

Simulation of the Effect of Temperature on the Bandgap Energy of CdSe, CdS, and ZnS Semiconductors

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Abstract: This study provides a theoretical analysis of how temperature affects the bandgap energies of the II–VI semiconductors CdSe, CdS, and ZnS, using both the Varshni equation and the Bose–Einstein phonon model. The bandgap is a key factor controlling the optical and electronic properties of semiconductors, and its variation with temperature has a direct impact on the performance of optoelectronic devices. The investigation considers a temperature range from 0 to 500 K and accounts for the effects of lattice thermal expansion and electron–phonon interactions. The results indicate a nonlinear decrease in bandgap energy with increasing temperature for all three materials, with CdSe showing the greatest reduction and highest thermal sensitivity, CdS exhibiting moderate sensitivity, and ZnS maintaining the greatest thermal stability. Comparison of the two models demonstrates consistent trends: the Varshni equation reflects empirical lattice expansion effects, while the Bose–Einstein model captures the influence of phonon-mediated interactions. The results underscore the critical role of temperature-dependent bandgap behavior in designing and optimizing optoelectronic devices that require thermal stability, such as solar cells, light-emitting diodes, laser diodes, and photodetectors.

Key words: CdSe, CdS, ZnS, Bandgap, Temperature Dependence, Varshni Equation, Bose–Einstein Model, Electron–Phonon Interaction, Semiconductors, Thermal Stability.

1. INTRODUCTION

The energy bandgap (E_g) represents the energy separation between the valence band and the conduction band in a semiconductor and serves as a key parameter governing its electrical and optical characteristics^[1, 2]. This energy separation determines the threshold for electron excitation, thereby influencing light absorption, emission wavelength, carrier generation, and transport processes. In direct bandgap II–VI materials such as CdSe, CdS, and ZnS, efficient radiative recombination makes the bandgap particularly important for practical applications including solar cells, light-emitting diodes, laser systems, and photodetectors^[3, 4]. Accurate knowledge of the electronic band structure is therefore necessary for spectral tuning and performance optimization in optoelectronic devices^[5].

It is well established that the bandgap of a semiconductor is not constant but varies with temperature due to changes in lattice structure and electron–phonon coupling^[6, 7]. An increase in temperature enhances lattice vibrations, which alters interatomic spacing and modifies the electronic energy levels. As a consequence, the bandgap typically decreases with rising temperature, producing a redshift in absorption and emission spectra. Experimental investigations and theoretical analyses in II–VI semiconductors have

consistently reported this temperature-induced bandgap narrowing^[8, 9]. Furthermore, first-principles calculations based on electron–phonon interaction theory provide deeper insight into the microscopic mechanisms responsible for thermal bandgap renormalization^[10, 11].

To describe this temperature dependence quantitatively, several models have been developed. The Varshni equation remains one of the most widely applied empirical relationships, using material-dependent parameters to represent thermal effects on the bandgap^[12]. While it often reproduces experimental trends within moderate temperature ranges, its semi-empirical nature limits its ability to fully explain the underlying physical processes, particularly in extreme or nanoscale conditions^[13]. Alternatively, the Bose–Einstein phonon model incorporates statistical phonon occupation explicitly and provides a more physically grounded interpretation of how lattice vibrations influence electronic states^[14].

Recent investigations indicate that temperature coefficients and electron–phonon coupling strengths vary considerably among semiconductor materials, especially in wide-bandgap and quantum-confined systems^[15]. In nanostructured II–VI compounds, confinement effects alter the effective bandgap and modify its sensitivity to temperature, highlighting the interplay between electronic structure and lattice dynamics^[16, 17].

A thorough understanding of temperature-dependent bandgap behavior is therefore crucial for the reliable design of semiconductor devices intended for operation under varying thermal conditions. Integrating the empirical flexibility of the Varshni model with the physical insight provided by the Bose–Einstein approach offers a comprehensive framework for evaluating thermal bandgap variation. Accordingly, this study applies both models to CdSe, CdS, and ZnS to examine their comparative thermal responses and to clarify the role of lattice expansion and electron–phonon interactions in II–VI semiconductors.

2. THEORETICAL BACKGROUND

2.1. Energy Band Structure in Semiconductors

The energy band structure of a semiconductor explains how electron energy levels are arranged within a crystalline solid. Because atoms in a crystal are closely packed, their discrete atomic energy levels broaden into continuous bands of allowed energies separated by regions where no electron states exist. These regions of forbidden energy define the electronic behavior of the material and largely determine its electrical, optical, and thermal characteristics.

In a semiconductor, electrons fill the valence band, which lies at lower energy, while the conduction band is positioned at a higher energy level. The separation between these two bands is known as the bandgap (E_g), as illustrated in Figure 1. More precisely, the bandgap is the energy difference between the valence band maximum (VBM) and the conduction band minimum (CBM). This energy represents the minimum requirement for promoting an electron from a bound state within the lattice to a mobile state where it can participate in conduction.

