

## Study of the impact of quantum confinement energy on the energy gap and activation energy of indium phosphide (InP) and indium arsenide (InAs)

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This study examines how quantum confinement energy affects the electrical characteristics represented by the energy gap. and the activation energy of indium arsenide (InAs) and indium phosphide (InP) was studied using a computer program (MATLAB) version (R2012a), which is based on the characteristic matrix theory and Bruce's model, we found that the energy gap increases with the quantum confinement energy at small nanoscales, as well as the activation energy due to the quantum confinement effect, but these electrical properties decrease with the quantum confinement energy at large nanoscales.

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### 1. Introduction

The properties of nanomaterials are different compared to bulk materials due to the unique nano size (1–100 nm), in terms of their physical, chemical, electrical and magnetic properties [1]. Quantum dots (QD) play an important role in the construction of optical and electronic devices [2]. (QD) are semiconductor nanoparticles that exhibit three-dimensional confinement, and thus represent the limit for low-dimensional structures due to their three-dimensional carrier configuration. Charge carriers become spatially confined when the radius of the (QD) conductor becomes smaller than the Bohr radius of the exciton (which is the average distance between an electron in the conduction band and the hole it leaves behind in the valence band) [3]. Discrete quantum energy levels of (QD) are more closely related to atoms [4]. Due to this similarity between (QD) and atoms, they are often termed as artificial atoms [5], the behavior of (QD) depends mainly on the confinement energy of the charge carriers (electrons and holes) [6]. For this reason, a deeper understanding of confinement energy in (QD) is critical. Trapping charge carriers in QD results in quantization of size [7], and this has important implications for the blue-shifting absorption and emission spectra with decreasing point size [8]. The band gap is tunable by changing the size of quantum dots (QD) based on the quantum confinement effect which plays an essential role in the optical and electrical properties of (QD).

### 2. Experimental

#### 2.1. Quantum confinement energy

Quantum confinement energy is a very important property of QD, this energy is observed when there is an increase in the energy gap, it is very important because it determines the emission energy of the quantum dot, quantum confinement energy mainly deals with the trapping of electrons [9]. Quantum mechanics describes a particle in the box model, that is a particle that moves freely in a small space surrounded by insurmountable barrier. The simplest model is a one-dimensional system in which a particle is constrained by the length of a box from which it cannot escape [10]. Given the energy of confining the particle in a one-dimensional box [10].

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$$E_{con} = \frac{n^2 \hbar^2 \pi^2}{2mL^2} \quad (1)$$

where (m) the mass of the particle, (n) the quantum number, (L) the length of the box, the above equation was measured as a result of fulfilling the boundary conditions imposed on the system. In addition, the minimum energy of the particle is at  $n = 1$  i.e. the minimum energy of the particle is not zero so the above equation becomes.

$$E_{con} = \frac{\hbar^2 \pi^2}{2mL^2} \quad (2)$$

The electron and the hole in (QD) are arranged like particles in a box., move freely but cannot move outward. Although we used the model for particles in a box to study the effect of quantum confinement, there are some differences in the quantum dots. There are two particles (an electron and a hole) inside them instead, of one particle in a box. Secondly the QDs are geometrically spherical and not square, so the box length is changed to the radius ( $r_{ps}$ ). Also, the electron and hole masses are replaced by their effective masses due to their interaction with the crystal lattice. Thus, the ground state quantum confinement energy equation for quantum dots becomes the following for [11].

$$E_{con} = \frac{\hbar^2 \pi^2}{2r_{ps}^2} \left[ \frac{1}{m_e^*} + \frac{1}{m_h^*} \right] \quad (3)$$

$E_{con}$ : represents the quantum confinement energy

$r_{ps}$ : is the radius of a spherical quantum dot

$m_e^*$ : electron's effective mass

$m_h^*$ : the gap's effective mass

## 2.2. Effective mass approximation (EMA) mode

This model display how the energy gap of a quantum dot in a semiconductor depends on the size of the (QD). It is often called the Bruce model. It is an important theoretical model that considers both the effective masses' values of an electron and a hole, which change according to the type of material. Moreover, the quantum dot energy gap variation value ( $\Delta E_g$ ) is given according to this model according to the Bruce equation in the following formula [12].

$$\Delta E_g = \frac{\hbar^2 \pi^2}{2r_{ps}^2} \left[ \frac{1}{m_e^*} + \frac{1}{m_h^*} \right] - \frac{1.786 e^2}{\epsilon r_{ps}} - \frac{0.124 e^4}{h^2 \epsilon^2} \left[ \frac{1}{m_e^*} + \frac{1}{m_h^*} \right]^{-1} \quad (4)$$

When  $r_{ps}$  represents the radius of the particle and  $m_e^*$  the effective mass of the electron,  $m_h^*$  the effective mass of the hole, and the  $\epsilon$  relative permittivity, also known as the dielectric constant.

