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Theoretical Studies of the Optical Properties of ZnS , ZnO and CdS Nanopartical Using the Brus Equation

Assim Ahmed Issa[1], Tamathir Abbas Hamoudi[2]
1 Department of New and Renewable Energies, College of Science, Mosul University, Mousl , Iraq
[2] Department of Chemistry and Biochemistry, Nineveh College of Medicine, Nineveh University, Mousl, Iraq

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Corresponding Author:
Name: Tamathir Abbas Hamoudi
E-mail:
tamathir.hamoudi@uoninevah.edu.iq
Tel:

ABSTRACT

In the present work, Brus equation has been used to study the size effect of the quantum dot on the optical properties of some semiconductor compounds (CdS, ZnS and ZnO). It is found that the absorption wavelength and bandgap energy are dependent on the size of the QD. As the size of the QD decreases, the bandgap energy increases and the absorption wavelength decreases. There is good agreement of the theoretical results of the bandgap energy and absorption wavelength obtained in this study using Brus equation with the published experimental results for the semiconductor compounds mentioned above.

1. Introduction

A semiconductor nanostructure that confines the motion of conduction band electrons is called A quantum dot (QD), excitons (bound pairs of conduction band electrons and valence band holes), or valence band holes, in all three spatial directions. In 1980s Alexei Ekimov discovered the QDs in a glass matrix [1].

In the past few years, Quantum- pent semiconductor structures, including quantum wells, quantum dots _QDs_ and quantum rods extensively investigated. Due to the special applications of nanodevices that differ from those of molecules and bulk solids, it has attracted great interests. Because the novel properties of nanomaterials depend on their size, structure, and shape, an understanding of their mechanism is worthy issues in nanoscience and nanotechnology [2]. Size-dependent blue shifts of absorption spectra and photoluminescence detected the quantum confinement effect. Recently, Semiconductor nanoparticles are attracted important heed for their role in technical applications and fundamental studies [3].

These semiconductor QDs have discrete electronic states, in contrast to the bulk band structure, with an effective bandgap blue shifted from that of the bulk[4,5]. The size-dependent optical properties of QDs are actively studied during the past decade. The synthesis and subsequent functionality of QDs for a variety of applications include photostable luminescent biological labels, photovoltaic devices [6-9].

If the dimensions are reduced sufficiently, the semiconductor nanoparticle band gap increases due to altering the light absorption, quantum confinement and emission properties of these ultra-small semiconductor nanoparticles that are now known as Quantum Dots (QDs). According to the Brus equation, the quantum reservation involves restricting the motion of a part particle size was also calculated. The fabricated a dye-sensitized solar cell using _ 2014 The Korean Society of Industrial and Engineering Chemistry [10]. A number of researchers have studied the optical bandgap is broaden with decreasing particle size leading to a blue shift in the bandgap absorption spectrum, as a consequence, optoelectronic properties can be specifically tuned to have desired energy output by varying the dot size The vast applications of quantum dots in technology is emission based. The confinement energy is important because it determines the emission energy as well as the wavelength of the quantum dot[11-16].

Aim of the study

This research trying to look out at how the Brus equation can be used to obtain the band gab energy and wavelength at various dots radii and compare theoretical study with experimental.

2. Theoretical

1.2. Brus equation

The emission energy of quantum dot nano semiconductor, a function of the radius (R) and band gap energy of bulk semiconductor (E_g bulk) can be calculated by Brus equation which is used to calculate the theoretical energy gap as following : [17-18] .

$$\Delta E_g(qd) = E_g(bulk) + \frac{h^2}{8R^2}\left(\frac{1}{m_e^*} + \frac{1}{m_h^*}\right) ----(1)$$

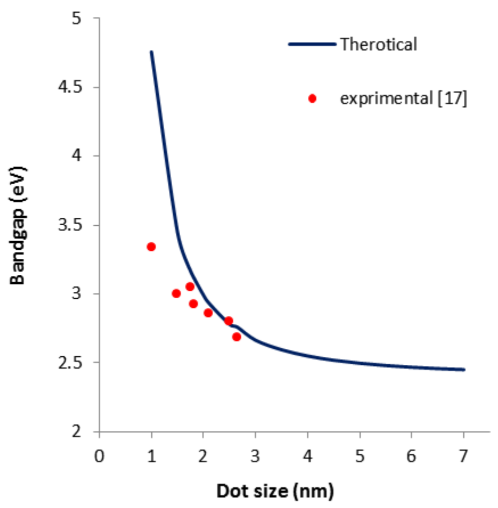
$\Delta E_g(qd)$ = band gap energy of quantum dot .

