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The Study of Optical Properties Exciton Based of Molecular Quantum Dot

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ABSTRACT

Optical properties of semiconductors, dielectrics and metals play a key role in the development of thin film solar cells. While these devices belong to photon photodetectors both the photon and wave nature of light affects their performance. Some of these problems are discussed. In this Paper we Solve the Schrodinger equation using the numerical method of finite difference approximation and assume that the structure of our quantum dot molecule is two cubic GaAs quantum dots in the $Al_xGa_{1-x}As$ medium with dimensions $L_X * L_Y * L_Z$ .By simulation the energy of exciton dependence with different molar coefficients, it was observed that: In sample, the exciton binding energy decreases with increasing molar coefficient. At a constant molar coefficient, the exciton dependence energy increases as the potential barrier width increases. At a constant molar coefficient, the exciton binding energy increases as the potential well width increases.

Keywords: Exciton binding energy; Quantum dots molecule; Molar coefficient; Photo generation

INTRODUCTION

Semiconductors are materials where the electronic band structure exhibits a relatively small band gap between the valence and conduction bands. They are of central importance for the electronics industry as base materials for diodes, transistors and other important electronic components, and semiconductor wafers are the starting point for electronic integrated circuits. However, semiconductors have also acquired a substantial role in the area of optics and photonics. [1]

The efficiency of photo generation of free carriers by light as well as its spatial distribution is taken into consideration. This distribution is strongly affected by light interfering in a structure of many thin films. The possible geometrical and optical inhomogeneities of the solar cell structure are discussed. A few methods of determining surface and averaged overall film thickness refractive indices of semiconductor materials are presented. Techniques for determining different

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components of absorption of light in semiconductors are also reported. Examples of optical methods useful for determining essential parameters of semiconductors (e.g., optical energy gap, carrier diffusion length, and parameters of electron states) are presented as well. [2,3].

THEORY

When electrons are excited in semiconductors, so that they can pass through the energy gap. The bottom of the conduction band is filled with electrons and the top of the capacitance band is filled with holes. As a result, both bands are now only relatively full, and if an electric field is applied, the electrons and holes can carry electric current. Although the conductivity of semiconductors (which have few electrons and holes) is small compared to the conductivity of small metals, this conductivity is still significant for scientific purposes. [4]

If we consider the simplest band structure of a semiconductor. The energy of the conduction band is as follows:

$$E_e(k) = E_g + \frac{\hbar^2 k^2}{2m_e^*} \qquad (1)$$

That k is the effective wave vector and m_e^* effective mass of the electron. Energy represents the energy of the gap. Zero energy level is located above the capacity bar. The capacity of bar can be written as follows: [5]

$$E_\upsilon(k) = -\frac{\hbar^2 k^2}{2m_h^*} \qquad (2)$$

Which m_h^* is the effective mass of the hole. Important structural parameters of the band are: electron and hole masses (m_e و m_h) and band gap energy (E_g)[6].

In crystalline materials, the band structure of matter is expressed by the density of states, N (E) [7]. The density of states is defined as N (E) dE is the specific number of states per unit volume for an electron with a specific spin direction whose energy is between E and E + dE.

In many cases, the density of states is determined mainly by the potential of the atom, and its nearest neighbors. The main factors that affect the density of states are the Correlation number and the distance between the atoms. If the Correlation number remains constant, there will be little change in the density of the states, unless the density of the state’s changes due to the change in volume. [8,9]

