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Examining the impact of quantum confinement energy on the optical characteristics of zinc sulfide and gallium nitrate in the ultraviolet spectral range

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The study of confined quantum systems exhibit distinct behavior compared to that in bulk solids. This enables the design of materials with tunable chemical, physical, electrical and optical properties. In this paper, the effect of quantum confinement energy on the optical properties (gap energy, refractive index) of semiconductors gallium nitrate (GaN) and zinc sulfide (ZnS) is studied. The study is done using the MATLAB computer program (20a). This software is based on the Brus model and the particle in-a-box model. The results indicate that the optical properties depend on the quantum confinement energy, with an increase in quantum confinement energy corresponding to an increase in the energy gap and a decrease in refractive index.

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1. Introduction

In general, quantum correlation can be found when a material's dimensions match the wavelengths of electrons in the sample. Quantum correlation causes a change in the material's electronic structure, and the electrical and optical properties are different from those of the bulk material [1]. Nanomaterials having size-dependent characteristics can be three-dimensional (3D) colloids or two-dimensional (2D) quantum wells. Quantum wires (1D) and quantum dots (0D)[2]. The increase in surface area relative to the size of the nanomaterial, along with the wide energy gap, are the two characteristics of semiconductor nanoparticles that are most significant because they play a significant role in the electrical and optical properties of semiconductor materials. This change in properties manifests itself primarily in the estimation of the energy levels of electrons. This phenomenon is referred to as quantum confinement[3].

2. Theoretical Framework

2.1. Brus model

Energy level formation in semiconducting nanomaterials is unique due to the quantum correlation effect. The Bruce model in one of the most common theoretical models that allow studying the relationship between the volume of materials and the energy gap [4-5].
The model of particles in -a -box of quantum mechanics portrays a particle traveling freely in a limited space surrounded by an impenetrable barrier. The most fundamental model is a one-dimensional system in which the particle's mass is proportional to the length of a box from which it cannot escape. Here we use the Schrödinger equation to obtain the wave function and energy levels of a particle trapped in a one-dimensional box [6].

$$E_n = \frac{n^2 \hbar^2 \pi^2}{2L^2 m} = \frac{n^2 h^2}{8L^2 m} \quad (1)$$

$E_n$is the confinement energy, n is the fundamental quantum number, L is the length of the box, m is the mass of the particle (electron), $\hbar$ is Planck's constant divided by 2π. The 1-dimensional

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particle-in-a-box model can be easily extended to a 3-dimensional box, which is more relevant and describes the behavior of quantum dots that confine an electron in three dimensions selting the energy of the particle [7].to:

$$E_n = E_x + E_y + E_z = \frac{h^2}{8m}\left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2}\right) \quad (2)$$

In quantum dots (QDs), the electron and hole are restricted such that they move freely inside the dot but cannot depart, just like a particle in a box. As a result, quantum dots (QDs) are genuine particles in a box. Due to their similarities, we employed the particle-in-a-box model to investigate the effect of quantum confinement on the properties of quantum dots. However we have made some adjustments to compensate for the discrepancies.

First, there are two particles inside the quantum dots (an electron and a hole) instead of one as shown in the particle-in-the-box model.

Second, quantum dots (QDs) are geometrically spherical infinite square well in, so the square length L is replaced by the radiusr_{ps}.

Third, the electron and hole masses are replaced by their effective masses due to their interaction with the crystal lattice. Thus, it becomes the quantum confinement energy in quantum dots (QDs).

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

where r_{ps} quantum dot's radius , m_e^* effective mass of excited electron, m_h^* effective mass of excited hole. However, electrons in QDS do not move in a vacuum unlike particles in a box, but rather move inside a semiconductor crystal with an energy gap which contribute to the basic energy of the system. Quantum dot energy gap (QDS) It is the sum of the energy gap in the semiconductor plus the energy of the quantum confinement on the quantum dots [8].

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

$E_g^{nano}(r_{ps})$ is the band gap energy of quantum dot , E_g^{bulk} band gap energy of bulk semiconductor. We see that the energy gap widens with the reduction in body size as a result of the quantum confinement effect. The following relationship (5) describes how the quantum confinement increases when the radius of matter particles approaches or equals the natural Bohr radius of the exciton[9]:

$$\alpha_\circ = \frac{4\pi\varepsilon_\circ\varepsilon_r\hbar^2}{e^2}\left[\frac{1}{m_e^*} + \frac{1}{m_h^*}\right] \quad (5)$$

where $\varepsilon_r and\ \varepsilon_\circ$ represent the dielectric constants of the vacuum and the semiconductor material, respectively, and e denotes the electron charge.