$E_g(bulk)$= band gap energy of bulk semiconductor.

h = Planck constant .

m_e^* = effective mass of excited electron.

Considering the values of m^*_h, m^*_e and E_g (bulk) shown in Table-1 and substituting them into equation 1 (brus equation) , the obtained results for variation of bandgap energies as a function of quantum dot size for CdS , ZnS, and ZnO are are plotted in Figures - 1 , 2 and 3 respectively. The experimental bandgap values [3,21,22] are in good harmony with theoretical bandgap values, It is evident that the bandgap energy decreases with increase QD size . Figures - 1 , 2 and 3 respectively indicates the change in the energy gap due to the decrease in the quantum dot size, it is noted that; the energy gap value changes lightly when the quantum size decreases from 7 nmto 3 nm. But when the size is smaller than a size 3 nm, the energy gap begins to increase very significantly until it reaches the highest values at 1 nm. In fact, that is due to the effect of quantum confinement that shifts the energy state to higher (lowest) levels at the conduction band (valence band), which increases the size of the energy gap [15].



m_h^*= effective mass of excited hole.

R = radius of quantum dot.

e = electronic charge.

Equation used to calculate the wavelength of the materials (ZnS, ZnO and CdS) [14].

$$\lambda = \frac{hc}{Eg} ------(2).$$

λ = wavelength.

Eg = band gap energy.

C = Velocity of light (3x108 m/s) .

3. Calculation and Results

1.3.Evaluation of bandgab energy and wave length

Table 1 shows the material parameters used for the cmputation of the band gap energy and wave length of quantum dot

Table 1: ZnS, ZnO and CdS quantum dot material parameters

Quantum dots	m^*_h	m^*_e	$E_g(bulk)$ at 300 K	Ref
ZnS	0.23 m_o	0.34 m_o	3.68	(19)
ZnO	0.45m_o	0.24m_0	3.35	(3)
CdS	0.64 m_o	0.21 m_o	2.48	(20)

Fig. 1: The variation the bandgap and Dot Size (nm) for CdS

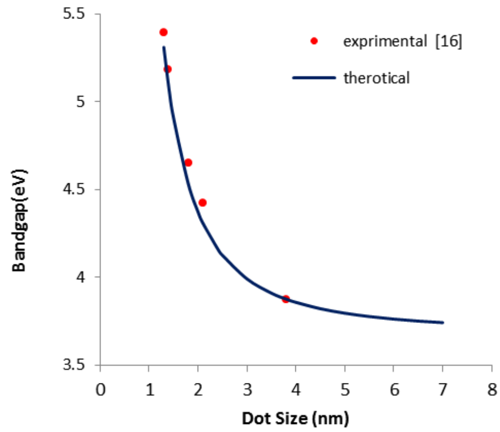


Fig. 2: The variation the bandgap and Dot Size (nm) for ZnS

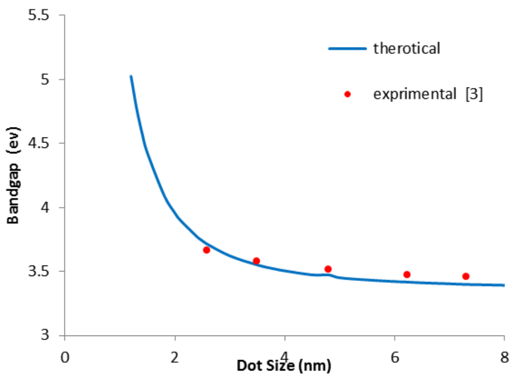


Fig. 3: The variation the bandgap and Dot Size (nm) for ZnO.