And also

$$\Delta E_g = E_g^{nano}(r_{ps}) - E_g^{bulk}$$

With which equation (4) takes the form [13].

$$E_g^{nano}(r_{ps}) = E_g^{bulk} + \frac{\hbar^2 \pi^2}{2r_{ps}^2} \left[ \frac{1}{m_e^*} + \frac{1}{m_h^*} \right] - \frac{1.786 e^2}{\epsilon r_{ps}} - \frac{0.124 e^4}{h^2 \epsilon^2} \left[ \frac{1}{m_e^*} + \frac{1}{m_h^*} \right]^{-1} \quad (5)$$

The energy gap is inversely proportional to  $r_{ps}^2$ , as shown by the second component on the right-hand side of equation (5), implying that the energy gap narrows as the nano particle size increases. Because the strength of the columbic interaction has increased, the third term in the

equation can be ignored, resulting in a drop in the energy gap with decreasing  $r_{ps}$ . Because the third and final terms are so small in comparison to the second term, they can be overlooked. As a result, equation (5) becomes.

$$E_g^{nano}(r_{ps}) = E_g^{bulk} + \frac{\hbar^2 \pi^2}{2r_{ps}^2} \left[ \frac{1}{m_e^*} + \frac{1}{m_h^*} \right] \quad (6)$$

We observe that the energy gap widens with decreasing nanoparticle size as a result of quantum confinement. However, when a substance's (QD) radius approaches or equals the natural Bohr radius  $\alpha_o$  of the exciton, which is determined by the following relation [14], the quantum confinement is significant.

$$\alpha_o = \frac{4\pi\epsilon_o\epsilon_r\hbar^2}{e^2} \left[ \frac{1}{m_e^*} + \frac{1}{m_h^*} \right] \quad (7)$$

When  $\epsilon_r$  and  $\epsilon_o$  represent the dielectric constant of the vacuum and the semiconductor material, respectively, and  $e$  represents the electron charge.

### 2.3. Characteristic matrix theory

When electromagnetic radiation strikes a single thin film with two dividing borders that has been produced on the substrate material as shown in Fig. 1.

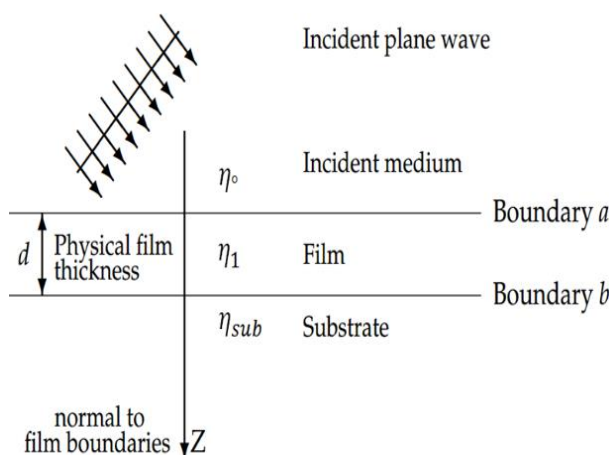


Fig. 1. Depicts the impact of a plane wave on a thin film [15].

Using the characteristic matrix [16], which connects the optical permittivity of the system for any polarization and for both vertical and oblique incidence, the continuous tangential elements of the magnetic and electrical fields entering and leaving the system, and it is provided as the following formula [17].

$$\begin{bmatrix} B \\ C \end{bmatrix} = \begin{bmatrix} \cos\delta & i\sin\delta/\eta_1 \\ i\eta_1\sin\delta & \cos\delta \end{bmatrix} \begin{bmatrix} 1 \\ \eta_{sub} \end{bmatrix} \quad (8)$$

The matrix's elements, which stand in for the electric and magnetic fields, are represented by the letters (B, C). The membrane's optical permittivity is represented by the number  $\eta_1$ , and the substrate's optical permittivity is represented by the number  $\eta_{sub}$ .