2.2. Index of refraction and energy gap

There have been numerous attempts to link the refractive index and energy gap E_g using straightforward relationships because the refractive index and the material's energy band structure are closely related[10–11]. However these correlations are not affected by the temperature or the energy of the incident photons[11]. Several correlations between n andE_g are examined. Various correlations between the band gap and the high-frequency refractive index are also proposed, as is a linear form of n as a function of E_g.

$$n = \alpha + \beta E_g \quad (6)$$

where α = 4.048&˘β = −0.62 ev^{-1}

Using the basic physics of light refraction and dispersion, an empirical relationship is proposed as [1 2] .

$$n = \sqrt{1 + \left(\frac{A}{E_g + B}\right)^2} \tag{7}$$

3. Results

The particle in-a-box model was used to investigate the link between quantum confinement energy and nanoscale particle size in semiconducting materials.

We are study its effect on the optical properties using the MATLAB program. The program was prepared using the Brus model, as fifteen different granular sizes were determined for each material, starting with the sizes at which the materials behave similarfy to the Bulk and were between (40-60 nm), then gradually reducing the size until we reach a bohr diameter of the exciton of that substance, and let us end with a granular size close to (2nm). Thus, the granular size of each material we determined, and then the quantum energy gap was calculated at each size.

Table 1. Some physical properties of used optical materials [13-14-15].

Material	Refractive Index	E_g^{bulk} (eV)	m_e^*	m_h^*	Bohr radius $a_\circ(nm)$
GaN	2.4	3.4	0.20	0.80	3.1
ZnS	2.4	3.68	0.34	0.23	5

4. Discuss the results

4.1. Quantum confinement energy

The quantum confinement energy graph is shown as a function of the nanoscale grain size of the quantum dots. Inversely depending on the size of the quantum dots which is given by the following relation ($Ps = 2r_{ps}$).With r_{ps} the radius of the quantum dots. The confinement energy reduces with increasing quantum dot size but never reaches zero for the various QDs under consideration. Thus, the ground state of electron confinement in QDs is not zero, which means that electrons in QDs are not stationary, but have kinetic energy in a similar way to a particle in a box [16]. We also notice from the Figure 1&2 when the size of the quantum dots is (40-10) nm the values of the energy of the quantum confinement are low this is called weak quantum confinement and the reason for this is that the size of the quantum dots is greater than the Bohr diameter of the exciton. The energy levels are semi-continuous. And when the size of the quantum dots is less than 10 nm, the effects of severe quantum confinement begin to appear, as the size of the quantum dots is less than the bohr diameter of the exciton ($r_{Boher} = 2a_\circ$). In relation to zinc sulfide (zns), strong quantum confinement appears when the size of the quantum dots is 10 nm where the is bohr diameter of the exciton ($r_{Boher} = 2a_\circ$ =10nm) where ($a_\circ$ was the Bohr radius of the exciton) and at this size the quantum confinement energy is E_{con}=0.10ev and up to E_{con} =1.21ev of a size 3nm.Also, with respect to gallium nitrate (GaN), the strong quantum confinement starts at r_{Boher} =6.2, and the quantum confinement energy at this size is E_{con} =0.26ev and reaches E_{con} =1.39ev of a size 2.6nm.

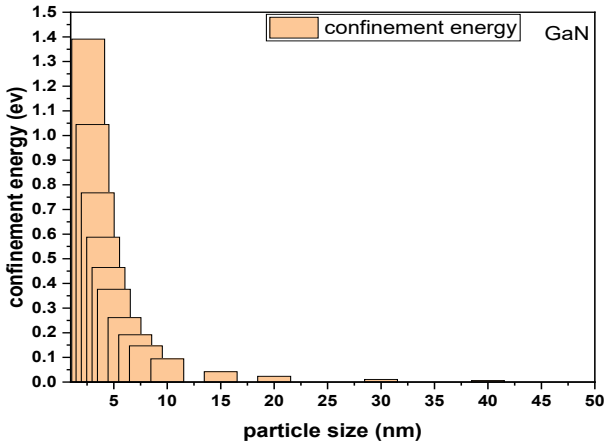

Fig. 1. The change in the energy of quantum confinement of gallium nitrate (GaN) as a function of nanoparticle size.

