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Investigation of Size- and Temperature-Dependent Bandgap Modulation in CdSe, CdS, and ZnS Semiconductor Nanostructures

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Abstract: - This theoretical study investigates the combined effects of nanoparticle size and temperature on the bandgap energy of Cadmium Selenide (CdSe), Cadmium Sulfide (CdS), and Zinc Sulfide (ZnS) semiconductor nanomaterials. The Brus model was employed to examine the size-dependent bandgap variation, while the Varshni equation was used to evaluate the temperature-dependent behavior. The results show that decreasing nanoparticle size leads to a significant increase in bandgap energy due to quantum confinement, causing a blue shift in optical properties. In contrast, increasing temperature causes a gradual decrease in bandgap energy owing to lattice expansion and electron–phonon interactions. Among the three materials, ZnS exhibits the highest bandgap and thermal stability, CdS shows intermediate values, and CdSe has the lowest bandgap energy, and greatest temperature sensitivity. The study highlights that the electronic and optical properties of these semiconductor nanomaterials can be finely tuned by controlling particle size and accounting for temperature effects. These findings provide critical insights for the design and optimization of optoelectronic devices, quantum dot LEDs, solar cells, photodetectors, and UV electronic applications.

Key words: Semiconductor Nanomaterials, Bandgap Energy, Quantum Confinement, Nanoparticle Size, Temperature Effects, Brus Model, Varshni Equation.

1. INTRODUCTION

Semiconductor nanomaterials have gained significant attention in recent decades due to their tunable electronic and optical properties, which are highly dependent on particle size and environmental factors [1, 2,]. When the size of a semiconductor particle approaches the nanometer scale, quantum confinement effects dominate, resulting in discrete energy levels and a size-dependent bandgap energy [3, 4]. These effects are particularly pronounced in II–VI semiconductor nanocrystals such as Cadmium Selenide (CdSe), Cadmium Sulfide (CdS), and Zinc Sulfide (ZnS), which possess direct bandgap structures suitable for optoelectronic and photonic applications [5,6].

The bandgap energy of these nanomaterials determines the wavelength of light absorbed or emitted and thus directly influences their optical performance [7,8]. In nanoparticles, electrons and holes are confined within small spatial regions, causing an increase in kinetic energy and a corresponding blue shift in emission spectra [10]. This size-dependent tunability is critical for applications such as quantum dot light-emitting diodes, lasers, and biological imaging [11, 12].

Temperature is another crucial factor affecting the bandgap energy. As temperature rises, thermal vibrations within the lattice increase, resulting in electron–phonon interactions and lattice expansion, which reduce the bandgap energy [13,14]. Empirical models, such as the Varshni relation, are widely used to describe the temperature dependence of the bandgap for various semiconductors [15, 16].

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Understanding the combined effect of particle size and temperature is essential because real-world devices operate under varying thermal conditions and require precise tuning of optical properties. For instance, quantum dot displays, photodetectors, and nanoscale lasers depend on both the size of nanoparticles and the operational temperature to maintain performance and color fidelity. Several studies have explored size-dependent bandgap tuning and temperature-dependent bandgap shifts but relatively few have systematically examined the interplay between size and temperature in CdSe, CdS, and ZnS nanomaterials[17, 18],.

Consequently, this study aims to provide a theoretical investigation of the bandgap energy of CdSe, CdS, and ZnS nanomaterials as a function of particle size and temperature. The Brus model is employed to describe the size-dependent bandgap variations, while the Varshni equation models the temperature-dependent behavior. The results will offer insights into how nanoscale confinement and thermal effects jointly influence the electronic and optical properties, guiding the design of efficient and thermally stable nanoscale devices [19, 20].

2. Theoretical Framework

The electronic and optical behavior of semiconductor nanomaterials is primarily governed by the structure of their energy bands. In crystalline semiconductors, electrons occupy allowed energy regions known as the valence band and the conduction band, which are separated by an energy gap referred to as the bandgap energy. The magnitude of this bandgap determines the electrical conductivity, optical absorption, and emission characteristics of the material. For many II–VI semiconductors such as Cadmium Selenide (CdSe), Cadmium Sulfide (CdS), and Zinc Sulfide (ZnS), the bandgap is direct, meaning that electrons can transition between the valence and conduction bands without a change in momentum. This property makes these materials highly suitable for optoelectronic devices such as light-emitting diodes, lasers, and photodetectors.

In bulk semiconductors, the bandgap energy is mainly determined by the intrinsic electronic structure of the material. However, when the size of the semiconductor crystal is reduced to the nanometer scale, significant changes occur in its electronic properties due to the phenomenon known as quantum confinement. Quantum confinement arises when the dimensions of a semiconductor particle become comparable to or smaller than the exciton Bohr radius. Under such conditions, the motion of electrons and holes is restricted within a limited spatial region, resulting in the quantization of energy levels. Consequently, the bandgap energy becomes dependent on the particle size.

