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The Band Gap Energy Calculated for $Cd_{1-x}Zn_xS$ Quantum Dots grown by the Sol gel Method

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Abstract

This work reports on a theoretical investigation of a band gap energy in the case of $Cd_{1-x}Zn_xS$ quantum dots embedded in an insulating material by the Sol gel method. Calculations have been computed as a function of Zn composition going from CdS to ZnS taking account on the excitonic binding energy. The obtained results showed a good agreement with experimental data. Thus, this study confirms the validity of the adopted model and can be considered as a helpful support for designing a variety of devices.

Keywords: Quantum dots, $Cd_{1-x}Zn_xS$, band gap energy, excitonic binding energy, devices.

INTRODUCTION

Since several decades, Films of $Cd_{1-x}Zn_xS$ are technologically useful materials [1-10]. This is due to the potentiality of this material which is used as a window material in hetero junction solar cells with a p-type absorber layer such as $CuInSe_2$ [6] or for fabricating p – n junctions without lattice difference in devices based on quaternary compounds like $CuIn_xGa_{1-x}Se_2$ or $CuSnS_zSe_{1-z}$ [5].

Concerning $Cd_{1-x}Zn_xS$ quantum dots (QDs), the study of their properties is being one of the main interests in both fundamental and applied research. Moreover, their

technological potentialities do not cease to be proved [11-15]. From a fundamental view point, it is well known that QDs exhibit a quantum confinement effect [16-21]. Thus, when the radius R of a quantum dot is smaller than double the exciton Bohr radius a_x, electrons and holes are supposed as two confined particles bound by an enforced Coulomb interaction. Consequently, in QDs with relatively low radii, the energies of both electrons and holes are quantized and this effect leads to a widening in the band gap [16-20, 6]. To study the electronic properties of $Cd_{1-x}Zn_xS$ QDs, we have, adopted, in a first time, the spherical geometry and a potential with a finite barrier at the boundary [22, 23]. We have suggested, in a second time, the flattened cylindrical geometry with a finite potential barrier at the boundary [24-33]. In this context, we have studied the electronic properties for a single and double quantum dot [24-25, 33] and also for super lattices based on $Cd_{1-x}Zn_xS$ QDs embedded in an insulating material [26-32]. Nevertheless, in all these works, we have not taken account on the Coulomb potential associated with the electron – hole interaction.

The goal of the present work is to study the band gap energy of $Cd_{1-x}Zn_xS$ QDs having a spherical geometry with an infinite potential barrier at the boundary. Calculations have been computed as a function of Zn composition going from CdS to ZnS taking account on the excitonic binding energy. The paper is organized as follows: after an introduction, modeling, results and discussion are presented. Conclusion of this study is reported in the last section.

MODELING

As a system, we consider a pair of an electron and a hole, both confined in a spherical quantum dot of radius R. The semiconductor material is capped inside a dielectric matrix [6].

The band gap energy for a QD is given by the following relation:

$$E_g^{QD} = E_g^{bulk} + \frac{\hbar^2 \pi^2}{2R^2}\left(\frac{1}{m_e^*} + \frac{1}{m_h^*}\right) - \frac{1.8\, q^2}{4\pi\varepsilon_0\, \varepsilon_r\, R} \qquad (1)$$

where E_g^{bulk} is the band gap for bulk $Cd_{1-x}Zn_xS$, $\hbar$ is the Plank's constant, m^* is the effective mass of free carriers, q is the elementary charge, ε_0 is the dielectric constant vacuum and ε_r is the relative permittivity. The subscripts e and h refer to the electron and hole particles respectively. In deriving Equation (1), we have adopted the effective mass theory (EMT) and the band parabolicity approximation (BPA) as well.

RESULTS AND DISCUSSION

Table 1. shows the exciton Bohr radius a_x in the case of $Cd_{1-x}Zn_xS$ alloys. Consequently, it is clear that, for all the compositions studied, the adequate values of quantum dot radius should approximately be inferior to 3.5 nm.