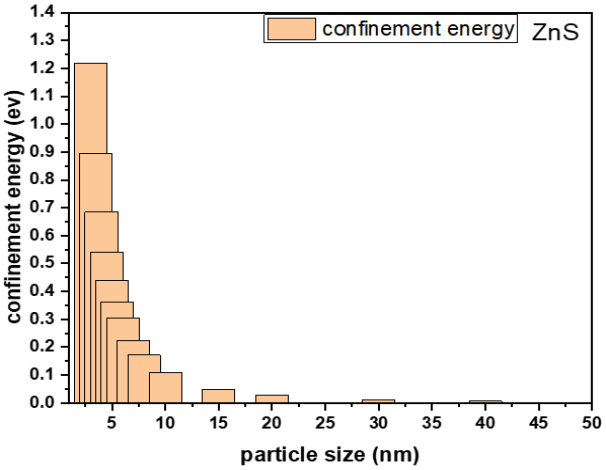

Fig. 2. The change in the energy of quantum confinement of zinc sulfide (ZnS) as a function of nanoparticle size.

4.2. Energy gap

The relationship between the quantum confinement energy and the energy gap was studied using the Bruce model (effective mass approximation model) As the figures show 3 &4.

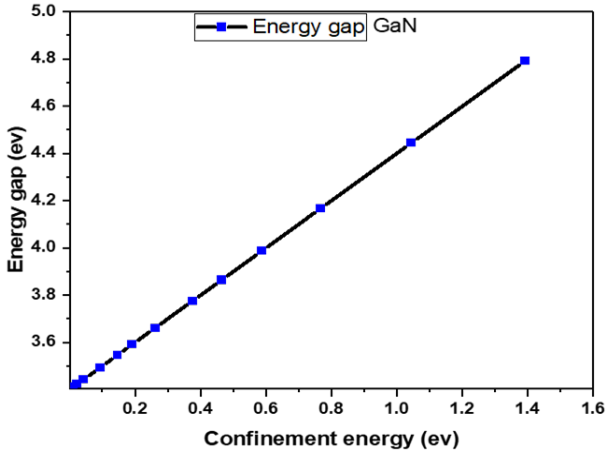

Fig. 3. the variation in the energy gap of semiconductor materials (GaN) is depicted as a function of the quantum confinement energy.

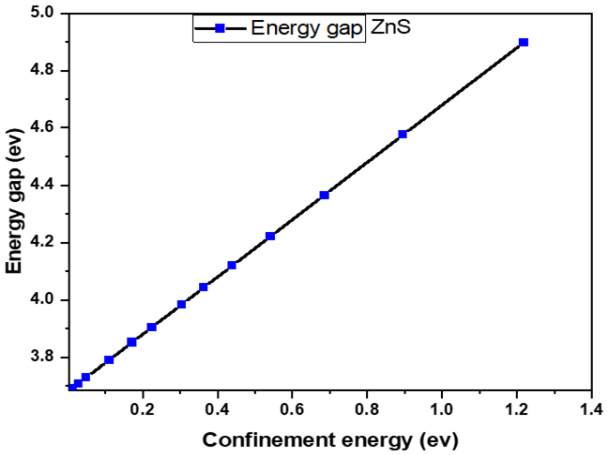

Fig. 4. the variation in the energy gap of semiconductor materials (ZnS) is depicted as a function of the quantum confinement energy.

Most semiconductor materials behave similarly. As we notice that the value of the energy gap is large when the reservation energy. The quantum is large and then gradually decreases when the quantum confinement energy decreases. On the other hand, the increase in the energy gap at very small nano-sizes is produced to increase the quantum confinement of electrons, which leads to an edge splitting.

4.3. Refractive index

We note from the figures 5&6 that the refractive index is almost stable for nanosizes (20-60nm)where the quantum confinement is weak and with a decrease in the nanogranular size that leads to an increase in the quantum confinement energy and a decrease in the refractive index .

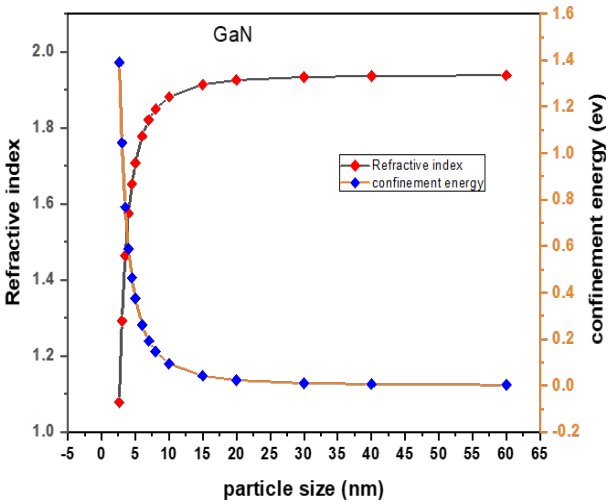

Fig. 5. Depicts the relationship between the refractive index and the quantum confinement energy of (GaN) material as a function of nanoparticle size.