At temperature T, the number of electrons in the energy range E and E + dE for each spin direction is N (E) .f (E) dE, where f (E), the Fermi distribution function, is as follows: [10]

$$F(E) = \frac{1}{e^{(E-\in)/KT} + 1} \qquad (3)$$

If a photon with energy comparable to the energy gap lands on a semiconductor, it is absorbed by the electrons in the semiconductor. This light energy absorbed by the electrons frees them from the bonds of neighboring atoms, and eventually the electrons move freely in the crystal. This, in theory, is the excitation of electrons from the capacitance band to the conduction band. If the energy of the incident photon is greater than the energy of the band gap, this excitation is considered a strong energy excitation and the electron goes to the conduction band and is released, and its vacancy in the capacitance band is defined as a hole. The hole has a positive charge, so it binds to the electron in the conduction band, which is called the electron pair of the hole under Coulomb potential attraction, or exciton and the amount of energy reduced by the electron and the hole due to the Coulomb potential is called the dependence energy, which is denoted by. Photons with energies equal to the band gap energy can also be absorbed and produce excitons directly. This type of excitation is called resonant excitation, which is shown in Figure (1). The exciton system is a relatively stable structure and has a relatively long life of its kind, ranging from 100 picosecond to nanoseconds. [11,12,13]

Excitons are very similar to hydrogen atoms because of the very large mass of the hole relative to the electron, so Bohr theory can be used to study the properties of excitons. The exciton radius or the relative distance between the electron and the hole is therefore often called the exciton buohre radius.

Figure (1) shows a simple picture of exciton production. An electron absorbs a photon and is excited to a higher level, leaving a positive charge (hole). [14]

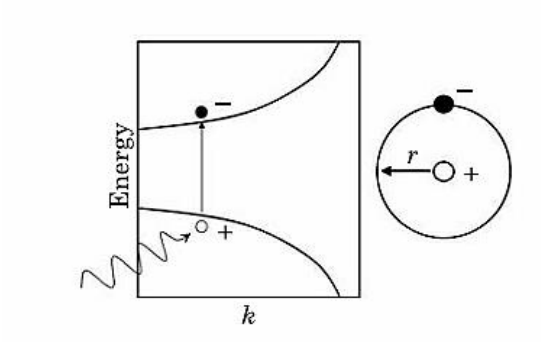

Fig. 1. formation of excitons.

The exciton dependence energy varies greatly depending on the material, for example in neon (a large gap insulator) the exciton attachment energy is 4 eV and in GaAs (a semiconductor with a small gap) this dependence energy is a few meV. Also in metals, due to the metal camouflage of the electron-hole interaction, the exciton dependence energy is very small and even zero in some cases. [15,16]

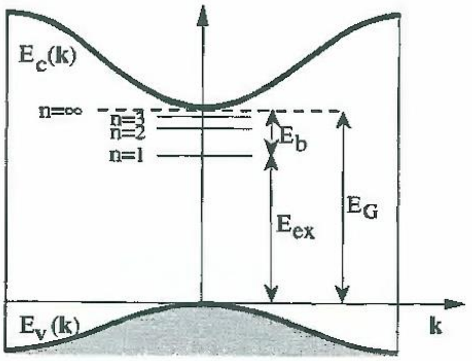

Fig. 2. The binding energy depend on the energy gap and the exciton energy.

A simple representation of the energy dependence of excitons and their importance in different materials can be obtained by considering the expression for the lowest energy level of a hydrogen atom: [17]

E_{Hb}=-m_0e48$h^2r^2\varepsilon^2{}_0$=-13.6 eV (4)

m_0 is the mass of the free electron and ε_0 is the vacuum constant r of the boron radius. The dependence energy of solids decreases for two reasons: first, that the effective mass is less than that of the free electron; and second, that interaction occurs due to the presence of a large dielectric constant. [18]

For GaAs, the effective mass of the electron is estimated to be m^* = 0.067 and ε = 12.85 ε_0, resulting in an excitation energy of 5meV.

Coulomb interaction plays a definite role in reducing energy dependence. For quasi-one-dimensional materials, however, electrostatic interaction is weak and the dependence energy increases significantly.

MODELLING AND SIMULATION

We Solve the Schrodinger equation using the numerical method of finite difference approximation. Assume that the structure of our quantum dot molecule is two cubic

GaAs quantum dots in the $Al_xGa_{1-x}As$ medium with dimensions Lx * Ly * Lz.

