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Original Article

Theoretical Study on the Absorbance Bandgap of the Group II-VI Semiconductor Quantum Dots

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Abstract *- A theoretical study on the absorbance bandgap of the CdSe, CdS and ZnS QDs has been studied using effective mass approximation. The results strongly indicate that the quantum confinement effect on QDs leads to a size-dependent increase in the absorbance bandgap. This property allows for the tuning of optical and electronic characteristics, making these materials highly valuable in various advanced technological applications. It is found that CdSe with a bulk bandgap of ~1.7 eV increases as the dot size decreases, resulting in a shift from red to blue emission; CdS begins at ~2.42 eV and increases as the size decreases, shifting from green to violet emission and ZnS with largest initial bandgap of ~3.68 eV is pushed further into the UV range as the size decreases. Thus, by controlling the size of the QDs, it is possible to precisely tailor their properties for specific uses, making them highly versatile for a range of applications in optoelectronics, biomedical imaging, and quantum computing.*

Keywords *- Absorbance spectrum, Bandgap, Quantum confinement, Quantum dot, Effective mass approximation.*

1. Introduction

Group II-VI semiconductor Quantum Dots (QDs) such as CdSe, CdS, and ZnS are of great importance and have attracted tremendous research interests for future-generation device applications due to their unique optical and electronic properties, such as such as broad absorption spectrum, low-cost manufacturing, and size-tunable optoelectronic properties. By controlling the size of the QDs, manufacturers can precisely tailor their optical and electronic properties for specific applications, harnessing the unique benefits of quantum confinement. Thus, understanding the impact of the quantum confinement effect in Group II-VI QDs opens up numerous possibilities for advanced technological applications in optoelectronics, solar energy, biomedical imaging, and quantum computing. [1]

Quantum confinement is a quantum mechanical phenomenon that occurs when the sizes of semiconductor materials are reduced to the nanoscale, typically below the exciton Bohr radius (the average distance between an electron and a hole in a material). [2][3] At this length scale, the motion of charge carriers (electrons and holes) is restricted, leading to discrete energy levels rather than the continuous bands observed in bulk materials, which alters the electronic and optical properties of the material, including the absorbance bandgap. [4]

A quantum dot is a semiconductor nanostructure with three-dimensional confinement [5][6]. Due to this size limitation, QDs possess a strong quantum confinement effect, which results in the quantization of electronic energy states different from those of corresponding bulk semiconductors. In bulk materials, continuous conduction and valence bands are separated by the energy gap of empty states in between [7].

On the contrary, in QDs, the energy levels are discrete, and the absorbance bandgap increases with decreasing dot size, as shown in Figure 1.1, leading to size-dependent optoelectronic properties [8]. Such an effect permits us to precisely modulate the absorption spectrum of QDs by adjusting their size, shape, and chemical composition.

In this paper, the effective mass approximation is used to investigate the quantum size effect on the absorption bandgap of CdSe, CdS, and ZnS and provides a clear view of the analytical approach to study the optical properties of QDs.

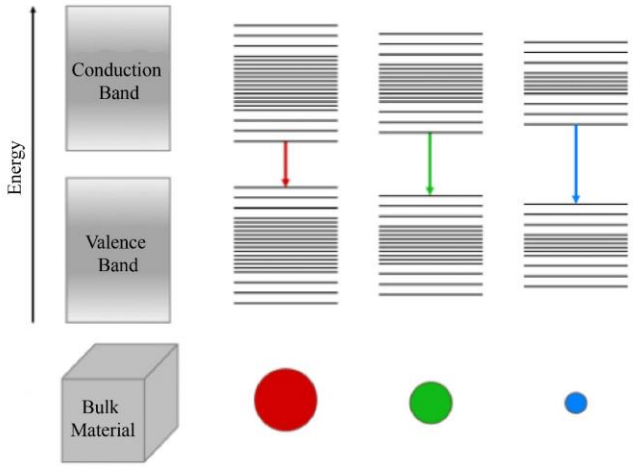

Fig. 1 Electronic structures of inorganic semiconductors QDs of different diameters

2. Theoretical Background

The relationship between the bandgap Eg and the QDs size (R) can be explained by the Effective Mass Approximation (EMA) model, which for spherical quantum dots is given by [9]:

$$E_{gap}(R) = E_{gap}^{bulk} + \frac{h^2\pi^2}{2R^2}\left(\frac{1}{m_r^*} + \frac{1}{m_h^*}\right) - \frac{1.8e^2}{4\pi\epsilon_0\epsilon_r R} \quad (1)$$

Where:

$E_{gap}(R)$ is the size-dependent energy gap of the QDs., E_{gap}^{bulk} is the bulk energy gap of the material, $\hbar$ is the reduced Planck's constant, R is the radius of the QDs, m_e^* is the effective mass of the electron, m_h^* the effective mass of the hole, e is the elementary charge, ϵ_0 is the permittivity of free space, ϵ_r is the relative permittivity (dielectric constant) of the material.

2.1. Terms Explained

2.1.1. Bulk Bandgap Energy (E_{gap}^{bulk})

This is the bandgap energy of the bulk material (the semiconductor in its bulk form, not in nanocrystal form).

2.1.2. Kinetic Energy Term

$$\frac{h^2\pi^2}{2R^2}\left(\frac{1}{m_e^*} + \frac{1}{m_h^*}\right) \quad (2)$$

This term accounts for the quantum confinement effect, where R is the radius of the quantum dot. It increases the bandgap energy as the size of the quantum dot decreases.

