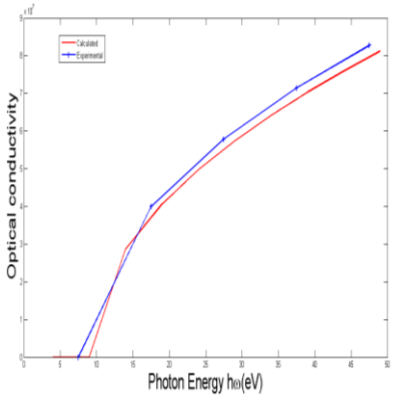

Figure 20: Calculated and Experimental Optical Conductivity Vs Photon energy

Figure 13 shows that there is no absorption in the energy range between 0 to 8.99 eV. It is important to emphasis that the energy at which the absorption starts corresponding to its direct band gap is at 9.0eV. Silicon oxide nanoparticle shows no absorption below its band gap. The absorption coefficient increases with increase in photon energy; this shows that absorption coefficient is photon energy dependent. The degree of absorption depends among other things on the number of free electron capable of receiving the photon energy [30]. The extinction coefficient is zero in the photon energy range 0-8.99 eV as shown in figure 14 which means that, silicon oxide nanoparticle is transparent in this energy region. The increase in extinction coefficient with increase in photon energy shows that the fraction of light due to scattering and absorbance increases in this energy. The peak is mainly due to the transitions from the last valence band to the first conduction band. Also the peak depict region of deep penetration of the electromagnetic wave [31].

Figure 15 indicates that, the real part of the dielectric constant decreases with increase in photon energy; this shows that the loss factor, decreases with increase in photon energy. At higher photon energy, the propagation of the electromagnetic wave drops drastically thus silicon oxide nanoparticle tends to become an insulator at this energy. The increase in the imaginary part of the dielectric constant with photon energy as depicted in figure 16 shows the loss factor increases with increase in photon energy. Optical conductivity of silicon oxide nanoparticle is constant in the energy range 0-8.99 eV as shown in figure 17, which means that, silicon oxide nanoparticle do not conduct in this energy range. The increase in optical conductivity with increase in photon energy can be attributed to the increase in absorption coefficient.

3.2 Comparison of theoretical values of the optical properties with experimental values.

The theoretical model used for the calculation of the optical properties of silicon oxide nanoparticle was verified experimentally using a relationship known as Tauc plot that determines band gap (E_g) for silicon oxide nanoparticle which is used to calculate the optical properties empirically [32].

Figure 18 shows a good correlation between theoretical and experimental values in the energy range of 17eV-26.8eV. However, noticeable discrepancies exist between the energies of 26.8eV-48.5eV; also the experimental curve indicates the band gap value of 8.4eV while the theoretical curve absorption start at 9.0eV which is the band gap theoretical value of silicon oxide nanoparticle. The variation of E_g originated due to the difference in temperature since E_g reduce as temperature increase. The peak on the curves which indicate the highest point of penetration of electromagnetic wave has a theoretical value of 0.235 and 0.22 as experimental value. Extinction coefficient curves indicate more correlation than the absorption as shown in figure 19. The energy range 14.9eV-29.5eV shows a good agreement exist between the theoretical and experimental values. Figure 20 shows that the theoretical and experimental curves of optical conductivity have a lot of discrepancies. This suggests that the theoretical model need refinement to yield better agreement and this is left for future consideration.

4. Conclusions

In conclusion, the Schrödinger equation for the reduced mass of oxygen and silicon nuclei with coulomb and Born-Mayer repulsive interaction in the attractive field of the electron –nuclei was obtained. The solution of the equation was obtained numerically using Runge-Kutta fourth order method. The ODE45 module in matlab which is built based on Runge-Kutta fourth order method is used to implement Runge-Kutta algorithm in matlab. The energy used for the numerical solution is guess energy based on the hydrogen atom model. A sinusoidal wave of one wavelength is observed at the initial value of the principal quantum number. The periodic nature of the wave is that, the amplitude decay all through along the direction of propagation and this is due to the core-shell nature of silicon oxide nanoparticles. As the principal quantum number increases there is formation of wave packet due to constructive interference of the waves over a small region of space. The wave function obtained was used to evaluate the "expectation energy" of the system which is considered to be the average energy. Hence, the expectation energy is used to evaluate the optical properties of the system such as absorption coefficient, extinction coefficient, real and imaginary dielectric constant and optical conductivity. The curves of the optical properties mostly show a band gap value of 9.0 eV which is the theoretical band gap value of silicon oxide nanoparticle. As the photon energy increases all the optical properties shows different characteristics. The theoretical model use for the calculation of the optical properties of silicon oxide nanoparticle was verified experimentally using a relationship known as Tauc plot that determined band gap (E_g) of silicon oxide nanoparticle which is use to calculate the optical properties empirically. The comparison between theoretical and experimental calculated optical properties shows a good correlation, however, noticeable discrepancies exist in the curve of optical conductivity.

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