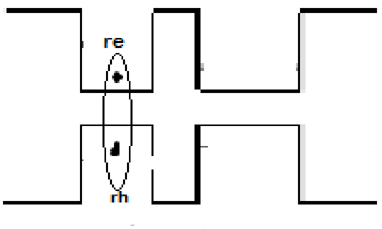

Fig. 3 . structure of the quantum dot molecule.

In the absence of any external force, the Schrodinger equation in approximating the effective mass for such a structure is expressed as follows:

$$[-\frac{\hbar^2}{2}(\nabla.(1/m^*(x,y,z))\nabla)+V(x,y,z)]\psi(x,y,z)=E\psi \tag{5}$$

In the above relation m * is the effective mass of the carriers. We consider its value for carriers inside the well area m_w for carriers outside the well area m_b. To determine the potential V (x, y, z), we consider the dimensions of the well area $L_X * L_Y * L_Z$, so for the area inside the well V (x, y, z) = 0, and for the points outside the well V (x, y, z) = V_0. By solving the equation (5), the energy values of the carriers are obtained. [19]

Since the above equation has no analytical answer for the mentioned structure. Numerical approximations should be used to solve it. One of the methods used is the use of finite difference approximation method. In this method, we first divide the desired spatial range (between zero and L) into N parts and number them so that the zero point shows the left border and the N_{th} point shows the right border.

The value of the wave function at the zero and nth points is given by the boundary conditions that are part of the problem statement. The purpose of the calculations is to obtain the wave function at the N-1 point inside the piece. For this purpose, with the help of the finite difference approximation, we write the second derivative term as follows:

$$\frac{d^2\psi}{dx^2}=\frac{\psi(x-\Delta x)-2\psi(x)+\psi(x+\Delta x)}{\Delta x^2} \tag{6}$$

By placing this approximation of the second-order derivative in the Schrodinger equation, we arrive at the following category of equations:

$$if\,n=1 \rightarrow \frac{-\hbar^2}{2m}\left[\frac{\psi(2)-2\psi(1)+\psi(0)}{\Delta x^2}\right]+V(1)\psi(1)=E\psi(1)$$

$$if\,n=2 \rightarrow \frac{-\hbar^2}{2m}\left[\frac{\psi(3)-2\psi(2)+\psi(1)}{\Delta x^2}\right]+V(2)\psi(2)=E\psi(2)$$

$$\vdots$$

$$if\,n=n \rightarrow \frac{-\hbar^2}{2m}\left[\frac{\psi(n+1)-2\psi(n)+\psi(n-1)}{\Delta x^2}\right]+V(n)\psi(n)=E\psi(n)$$

$$if\,n=N-1 \rightarrow \frac{-\hbar^2}{2m}\left[\frac{\psi(N)-2\psi(N-1)+\psi(N-2)}{\Delta x^2}\right] + V(N)\psi(N)=E\psi(N) \tag{7}$$

With a little care we realize that we have N-1 unknowns. Our unknowns are ψ (1) to ψ (N-1) and ψ (0) and ψ (N) are known by boundary conditions.

$$-\frac{\hbar^2}{2m}(A\psi+A_n)+V*\psi=E\psi \tag{8}$$

$$\begin{pmatrix} \frac{2}{\Delta x^2}+V_1 & -\frac{1}{\Delta x^2} & & & & \\ -\frac{1}{\Delta x^2} & \frac{2}{\Delta x^2}+V_2 & -\frac{1}{\Delta x^2} & & & \\ & \ddots & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & & & -\frac{1}{\Delta x^2} & \frac{2}{\Delta x^2}+V_{n-1} & -\frac{1}{\Delta x^2} \\ & & & & -\frac{1}{\Delta x^2} & \frac{2}{\Delta x^2}+V_n \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \vdots \\ \psi_{n-1} \\ \psi_n \end{pmatrix} = E \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \vdots \\ \psi_{n-1} \\ \psi_n \end{pmatrix} \tag{9}$$

