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Confinement Effect on the Excitonic Kinetic Energy of CdSe, CdS, and ZnS Semiconductor Nanostructures Using the Brus Effective Mass Model

H.I. Ikeri[1], N A. Akonjom[2], G. C. Ogbu[3], N.N. Tasie[4], C.I. Elekalachi[5], O. K. Asielue[6], A.N. Nwobodo[7]
[1]Department of Physics, Kingsley Ozumba Mbadiwe University, Ogboko Ideato, Imo State
[2]Department of Physics, University of Cross Rivers State.
[3]Department of Industrial Physics, Enugu State University of Science and Technology.
[4]Department of Physics, Rivers State University
[5]Department of Industrial Physics, Chukwuemeka Odimegwu Ojuchukwu University.
6Department of Science Laboratory Technology Delta State Polytechnic Ogwashi.
[7]Department of Industrial Physics, Enugu State University of Science and Technology.

Abstract – Quantum confinement profoundly modifies the electronic and optical properties of semiconductor quantum dots (QDs), primarily by increasing excitonic kinetic energy as particle size decreases. This study examines the size-dependent excitonic kinetic energy of CdSe, CdS, and ZnS quantum dots using the Brus effective mass model. Analytical calculations reveal that excitonic kinetic energy rises sharply with decreasing quantum dot radius, following inverse-square dependence consistent with the spatial confinement of charge carriers. Among the materials studied, ZnS exhibits the strongest confinement due to its large reduced exciton mass and low dielectric screening, followed by CdS with intermediate behavior, and CdSe, which shows the weakest confinement owing to its small reduced mass and higher dielectric constant. These trends underscore the dominant role of intrinsic material parameters in determining excitonic sensitivity to confinement. The results provide critical theoretical guidance for the design and optimization of quantum dot–based optoelectronic devices, including photodetectors, light-emitting diodes, fluorescence probes, and other quantum-enabled technologies, where precise tuning of excitonic energy levels is essential.

Keywords: Quantum dot, **exciton Bohr radius, semiconductor nanostructures,** ***confinement***

1. INTRODUCTION

Quantum dots (QDs) are semiconductor nanostructures whose optical and electronic properties are substantially modified when their dimensions approach or fall below the exciton Bohr radius, leading to discrete, atom-like energy levels and strong size tunability (Alivisatos, 1996; Bimberg et al., 1999). This size-dependent discretization of energy states, known as quantum confinement, alters carrier wavefunctions, enhances excitonic kinetic energy, and increases the effective bandgap relative to the bulk material (Brus, 1984; Efros & Efros, 1982). Among II–VI semiconductor QDs, CdSe, CdS, and ZnS have been extensively studied due to their wide bandgaps, photostability, and applications in optoelectronics, bioimaging, and nanophotonics (Murray et al., 1993; Peng et al., 2000).

The excitonic kinetic energy is particularly important because it dominates the size-dependent energy shift predicted by the Brus effective mass model, scaling inversely with the square of the particle radius (Scholes & Rumbles, 2006; Rossetti et al., 1983). As QD radius decreases, the spatial restriction of electrons and holes produces a substantial increase in kinetic energy, resulting in pronounced blue-shifts in absorption and emission spectra (Qu et al., 2001; Klimov, 2000). Because CdSe, CdS, and ZnS differ in effective carrier masses and dielectric constants, they exhibit distinct confinement behaviors, making comparative analysis essential for materials engineering (Wang et al., 2003; Dabbousi et al., 1997).

CdSe QDs, with relatively low electron and hole effective masses, experience strong confinement at moderate sizes, significantly altering their excitonic structure (Leatherdale et al., 2002; Norris & Bawendi, 1996). In contrast, ZnS, characterized by a wider bandgap and higher effective masses, exhibits weaker confinement-induced kinetic energy enhancement, while CdS displays intermediate behavior, enabling broader tunability across the visible spectrum.

The Brus effective mass model provides a foundational framework for interpreting size-dependent excitonic energies, offering analytical expressions for the kinetic and Coulombic contributions to the exciton energy in spherical nanocrystals (Kayanuma, 1988; Sze & Ng, 2006). Despite its simplifications, it effectively captures the primary physics underlying bandgap expansion and excitonic energy modulation in II–VI nanoscale semiconductors.