The reflectivity value of the electromagnetic beam falling on a surface separating two different media is given by Vernel equations [18].

$$R = \left( \frac{\eta_o - \eta_1}{\eta_o + \eta_1} \right)^2 \quad (9)$$

where  $\eta_1$  and  $\eta_o$  denote the appropriate effective refractive index for the incidence and penetration modes, respectively

### 3. Results and discussion

The values of the energy gap and the activation energy were calculated as a function of the change in the quantum confinement energy at the small and large nanosizes for indium arsenide (InAs) and indium phosphide (Inp) using a computer program (MATLAB) version (R2012a).

#### 3.1. Energy gap of (InAs, Inp)

Initially, the relationship between the energy gap and the quantum confinement energy was studied as functions of the nanoscale grain size of the materials under study. We observed that the material behaves similarly to its behavior in the normal state (i.e., the bulk material) at large volumes, but with a gradual decrease in volume until we reach the Bohr exciton radius for that material. which ends with a nanoscale grain size close to (2.6 nm) it is found that there is a wide variation in energy gap and quantum confinement energy at nanosizes smaller than (10 nm) as shown in the figures below.

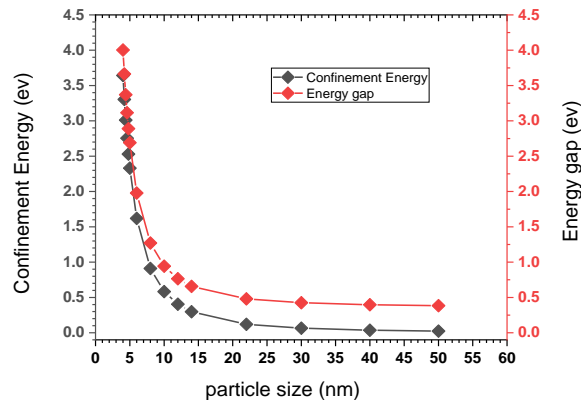


Fig. 2. Energy gap and quantum confinement energy for indium arsenide (InAs) as function of particle size at the nanoscale.

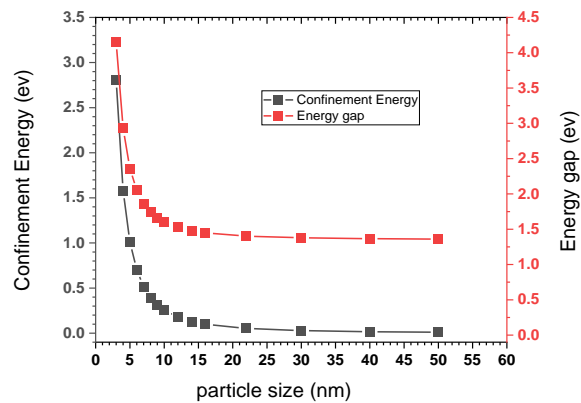


Fig. 3. Energy gap and quantum confinement energy for indium phosphide (Inp) as functions of nanoscale particle size.

Figure 2 & 3 indicate, energy gap value is high at tiny sizes. (PS=10nm), then it begins to decrease gradually when the particle size of the material exceeds the Bohr radius of the exciton, it becomes almost constant, due to quantization of its sizes (quantization of the density of states), this arises because the nanoparticle size is comparable to the de Broglie wavelength of its charge carriers (i.e., electrons and holes) [19]. On the other hand, we note that the quantum confinement energy is inversely proportional to the size of the nanoparticle, and this is shown from the above figures, where at large sizes (PS=50nm), we note that the quantum confinement energy is small, but does not approach zero, as the lowest possible energy for the quantum dot sample is not equal to zero, i.e. the confinement of the ground state of the electrons in (QD) is not zero. This means that the electrons in the (QD) are not fixed, but rather have kinetic energy in a manner similar to a particle in a box, and on the contrary, it increases when the sizes are as small as (PS=10nm) [20].