Hamilton exciton is an equation (7) that can be written as equations (8), (9) and (10) for electrons and holes.

$$H_{ex}=-\frac{\hbar^2}{2m_e^*}\nabla_e{}^2-\frac{\hbar^2}{2m_h^*}\nabla_h^2-\frac{e^2}{4\pi\varepsilon_0|\vec{r}_e-\vec{r}_h|}+V_e(\vec{r}_e)+V_h(\vec{r}_h) \tag{10}$$

$$H_e = -\frac{\hbar^2}{2m_e^*}\nabla_e{}^2 + V_e(\vec{r}_e) \quad (11)$$

$$H_h = -\frac{\hbar^2}{2m_h^*}\nabla_h^2 + V_h(\vec{r}_h) \quad (12)$$

$$H^{'} = -\frac{e^2}{4\pi\varepsilon_0|\vec{r}_e - \vec{r}_h|} \quad (13)$$

The exciton wave function in a semiconductor structure can be thought of as a wave packet that is a linear combination of electron and hole Bloch wave functions.

$$\psi(r_e,r_h) = \sum_{k_e,k_h}\Phi(k_e,k_h)\phi_{ck_e}(r_e)\phi_{vk_h}(r_h) = \sum_{k_e,k_h}\Phi(k_e,k_h)u_{ck_e}(r_e)e^{ik_e.r_e}u_{vk_h}(r_h)e^{ik_h.r_h} \quad (14)$$

The exciton push function describes the relative motion of the electron-hole system at a scale greater than the atomic distance and will therefore follow the Schrodinger equation of two particles. [20]

$$[-\frac{\hbar^2}{2m_e}\nabla_e{}^2 - \frac{\hbar^2}{2m_h}\nabla_h{}^2 - \frac{e^2}{4\pi\varepsilon_0|r_e - r_h|}]\Phi = E\Phi \quad (15)$$

The Hamiltonian of the system is as above.

CONCLUSIONS

We calculated the Hamiltonian value of the whole system using MATLAB software and writing a program to solve the Schrodinger- Exciton equation.

On the other hand, the value of the exciton wave function can be defined as follows: α is the normalization coefficient

To calculate the amount of exciton energy, we use the following equation:

E_b=E_e+E_h- E_{ex} (16)

Our material of choice is GaAs/$Al_{0.15}Ga_{0.85}As$, and we considered the limit potential of electrons and holes in this structure to be the following values:

V_e=0.57 ΔE_g, V_h=0.43 ΔE_g

ΔE_g=E_{gb}-E_{gw}

ΔE_g =1.155x+0.37x^2(ev)

$Al_xGa_{1-x}As$ for $Al_{0.15}Ga_{0.85}$ As for molar coefficient x = 0.15 will be equal to:

ΔE_g =1.155x+0.37x^2= 1.155* 0.15+0.37*$(0.15)^2$= 0.24083(ev)

$$\frac{me*}{m0} = 0.0665$$

$$\frac{mhh*}{m0} = 0.34$$

$$\frac{mlh*}{m0} = 0.094$$

We performed the calculations with a heavy cavity and assumed a dielectric constant of K = 12.5.

We solved the Schrodinger equation in one dimension by the finite difference method and then generalized the program to three dimensions. In the next step, we extended the Schrodinger equation to electrons and holes and calculated the values of the electron wave function and the hole wave function Ψe, Ψh and r. Based on the calculations, we obtained the value of the exciton wave function. Then, by calculating the Hamiltonian of the electron and the hole, the Hamiltonian of the exciton was obtained, and by minimizing the excitonic energy relative to the input parameter α, the base state energy of the exciton was calculated from the following equation:

$$E_{ex}(\alpha)=\frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} \quad (17)$$

With investigation of the obtained values, the following results were obtained:

The energy of the exciton dependence is directly proportional to the width of the potential barrier width. Comes with an increase.