2.1.3. Coulombic Attraction Term

$$-\frac{1.8e^2}{4\pi\epsilon_0\epsilon_r R} \quad (3)$$

This term represents the Coulombic attraction between the electron and the hole. It decreases the bandgap energy and becomes more significant as the size of the quantum dot decreases.

3. Materials and Methods

In this paper, effective mass approximation described in equation 2.1 is used for the computation of absorption bandgap of different sizes of group II-IV (CdSe, CdS and ZnS) QDs. Absorbance bandgaps are plotted against various sizes in order to investigate the quantum size effect. The input parameters used are as shown in Table 1.

Table 1. The Group II-IV QDs material parameters used for the study

Quantum dots	M_e^x	M_h^x	$E_{g(bulk)}$ at 300k
CdSe	0.13m_o	0.45m_o	1.74Ev
ZnS	0.34m_o	0.23m_o	3.68Ev
CdS	0.21m_o	0.80m_o	2.42Ev

4. Results and Discussion

Figure 4.2 is a plot to visualize the relationship between the absorption bandgap and the size of CdSe, CdS, and ZnS QDs. This quantum potential effect on bandgap has a significant impact on the enhancement of device performance, thereby allowing for the engineering of their optical and electro-optical responses; as a matter of fact, optoelectronic properties can be specifically tuned to have desired energy output by varying the dot size.

As the dot size decreases, the bandgap increases. This is because the energy difference between the discrete energy levels in the conduction and valence bands grows larger.

This increase in the bandgap results in a blue shift of the absorption and emission spectra due to the quantum confinement effect compared to the bulk, as shown in Figure 2.

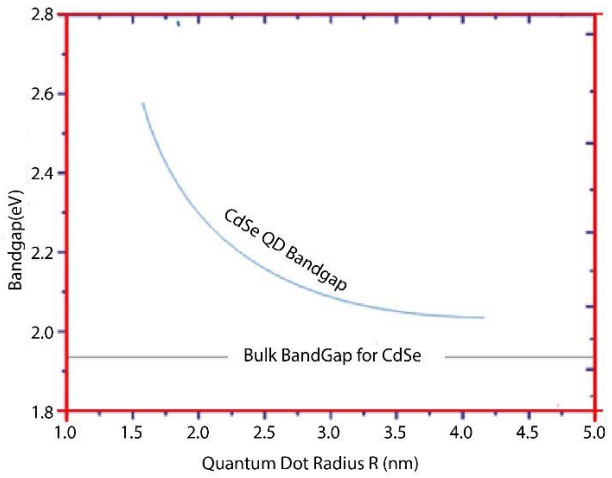

Fig. 2 Showing a large optical blue shift for CdSe

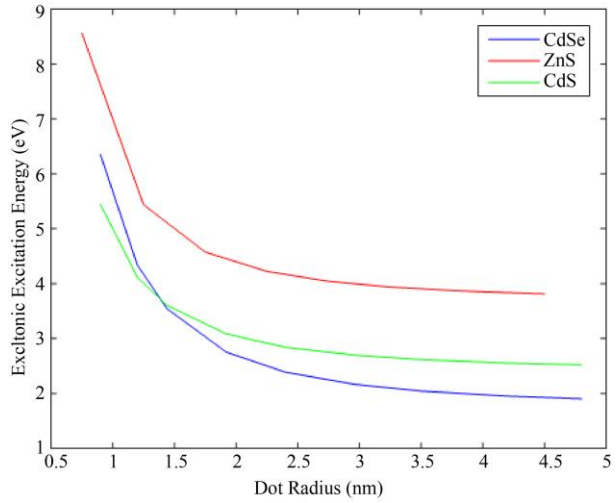

Fig. 3 Absorbance bandgap (excitation energy) versus QDs size

In general, as the size of CdSe QDs decreases, the absorbance bandgap increases, leading to a shift in emission from the red to blue part of the visible spectrum. Thus, QDs of CdSe can be tuned to emit light across the visible spectrum by varying their size. Similarly, CdS QDs exhibit an increase in band gap with decreasing size due to confinement causing the emission to shift from the visible towards the ultraviolet range as the size decreases. In addition, ZnS has a wider band gap compared to CdSe and CdS, leading to emission in the ultraviolet to the blue region of the spectrum and, therefore, can be used as shell materials to passivate QDs to improve their optical properties.

By controlling the size of the QDs, one can tune precisely their optical and electronic properties for specific needs and applications, including light-emitting diodes (LEDs), solar cells, biological imaging, and quantum computing. In LEDs, they can be used to produce light of specific wavelengths by tuning their size, enabling efficient and color-pure LEDs. In biomedical imaging, they provide bright, stable fluorescence useful for imaging biological samples, while in solar cells, they can be employed to enhance the absorption spectrum and improve efficiency. Furthermore, In quantum computing **t**he quantized energy levels in QDs can be used for quantum bits (qubits), crucial for the development of quantum computers. The results are compatible with those of the existing literature.

5. Conclusion

In conclusion, quantum confinement fundamentally changes the electronic and optical properties of CdSe, CdS, and ZnS QDs materials when they are reduced to nano-metric sizes. This effect permits the precise control of material properties such as absorption and emission bands by adjusting the size of QDs, making them highly versatile for a range of applications in optoelectronics, biomedical imaging, and quantum computing.

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