Substituting Eg, h, and c in equation 2. The obtained results for variation of wavelength with quantum dot size for CdS , ZnS, and ZnO are shown in Figure - 4

, 5 , and 6 respectively. The experimental wavelength values [21,23] are in good coincidence with theoretical wavelength values, it is evident that the bandgap energy increases with increasing the QD size. . In fact, that is due to the effect of quantum confinement that shifts the energy state to higher (lowest) levels at the conduction band (valence band), which increases the size of the energy gap [15]

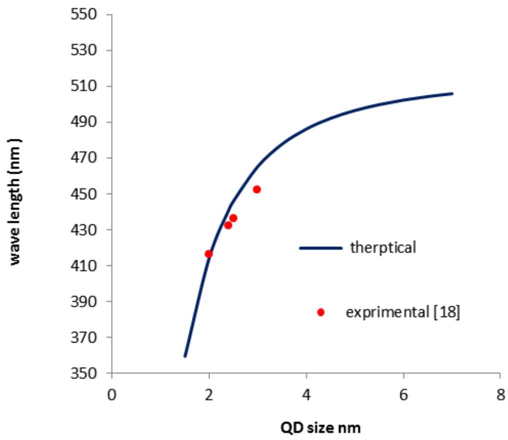


Fig. 4: The wave length variation with quantum dot size of CdS

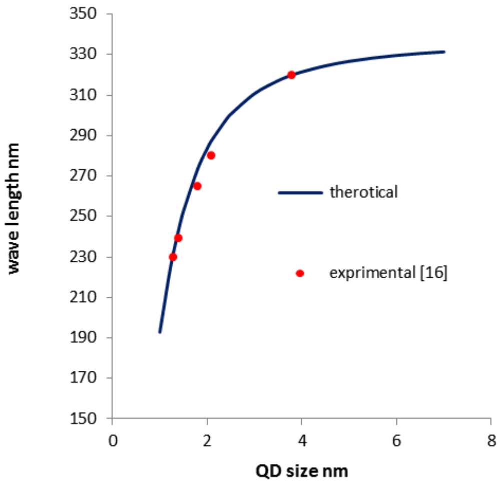


Fig. 5: The wave length variation with quantum dot size of ZnS

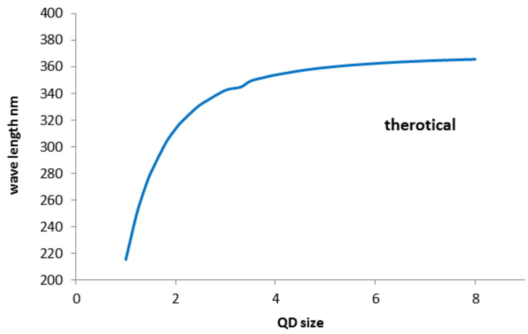


Fig. 6: The wave length variation with quantum dot size of ZnO

4. Discussion

1- Figures - 1 , 2 and 3 show that the results of band gab E_g variation with quantum dot size for CdS , ZnS, and ZnO calculated by using brus equation were the closest to the experimental . Also its show that the effect of quantum dot size on band gab for CdS , ZnS, and ZnO. The band gab inversely proportional to the quantum dot size.

2- Figures - 4 , 5 and 6 show that the results of wavelength varied with quantum dot size for CdS , ZnS, and ZnO calculated by using equation 2, are the close to the experimental and it shows that the effect of quantum dot size on wavelength for CdS , ZnS, and ZnO the wavelength increases with increasing the quantum dot size. This result is consistent with the research findings [11-16].

5. Conclusions

The results of present study work show the possibility of using the brus equation to calculate band gab and wavelength of quantum dot.

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دراسة نظرية للخواص البصرية للتراكيب النانونية ل ZnS و ZnO و CdS باستخدام معادلة بروس

عاصم احمد عيسى[1] , تماضر عباس حمودي[2]
[1]قسم الطاقات المتجددة , كلية العلوم ، جامعة الموصل ، الموصل ، العراق
[2]قسم الكيمياء والكيمياء الحياتية, كلية طب نينوى, جامعة نينوى, الموصل, العراق

الملخص

في هذا البحث تم استخدام معادلة بروس لدراسة تأثير حجم النقطة الكمومية على الخواص البصرية لبعض مركبات أشباه الموصلات (CdS، ZnS، ZnO). لقد وجد أن طول موجة الامتصاص وطاقة فجوة النطاق يعتمدان على حجم QD، حيث تزداد طاقة الفجوة كلما قل حجم النقطة الكمية ويقل طول موجة الامتصاص. في هذه الدراسة هناك توافق جيد للنتائج النظرية لطاقة الفجوة وطول موجة الامتصاص التي تم الحصول عليها باستخدام معادلة بروس مع النتائج التجريبية المنشورة لمركبات أشباه الموصلات المذكورة أعلاه.