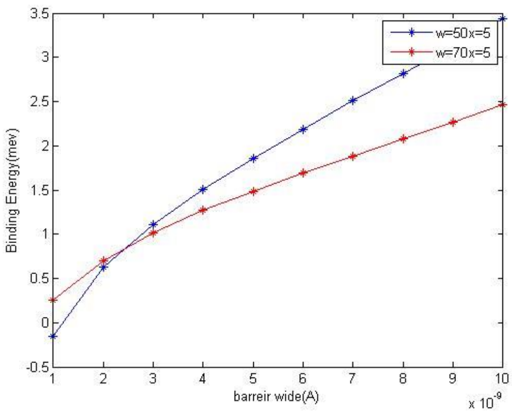

Fig. 4 . Energy changes of the exciton dependence on the width of the potential barrier width with the width of the potential well 50 and 70 angstroms and the coefficient of 5 molar.

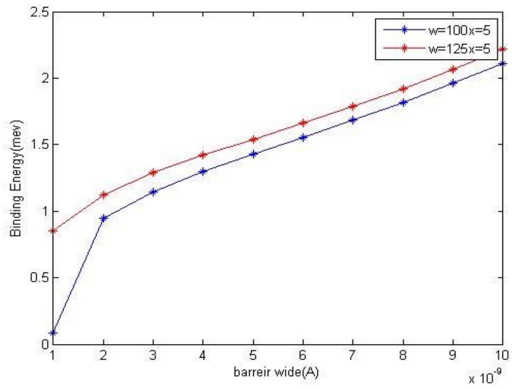

Fig 5. The energy changes of the exciton depend on the width of the potential barrier with the width of the potential well 100 and 125 angstroms and the coefficient of 5 molar.

Regarding the dependence of exciton dependence energy on changes in potential well width, the results show that at points with potential well width less than 100 angstroms, the dependence energy decreases, but more than this, the exciton dependence energy increases with increasing potential well width. increase. This increase in exciton-dependent energy also increases with increasing width of the potential barrier at such quantum points.

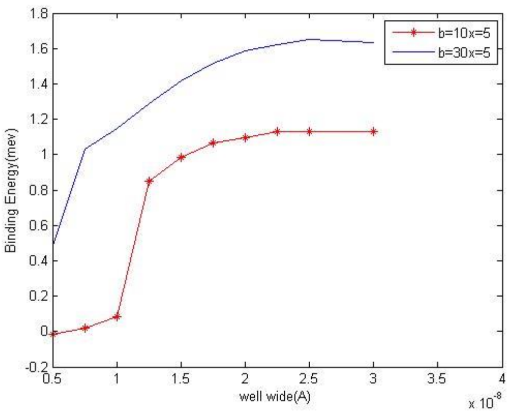

Fig. 6. Energy changes of the exciton dependence on the width of the potential well with the width of the potential barrier 10 and 30 angstroms and the coefficient of 5 molar.

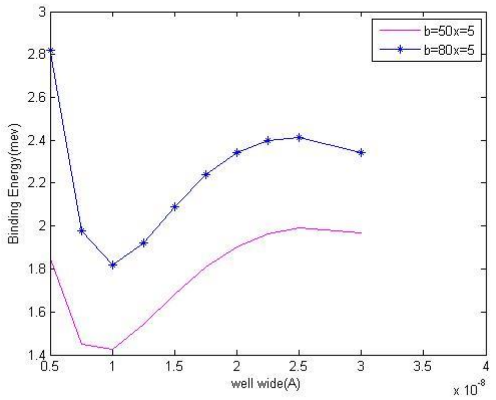

Fig. 7. Energy changes of the exciton dependence on the width of the potential well with the width of the potential barrier 50 and 80 angstroms and the coefficient of 5 molar.