2.1. Quantum Confinement Effect

The quantum confinement effect explains the size-dependent modification of the band structure in semiconductor nanoparticles. As the size of the nanoparticle decreases, the confinement of charge carriers becomes stronger, leading to an increase in the kinetic energy of the electrons and holes. This increase in kinetic energy effectively widens the bandgap energy of the material. As a result, smaller nanoparticles exhibit larger bandgap energies and emit light at shorter wavelengths compared to their bulk counterparts.

The size dependence of the bandgap energy in semiconductor nanocrystals can be theoretically described using the effective mass approximation (EMA) and the Brus model. According to this model, the bandgap energy of a semiconductor nanoparticle is influenced by three major contributions: the bulk bandgap energy, the quantum confinement energy of charge carriers, and the Coulomb interaction between the electron and hole [21]..

$$E(R) = E_g^{bulk} + \frac{h^2}{8R^2}\left(\frac{1}{m_e^*} + \frac{1}{m_h^*}\right) - \frac{1.8e^2}{4\pi\varepsilon R} \qquad (1)$$

where:

- $E_g(R)$ represents the bandgap energy of the nanoparticle
- E_g^{bulk} is the bandgap energy of the bulk semiconductor
- R is the radius of the nanoparticle

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- m_e^* and m_h^* are the effective masses of the electron and hole respectively
- h is Planck's constant
- e is the elementary charge
- ε is the dielectric constant of the material

The second term in the equation represents the quantum confinement energy, which increases as the particle size decreases. The third term accounts for the Coulomb attraction between electrons and holes, which slightly reduces the bandgap energy.

2.2. Temperature Dependence of Bandgap Energy

Temperature is another critical parameter influencing the bandgap energy of semiconductors. As temperature increases, thermal vibrations within the crystal lattice become more pronounced. These vibrations, known as phonons, interact with charge carriers and modify the electronic band structure. In addition, the expansion of the crystal lattice at higher temperatures alters the spacing between atoms, which affects the overlap of electronic orbitals and reduces the bandgap energy.

The temperature dependence of bandgap energy is commonly described using the Varshni empirical equation, which relates the bandgap energy to temperature through material-specific constants[22]..

$$E(T) = E_g(0) - \frac{\alpha T^2}{T + B} \quad (2)$$

where:

- $E(T)$ = bandgap at temperature T
- $E(0)$ = bandgap at 0 K
- α, B = material-dependent constants
- T = absolute temperature (K)

This equation shows that the bandgap energy decreases as temperature increases. The reduction in bandgap energy occurs because of enhanced electron–phonon interactions and lattice expansion at higher temperatures.

3. Materials and Methods

This study employed a theoretical and computational approach to investigate the combined effects of quantum size and temperature on the bandgap energy of CdSe, CdS, and ZnS semiconductor nanomaterials. The analysis was based on the Effective Mass Approximation (EMA), the Brus quantum confinement model, and the Varshni temperature-dependent bandgap equation. The selected materials were CdSe, CdS, and ZnS, with their respective physical parameters (bulk bandgap energy, effective masses, dielectric constants, and Varshni constants) obtained from established literature as shown in the Table 1 and 2 respectively. Nanoparticle radii ranging from 1–10 nm and temperatures between 100–500 K were considered.

The size-dependent bandgap energy was calculated using the Brus equation, while temperature effects were incorporated through the Varshni equation. Both models were combined to obtain a unified expression describing the bandgap energy as a function of nanoparticle size and temperature. Numerical simulations were performed using MATLAB/Python to compute bandgap energies for different size-temperature combinations. The results were analyzed through graphical plots of bandgap energy versus particle size, temperature, and three-dimensional size-temperature surfaces. Comparative and sensitivity analyses were also conducted to evaluate the response of each material to quantum confinement and thermal effects.

Table 1: Physical Parameters of the Semiconductor Materials

Material	Electron Effective Mass (m_e*)	Hole Effective Mass (m_h*)	Dielectric Constant	Bulk Bandgap (eV)

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CdSe	0.13 m_0	0.45 m_0	9.5	1.74
CdS	0.19 m_0	0.80 m_0	24.2	2.58
ZnS	0.28 m_0	0.59 m_0	8.1	3.68

Where: m_0 represents the free electron mass.