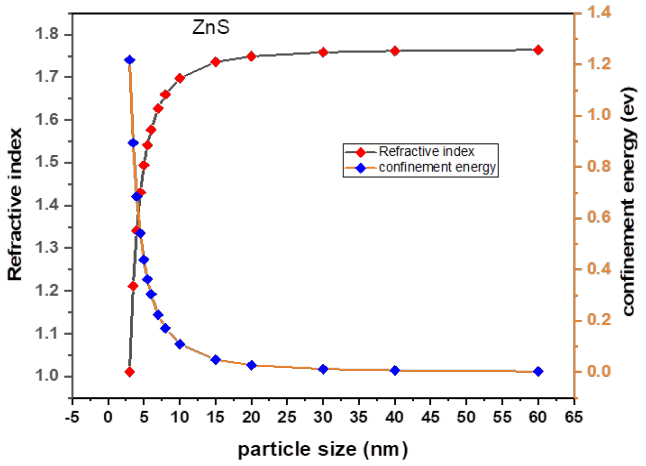

Fig. 6. Depicts the relationship between the refractive index and the quantum confinement energy of (ZnS) material as a function of nanoparticle size.

As an increase in the quantum confinement energy is accompanied by an increase in the energy gap, which It leads to a decrease in the refractive index according to equation (6).

5. Conclusion

We studied the effect of quantum confinement energy on wide energy gap semiconductors ZnS and GaN quantum dots (QDS) using Brus model. The optical properties appear depending on the quantum confinement energy, where the increase in the quantum confinement energy is accompanied by an increase in the energy gap and a decrease in the refractive index, which plays a vital role in the absorption of high-energy ultraviolet radiation, which is extremely important in optical and electronic devices.

References

[1] D .Koulentianos, Quantum confinement effect in materials for solar cell applications (Dissertation).Retrieved from http://urn.kb.se/resolve?urn=urn:nbn:se:uu:diva-237189 (2014).

[2] D. Bera, L. Qian, Semiconducting Quantum Dots for Bioimaging, Information Healthcare, New York, U.S. 191 (2009).

[3] A. Scaff, Introduction to Nanotechnology (Science, Engineering & Applications), Series of Strategic and Advanced Techniques, Arabic Compendium of Translation, INSB: 139789953824437. (2011).

[4] M. I. Ahamed and K. S. Kumar, Mater. Sci. Poland 37 (2019) 108; https://doi.org/10.2478/msp-2018-0103

[5] L. E. Brus, J. Chem. Phys. 80 (1984) 4403; https://doi.org/10.1063/1.447218

[6] A. I. Onyia, H. I. Ikeri, A. N. Nwobodo, Theoretical study of the quantum confifinement effects on quantum dots using particle in a box model, J. Ovonic Res. 14 (2018) 49.

[7] I, H.I. & O. Augustine & Asogwa, P.U. (2017) Chalcogenide Letters. 14. 49-54.

[8] O. Augustine & Ikeri, H.I. & Nwobodo, Anthonia, Journal of Ovonic Research. 14. 49-54 (2018).

[9] B. Bhattacharjee, D. Ganguli, K. Iakoubovskii, A. Stesmans and S. Chaudhuri, Indian

Academy of Sciences, Vol. 25, No. 3, pp. 175-180, (2002); https://doi.org/10.1007/BF02711150

[10] T.S. Moss, Proc. Phys. Soc. B 63 (1 950) 1 67.

[11] N.M. Ravindra, S. Auluck, V.K. Srivastava, Physica status solidi (b) 93 (1 979); https://doi.org/10.1002/pssb.2220930257

[12] P.J.L. Herve, L.K.J. Vandamme, J. Appl. Phys. 77 (1 995) 5476; https://doi.org/10.1063/1.359248

[13]G. Marius. The Physics of Semiconductors, An Introduction Including Nanophysics and Applications.(2016).

[14]C. Ephriam & O. Michael & Harry, Taylor, World Journal of Condensed Matter Physics. 2. 96-100.(2012); https://doi.org/10.4236/wjcmp.2012.22017

[15]S.M.Jesús, et al., Nanomaterials 12.14 (2022): 2501; https://doi.org/10.3390/nano12142501

[16] I,H.I. & Onyia, Augustine & Vwavware, Jude. The Dependence of Confinement Energy on the Size of Quantum Dots. 7. 27-30, (2019); https://doi.org/10.26438/ijsrpas/v7i2.2730