Now we explain more the change that occurs to the nanoscale energy gap and the quantum confinement energy through the following figures:

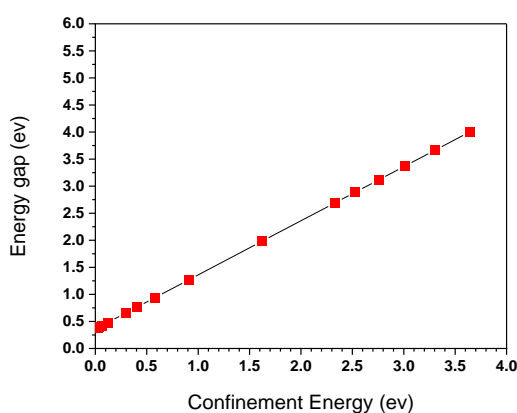


Fig. 4. The energy gap of indium arsenide (InAs) as a function of the the quantum confinement energy.

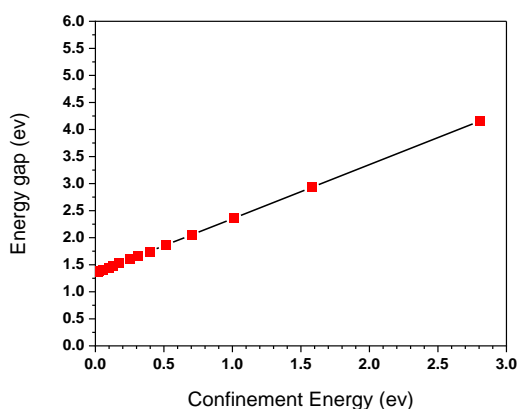


Fig. 5. The energy gap of indium phosphide (Inp) as a function of the quantum confinement energy.

We notice from the above figures that when it is large the quantum confinement energy is matched by an increase in the nanoscale energy gap this happens at small particle size as we said previously. On the contrary, the quantum confinement energy and the energy gap decrease at large nanovolumes. We notice in the material indium arsenide (InAs) when the confinement energy is (3.6ev) the nanoscale energy gap reaches (4.0ev) at a small size (PS = 4nm), but at large sizes (PS = 50nm) the quantum confinement energy is very small (0.02ev), and the energy gap (0.4ev) is also very small. There is a direct relationship between the nano-energy gap and the quantum

confinement energy resulting from the change in the particle size. Therefore, whenever the quantum confinement energy increases, that is, the quantum confinement of electrons increases. This increase leads to the division of the edge of the valence and conduction bands into separate and quantitative electronic levels. These electronic levels are similar to those in atoms and molecules and thus the value of the energy gap increases [21].

### 3.2. Activation Energy of (InAs, Inp)

In this part, at the beginning, we showed how the activation energy and the quantum confinement energy of materials (InAs), (InP) change as a function of nanoparticle size shown in the figures below:

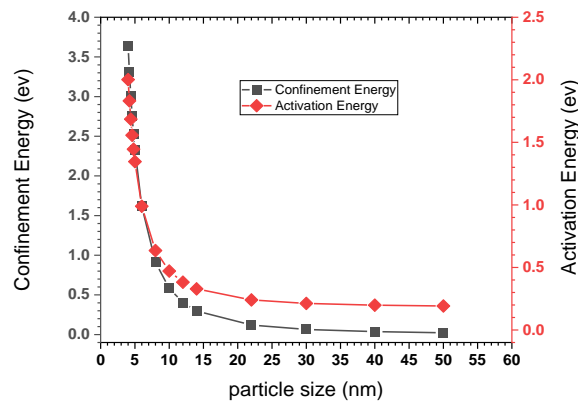


Fig. 6. Activation energy and quantum confinement energy for indium arsenide (InAs) as functions of nanoscale particle size.

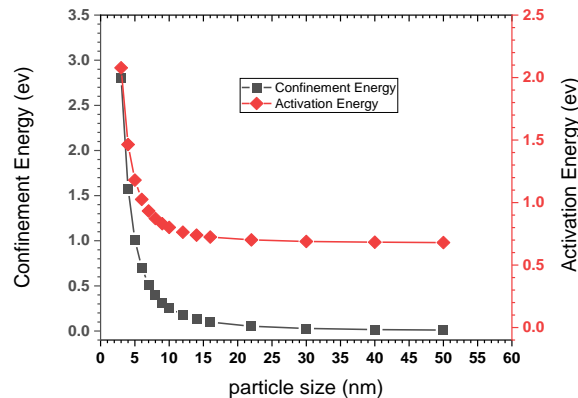


Fig. 7. Activation Energy and quantum confinement energy for indium phosphide (Inp) as functions of nanoscale particle size.