Table 1. The exciton Bohr radius a_x in the case of $Cd_{1-x}Zn_xS$ alloys

Compound	CdS	$Cd_{0.8}Zn_{0.2}S$	$Cd_{0.6}Zn_{0.4}S$	$Cd_{0.4}Zn_{0.6}S$	$Cd_{0.2}Zn_{0.8}S$	ZnS
a_B (nm)	2.36	2.16	2.01	1.98	1.80	1.75

Values of parameters used in these calculations are summarized in **Table.2**. These parameters are taken from Ref [22]. The effective masses and the dielectric constant for $Cd_{1-x}Zn_xS$ with different Zn compositions have been deduced using the Vegard's law.

We have calculated the band gap energy E_g^{QD} for $Cd_{1-x}Zn_xS$ quantum dots using the Eq (1). Table 3 shows the obtained results.

Table 2. Parameters used to calculate the band gap energy (eV) for $Cd_{1-x}Zn_xS$ QDs. (m_0 is the free electron mass)

x	$\frac{m_e^*}{m_0}$	$\frac{m_h^*}{m_0}$	ε_r	E_g^{bulk}(eV)
0.0	0.16	5.00	8.5	2.42
0.2				2.61
0.4				2.82
0.6				3.05
0.8				3.31
1.0	0.28	1.76	8.0	3.60

Table 3. The band gap energy E_g^{QD} as a function of radius for $Cd_{1-x}Zn_xS$ quantum dots

x **R(nm)**	**0**	**0.2**	**0.4**	**0.6**	**0.8**	**1.0**
2.0	2.755	2.988	3.141	3.228	3.596	3.814
2.1	2.716	2.946	3.104	3.295	3.564	3.787
2.2	2.683	2.909	3.072	3.266	3.436	3.764
2.3	2.656	2.878	3.045	3.236	3.512	3.744
2.4	2.631	2.851	3.021	3.221	3.491	3.727

2.5	2.610	2.827	3.001	3.202	3.472	3.712
2.6	2.591	2.806	2.982	3.186	3.456	3.698
2.7	2.574	2.788	2.966	3.172	3.442	3.687
2.8	2.559	2.772	2.952	3.159	3.429	3.677
2.9	2.546	2.757	2.939	3.148	3.418	3.668
3.0	2.535	2.744	2.928	3.138	3.408	3.660
3.1	2.524	2.732	2.918	3.129	3.399	3.653
3.2	2.515	2.721	2.909	3.121	3.392	3.646
3.3	2.506	2.712	2.901	3.144	3.384	3.641
3.4	2.498	2.703	2.893	3.143	3.378	3.635
3.5	2.492	2.695	2.886	3.102	3.372	3.631

One can easily remark that, (i) for the all compositions studied, E_g^{QD} decreases with increased R, (ii) for any composition, E_g^{QD} is sufficiently superior to the bulk band gap for the radius inferior to 3.0 nm, (iii) E_g^{QD} is slightly superior to the bulk band gap when the radii R exceeds 3.0 nm independently of the composition, (iv) For all the cases, the confinement of carriers becomes insignificant when R exceeds 3.5 nm, (v) E_g^{QD} shows a increasing tendency with increased zinc composition independently to the radii R. This result is mainly due to the hole effective masse which decreases with the zinc content x and to the bulk band gap which increases as a function of x, (vi) The E_g^{QD} values as deduced from our calculations do not show a significant discrepancy with respect to the relevant experimental values given by Refs [6, 21, 34-36]. This confirms the validity of the model used in the present work.

CONCLUSION

In summary, we have calculated the band gap energy as a function of radius for $Cd_{1-x}Zn_xS$ quantum dots. A particular attention has been paid to their compositional dependencies. Both electrons and holes are assumed to be confined in nanospheres with an infinite potential barrier at the boundary but taking account on the excitonic binding energy. The obtained results showed a good agreement with several experimental data. Moreover, in technological applications, this study is of great interest more especially for designing devices based on $Cd_{1-x}Zn_xS$ quantum dots.

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