Table 2: Varshni Parameters for the Selected Semiconductor Nanomaterials

Material	Bandgap at 0 K, E(0) (eV)	Temperature Coefficient (a, eV/K)	Varshni Constant (β, K)
CdSe	1.74	4.9×10^{-4}	245
CdS	2.58	5.4×10^{-4}	204
ZnS	3.68	7.0×10^{-4}	600

4.Results and Discussion

The theoretical calculations were performed to evaluate the influence of nanoparticle size and temperature on the bandgap energy of Cadmium Selenide (CdSe), Cadmium Sulfide (CdS), and Zinc Sulfide (ZnS) semiconductor nanomaterials. The results obtained from the Brus quantum confinement model and the Varshni temperature model are discussed in Figure 1 and 2.

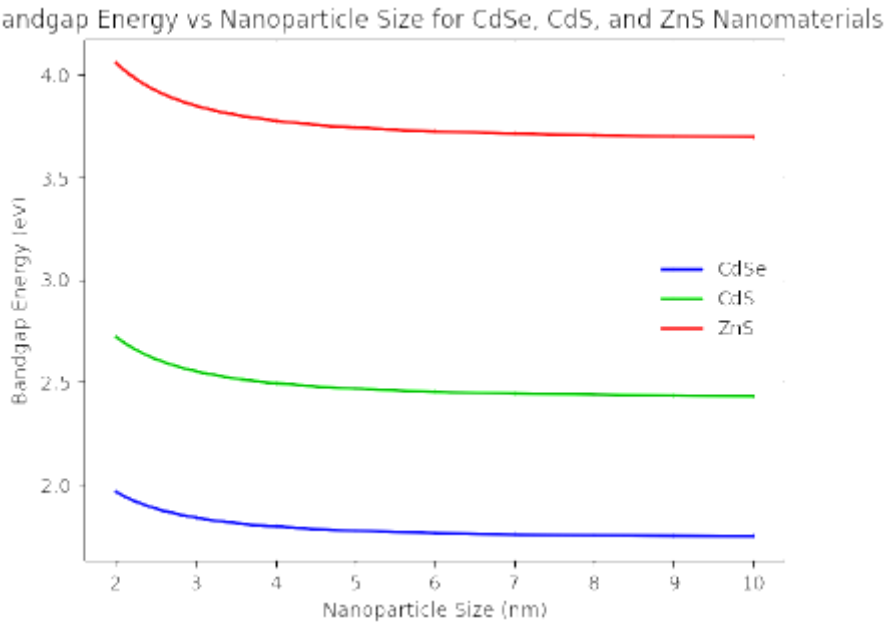

Figure 1: Bandgap versus size for CdSe, CdS and ZnS nanomaterials

The plotted relationship between nanoparticle size and bandgap energy for Cadmium Selenide (CdSe), Cadmium Sulfide (CdS), and Zinc Sulfide (ZnS) clearly demonstrates the influence of quantum confinement on the electronic properties of semiconductor nanomaterials. As the nanoparticle size decreases from about 10 nm to 2 nm, the bandgap energy of all three materials increases significantly. This behavior arises because the spatial confinement of electrons and holes within very small dimensions increases their kinetic energy, thereby widening the energy separation between the valence band and the conduction band.

The graph further reveals that ZnS exhibits the highest bandgap energy across the entire size range, followed by CdS, while CdSe shows the lowest bandgap energy. This trend is consistent with the intrinsic bulk bandgap values of the materials. As the particle size increases toward larger dimensions, the bandgap energy gradually approaches the bulk semiconductor value, indicating that the quantum confinement effect becomes weaker in larger nanoparticles. Another important observation from the graph is the blue shift in optical properties as nanoparticle size decreases. Smaller nanoparticles require higher photon energies for electronic

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transitions, which results in emission at shorter wavelengths. This size-dependent tunability of the bandgap is one of the most important advantages of semiconductor nanomaterials, particularly for optoelectronic applications.

From a technological perspective, these results have important implications for device design. Nanoparticles of CdSe are widely used in quantum dot displays, light-emitting diodes, and biomedical imaging because their relatively smaller bandgap allows efficient emission in the visible region of the electromagnetic spectrum. CdS nanomaterials, which possess intermediate bandgap values, are commonly employed in photoconductors, photodetectors, and solar cells where efficient absorption of visible light is required. In contrast, ZnS nanomaterials have a wide bandgap and therefore are suitable for ultraviolet optoelectronic devices, phosphor materials, and high-frequency electronic components.

The ability to control the bandgap energy through particle size manipulation enables the design of tunable nanoscale devices with specific optical and electronic properties. Consequently, understanding the relationship between nanoparticle size and bandgap energy in CdSe, CdS, and ZnS nanomaterials is essential for optimizing the performance of next-generation optoelectronic devices, quantum dot lasers, nanosensors, and photovoltaic technologies.