This study applies the Brus model to evaluate and

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compare the size-dependent excitonic kinetic energy in CdSe, CdS, and ZnS QDs, aiming to quantify the relative confinement strengths of each material and determine how intrinsic parameters such as effective mass and dielectric constant influence excitonic behavior. The findings provide theoretical insight critical for designing quantum dot–based photodetectors, LEDs, fluorescence probes, and other quantum-enabled optoelectronic devices.

2. THEORETICAL BACKGROUND

2.1 Excitons in Quantum Dots

An exciton is an electron–hole pair bound via Coulomb attraction. In bulk, the exciton behaves like a hydrogen-like quasiparticle. In a quantum dot with radius R, spatial confinement increases the energy due to quantization of particle motion. The total exciton energy in a QD is typically written as:

$$E(R) = E_g^{\text{bulk}} + E_{\text{kinetic}}(R) + E_{\text{Coulomb}}(R)$$

This work focuses on the excitonic kinetic energy term.

2.2 Brus Model

The baseline Brus equation for a Spherical QD is:

$$E(R) = E_g^{\text{bulk}} + \frac{h^2\pi^2}{2R^2}\left(\frac{1}{m_e^*} + \frac{1}{m_h^*}\right) - \frac{1.8e^2}{4\pi\varepsilon_0\varepsilon R}$$

The excitonic kinetic confinement energy is:

$$E_{\text{kinetic}}(R) = \frac{h^2\pi^2}{2R^2}\left(\frac{1}{m_e^*} + \frac{1}{m_h^*}\right)$$

Let the reduced mass be:

$$\frac{1}{\mu} = \frac{1}{m_e^*} + \frac{1}{m_h^*}$$

Then:

$$E_{\text{kinetic}}(R) = \frac{h^2\pi^2}{2\mu R^2}$$

3. MATERIALS AND METHODS

This study presents a theoretical and computational analysis of the size-dependent excitonic kinetic energy in CdSe, CdS, and ZnS semiconductor quantum dots. The Brus effective mass model was employed to derive analytical expressions for the kinetic confinement term, as described in Equation 2.34. No physical laboratory experiments were conducted; instead, the analysis relied on established analytical formulations and published semiconductor parameters. All input parameters were obtained from empirical data reported in the scientific literature, as summarized 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

The excitonic kinetic energy as a function of quantum dot size for CdSe, CdS, and ZnS, calculated using Equation 3.18, is presented in Figure 4.1. The graph reveals a pronounced inverse-square dependence of kinetic energy on quantum dot radius, in agreement with predictions from the Brus effective mass model. For all three II–VI semiconductor materials, excitonic kinetic energy increases sharply as the dot radius decreases, reflecting the enhanced spatial confinement of charge carriers at nanoscale dimensions. The magnitude and rate of this increase, however, differ markedly among the materials, owing to variations in intrinsic parameters such as electron and hole effective masses, the exciton reduced mass, and the dielectric constant. These differences underscore the material-dependent nature of quantum confinement and its impact on excitonic behavior in nanoscale II–VI semiconductors.