The figures above show that the values of the activation energy are large at small nano-sizes, that is, when there is a quantum confinement of the material, that is, when its size approaches the Bohr radius of the exciton, this corresponds to an increase in the quantum confinement energy, whose value increases as we said earlier at small nano-sizes, since the energy gap increases with the increase in the energy of quantum confinement due to the effect of quantum confinement of electrons [22], we note that the change in the activation energy with the particle size is similar to the change in the energy gap. When we compare the activation energy curve with the energy gap curve, we notice a great similarity between them. This is because the activation

energy is at the fermi level, which is located in the middle of the energy gap, meaning that the activation energy is equal to half of the energy gap [23]. We will now describe the change in the activation energy with the change in the quantum confinement energy resulting from the change in the nanoparticle size of the same studied materials:

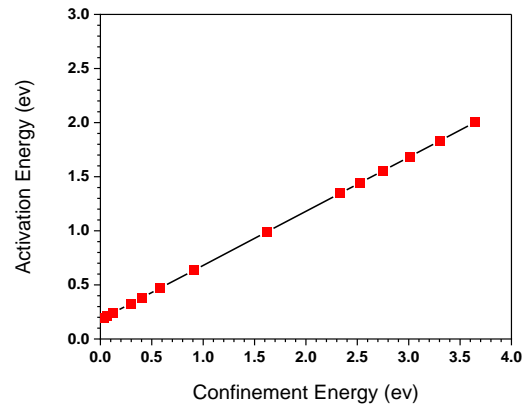


Fig. 8. Activation Energy of indium antimonide (InAs) as a function of the quantum confinement energy.

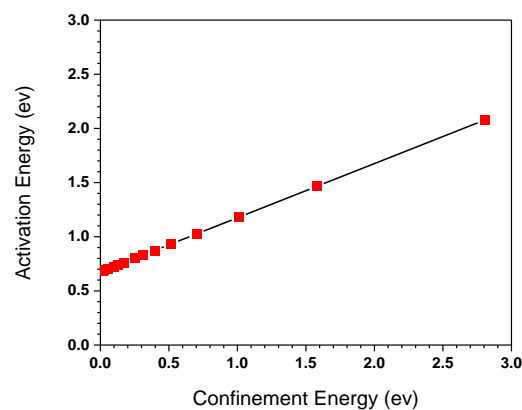


Fig. 9. Activation Energy of indium phosphide (InP) as a function of the quantum confinement energy.

We notice from these figures how the activation energy increases gradually with the increase in the quantum confinement energy, so let's take the material indium phosphide (InP) at small sizes (PS = 3nm) We note that the value of the quantum confinement energy is high (2.8eV), while the activation energy value is also high (2.1eV). As for large sizes (PS = 50nm), the value of the quantum confinement energy is very low (0.01eV), and the activation energy value is also low (0.7eV), the above increase at small sizes is explained by the effect of quantum confinement, as we explained at the beginning of our explanation. When a quantitative confinement is made on the material, that is, the size of the body will approach the Bohr radius of the exciton, in this case, the surface area will increase relative to the size [24], corresponding to an increase in the grain boundaries, and because of the large concentration of charge carriers in the grain boundaries, this leads to an increase in resistance. And since previous studies generally indicate that the activation energy is enhanced when the resistance is increased, therefore, we will notice a clear increase in the activation energy for small nanosizes [25].

#### 4. Conclusions

We noticed that the material exhibits a natural behavior similar to its behavior in the natural state (i.e. bulk material) at large sizes. But, with a gradual decrease in size until we reach the Bohr radius of the exciton, the quantum confinement energy increases, corresponding to an increase in the energy gap due to the effect of quantum confinement. We also noticed that the activation energy also increases with the energy gap, as the change in the energy gap is similar to the change in the activation energy, as the activation energy is located at the Fermi level, which is located in the middle of the energy gap, meaning that the activation energy is equal to half of the energy gap.

Quantum confinement energy is small, but does not approach zero, as the lowest possible energy for the sample of the quantum dot is not equal to zero, meaning that the confinement of the ground state of the electrons in (QD) is not zero. This change in the energy gap and the quantum confinement energy with the (QD) size of these materials makes them of great interest in many applications in optoelectronics, sensors, optical coatings, and solar cells.

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