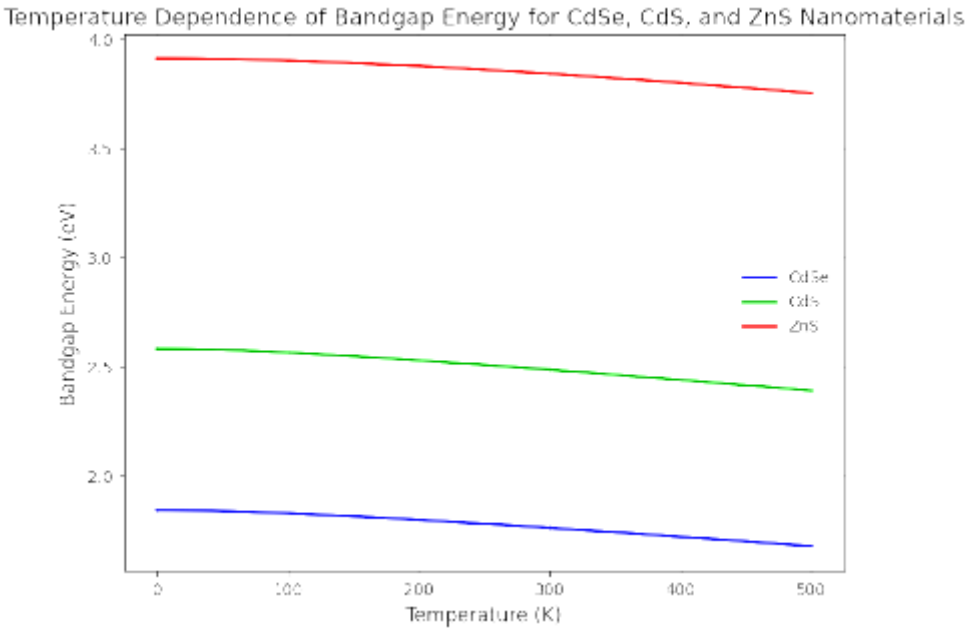

Figure 2: Bandgap versus temperature for CdSe, CdS and ZnS nanomaterials

The plotted graph showing the variation of bandgap energy with temperature for Cadmium Selenide (CdSe), Cadmium Sulfide (CdS), and Zinc Sulfide (ZnS) clearly demonstrates the influence of thermal effects on the electronic properties of semiconductor nanomaterials. As the temperature increases from 0 K to 500 K, the bandgap energy of all three materials decreases gradually. This behavior occurs due to lattice expansion, which increases the spacing between atoms, and electron–phonon interactions, which perturb the electronic energy levels. Both effects reduce the energy separation between the conduction band and the valence band, leading to a narrower bandgap at higher temperatures. Among the three materials, ZnS maintains the largest bandgap energy across the entire temperature range, reflecting its wide-bandgap nature and higher thermal stability. CdS exhibits intermediate bandgap values, while CdSe shows the lowest bandgap energy, which is consistent with their intrinsic bulk bandgap properties. The observed trends highlight that the bandgap of each material is sensitive to temperature changes, but the degree of sensitivity varies according to the material's electronic structure.

These temperature-dependent bandgap variations have significant implications for device applications. For instance, in CdSe-based quantum dots and light-emitting diodes (LEDs), the decrease in bandgap with temperature can cause a shift in emission wavelength, affecting color stability in displays. CdS nanomaterials, with moderate thermal sensitivity, are well-suited for solar cells, photodetectors, and sensors, where

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performance under varying temperatures is critical. In contrast, ZnS, with its wide bandgap and superior thermal stability, is ideal for ultraviolet optoelectronic devices, phosphors, and high-frequency electronic components, where maintaining consistent electronic and optical properties under high temperatures is essential. Understanding these temperature effects is therefore crucial for the design, optimization, and reliable operation of semiconductor nanomaterial-based devices across a range of thermal conditions.

5. CONCLUSION

The study demonstrates that both nanoparticle size and temperature significantly influence the bandgap energy of Cadmium Selenide (CdSe), Cadmium Sulfide (CdS), and Zinc Sulfide (ZnS) semiconductor nanomaterials. As particle size decreases, the bandgap energy increases due to quantum confinement, resulting in a blue shift in optical properties. Conversely, increasing temperature reduces the bandgap energy because of lattice expansion and electron–phonon interactions. ZnS maintains the highest bandgap and thermal stability, CdS exhibits intermediate behavior, and CdSe shows the lowest bandgap values. These trends indicate that controlling particle size and accounting for temperature effects are essential for optimizing the optical and electronic performance of these materials. Consequently, CdSe is well-suited for visible-light quantum dots and LEDs, CdS for solar cells and photodetectors, and ZnS for UV optoelectronic and high-temperature devices. Understanding these effects provides critical guidance for designing and developing efficient, stable, and tunable nanoscale semiconductor devices.

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