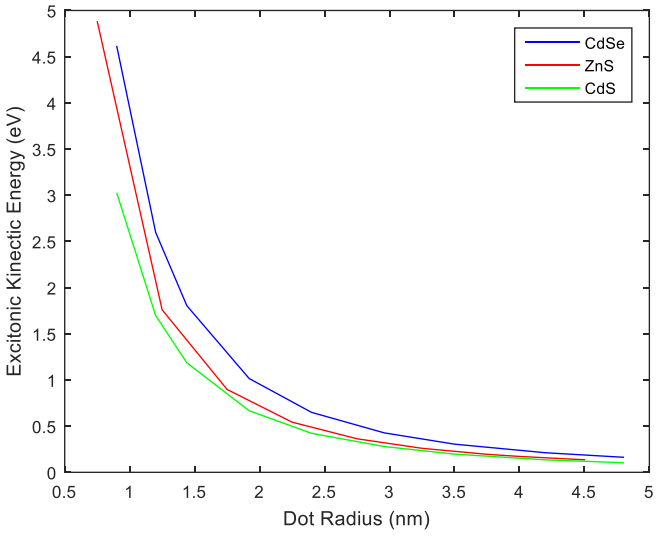

Fig. 1: Excitonic Kinetic Energy versus Dot Radius for CdSe, ZnS and CdS QDs

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Among the three materials, ZnS quantum dots exhibit the highest excitonic kinetic energy at any given size, indicating the strongest quantum confinement effect. This arises primarily from the large effective masses of electrons and holes in ZnS, resulting in a relatively large reduced exciton mass. A larger reduced mass amplifies the kinetic energy contribution, causing ZnS QDs to experience rapid energy increases as the dot size decreases. Additionally, the lower dielectric constant of ZnS provides weaker screening of electron–hole interactions, further enhancing confinement-induced energy shifts.

CdS quantum dots display intermediate confinement strength, with excitonic kinetic energies lower than ZnS but higher than CdSe across all radii. CdS possesses moderate effective masses and a dielectric constant that provides somewhat stronger Coulombic screening than ZnS, slightly softening the confinement effect. Nevertheless, its exciton reduced mass remains sufficient for pronounced size-dependent kinetic energy, particularly at radii below ~5 nm.

CdSe quantum dots show the weakest confinement among the three materials. With the smallest reduced mass and a relatively high dielectric constant, CdSe allows greater spatial delocalization of carriers. Consequently, excitonic kinetic energy increases more gradually with decreasing size, and even at very small radii, CdSe exhibits lower kinetic energy shifts, consistent with more weakly confined excitonic states.

Overall, the comparative analysis confirms the hierarchy of confinement strength as ZnS > CdS > CdSe, reflecting the dominant influence of reduced mass and dielectric screening on excitonic behavior. These trends demonstrate that intrinsic material parameters not dot size alone govern the sensitivity of excitonic kinetic energy to quantum confinement.

These findings are directly relevant for the design of quantum dot–based technologies. Materials with strong confinement, such as ZnS, are ideal for applications requiring large, size-tunable energy shifts, including high-efficiency ultraviolet photodetectors, wide-band-gap LEDs, and robust fluorescence probes. Conversely, materials with weaker confinement, such as CdSe, are better suited for devices demanding narrow emission linewidths, lower excitonic energies, and enhanced carrier mobility, including visible-light LEDs, quantum dot lasers, and biological imaging probes. Understanding how excitonic kinetic energy scales with both size and intrinsic material parameters enables precise engineering of energy levels, optical transitions, and overall device performance in next-generation quantum-enabled technologies.

5. CONCLUSION

The analysis of excitonic kinetic energy as a function of quantum dot size in CdSe, CdS, and ZnS semiconductor nanocrystals demonstrates that quantum confinement effects are strongly material-dependent and governed primarily by intrinsic parameters such as effective mass and dielectric constant. Across all three materials, excitonic kinetic energy increases sharply with decreasing radius, following the inverse-square dependence predicted by the Brus effective mass model. However, the magnitude of this increase differs markedly: ZnS exhibits the strongest confinement due to its large reduced exciton mass and low dielectric screening, CdS shows intermediate behavior, and CdSe exhibits the weakest confinement owing to its smaller reduced mass and higher dielectric constant.

These differences create distinct confinement regimes, with ZnS showing pronounced kinetic energy enhancement even at moderate sizes, whereas CdSe remains weakly confined until very small radii. The comparative trends confirm that ZnS > CdS > CdSe in terms of confinement strength, highlighting the decisive roles of reduced mass and dielectric response in determining excitonic energy shifts.

These insights are critical for optimizing quantum dot materials for specific technological applications. Strongly confined systems like ZnS are advantageous for ultraviolet and high-energy optoelectronic devices, while moderately confined CdS and weakly confined CdSe are better suited for visible-light emitters, photodetectors, fluorescence probes, and quantum dot–based lasers. Understanding how excitonic kinetic energy scales with size allows for precise tuning of electronic and optical properties, ultimately enhancing the performance and design of quantum-enabled devices.

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