By calculating the energy of exciton dependence with different molar coefficients, it was observed that: In each sample, the exciton dependence energy decreases with increasing molar coefficient. At a constant molar coefficient, the exciton dependence energy increases as the potential barrier width increases. At a constant molar coefficient, the exciton dependence energy increases as the potential well width increases.

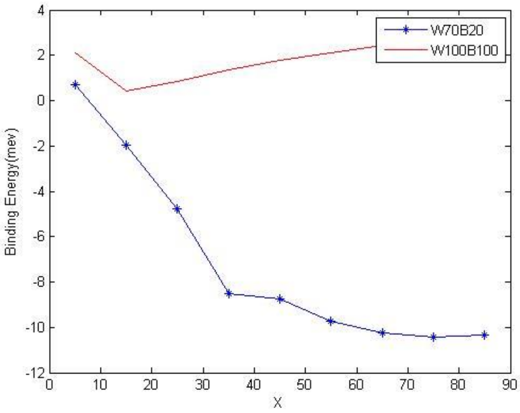

Fig. 8. Energy changes of exciton dependence on changes in molar coefficient with potential width of 70 and 100 angstrom wells and width of potential barrier of 20 and 100 angstroms.

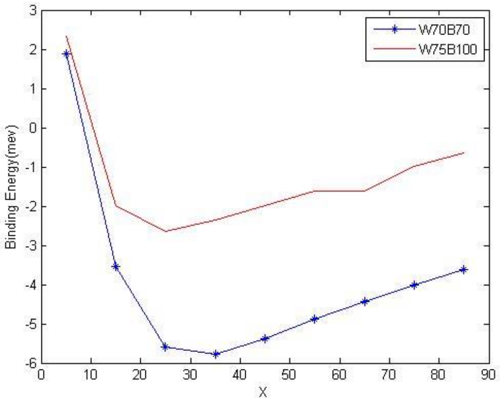

Fig. 9. Energy changes of exciton dependence on changes in molar coefficient with potential width of 70 and 75 angstrom wells and width of potential barrier of 70 and 100 angstroms.

The variation of exciton dependence energy were plotted for molecules with well widths of 10,100,60,70,75 angstroms and barrier widths of 20,100,40,70 and 100 angstroms of different values of the molar coefficient, respectively. The exciton in these molecules is inversely related to the molar coefficient, and as the values of the molar coefficient increase, the exciton dependence energy of the molecule also decreases.

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مجله شیمی فیزیک و شیمی نظری
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بررسی و مطالعه خواص نوری اکسایتون بر اساس نقطه کوانتومی مولکولی

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چکیده

خواص نوری نیمرساناها، دی الکتریک ها و فلزات نقش کلیدی در توسعه سلول های خورشیدی لایه نازک دارند. در حالی که این دستگاه ها متعلق به آشکارسازهای فوتونی هستند، طبیعت فوتونی و موجی نور بر عملکرد آنها تأثیر می گذارد. برخی از این مشکلات مطرح شده است. در این مقاله معادله شرودینگر را با استفاده از روش عددی تقریب تفاضل محدود حل می‌کنیم و فرض قرار داده که ساختار مولکول نقطه کوانتومی ما دو نقطه کوانتومی GaAs مکعبی $L_X * L_Y * L_Z$ در محیط AlxGa1-xAs بر این می یاشد که شبیه‌سازی انرژی وابستگی اکسایتون با ابعاد مختلف. ضرایب مولی مشاهده شد که: در نمونه با افزایش ضریب مولی انرژی اتصال اکسایتون کاهش می‌یابد. در یک ضریب مولی ثابت، انرژی وابستگی اکسایتون با افزایش عرض مانع بالقوه افزایش می‌یابد. در یک ضریب مولی ثابت، انرژی اتصال اکسایتون با افزایش عرض چاه بالقوه افزایش می‌یابد.

کلید واژه‌ها: انرژی بستگی پیوندی؛ نقطه کوانتومی مولکولی؛ ضریب مولار؛ تولید نوری

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