The magnitude of the bandgap directly controls how the material interacts with light and how it conducts electricity:

- **Optical Absorption:** When incident light carries energy equal to or greater than E_g , electrons can be excited from the valence band into the conduction band, resulting in absorption. Photons with energy below this threshold pass through the material without generating electronic transitions.

- **Optical Emission:** When electrons in the conduction band return to the valence band, they release energy approximately equal to E_g in the form of photons. Consequently, the bandgap determines the wavelength (or color) of the emitted radiation.
- **Electrical Conduction:** Electrical current arises when electrons occupy the conduction band. Since electrons must acquire at least E_g to reach this band, the bandgap effectively regulates the number of charge carriers available for conduction and, therefore, the overall conductivity of the semiconductor.

Thus, the bandgap serves as the central parameter linking electronic structure to optical response and charge transport in semiconductor materials.

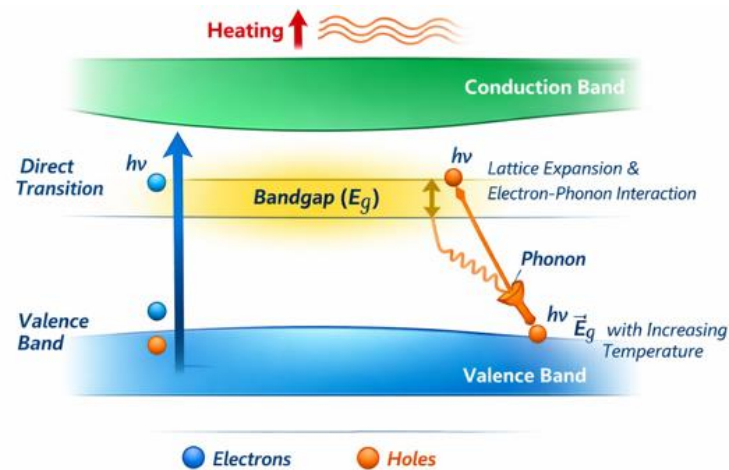


Fig. 1. Energy band structure in semiconductors

2.2. Mathematical Models of Bandgap–Temperature Dependence

2.2.1. Varshni Model

$$E(T) = E_g(0) - \frac{\alpha T^2}{T + B} \quad (1)$$

where:

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

This model predicts a nonlinear decrease in bandgap with increasing temperature.

2.3. Bose-Einstein Model

$$E_g(T) = E_g(0) - \frac{A}{\exp\left(\frac{\theta}{T}\right) - 1} \quad (2)$$

where:

- A = electron-photon coupling constant
- θ = characteristic photon temperature

This model directly links bandgap reduction to photon population statistics.

3. MATERIALS AND METHODS

This study employs a purely theoretical and analytical framework to examine the influence of temperature on the bandgap energies of CdSe, CdS, and ZnS semiconductors. Experimental procedures were not conducted. Instead, the temperature dependence of the bandgap was modeled using the Varshni and Bose–Einstein formulations, with material-specific parameters obtained from established literature sources and presented in Tables 1 and 2. The computed bandgap–temperature profiles were subsequently evaluated and compared for the three materials in order to assess their relative thermal sensitivity and stability.

Table 1: Material Parameters for Varshni Bandgap Models

Material	$E_g(0)$ (eV)	α (eV/K)	β (K)	Temperature Sensitivity
CdSe	1.84	4.5×10^{-4}	250	High
CdS	2.58	4.0×10^{-4}	300	Moderate
ZnS	3.91	2.5×10^{-4}	900	Low

Table 2: Material Parameters for Bose–Einstein Bandgap Models

Material	$E_g(0)$ (eV)	A (eV)	θ (K)	Electron–Phonon Coupling Strength
CdSe	1.84	0.060	180	Strong
CdS	2.58	0.050	220	Moderate
ZnS	3.91	0.030	340	Weak

4. RESULTS AND DISCUSSION

Figure 2 presents the relationship between bandgap energy and temperature for CdSe, CdS, and ZnS as determined from the Varshni equation. For each material, the bandgap decreases progressively as temperature rises, forming smooth downward curves across the considered temperature range. This trend aligns with established solid-state principles, where increased thermal energy intensifies lattice vibrations and modifies interatomic spacing, leading to a reduction in the energy difference between the valence and conduction bands.

A comparison of the three curves indicates that CdSe exhibits the most pronounced decline in bandgap with temperature. CdS shows a moderate reduction, while ZnS demonstrates the least variation. These differences can be attributed to variations in bonding characteristics and lattice stiffness among the materials. CdSe, having relatively softer bonding and stronger electron–phonon interaction effects, responds more significantly to thermal excitation. In contrast, the comparatively rigid lattice structure of ZnS limits bandgap shrinkage, contributing to its greater thermal stability.

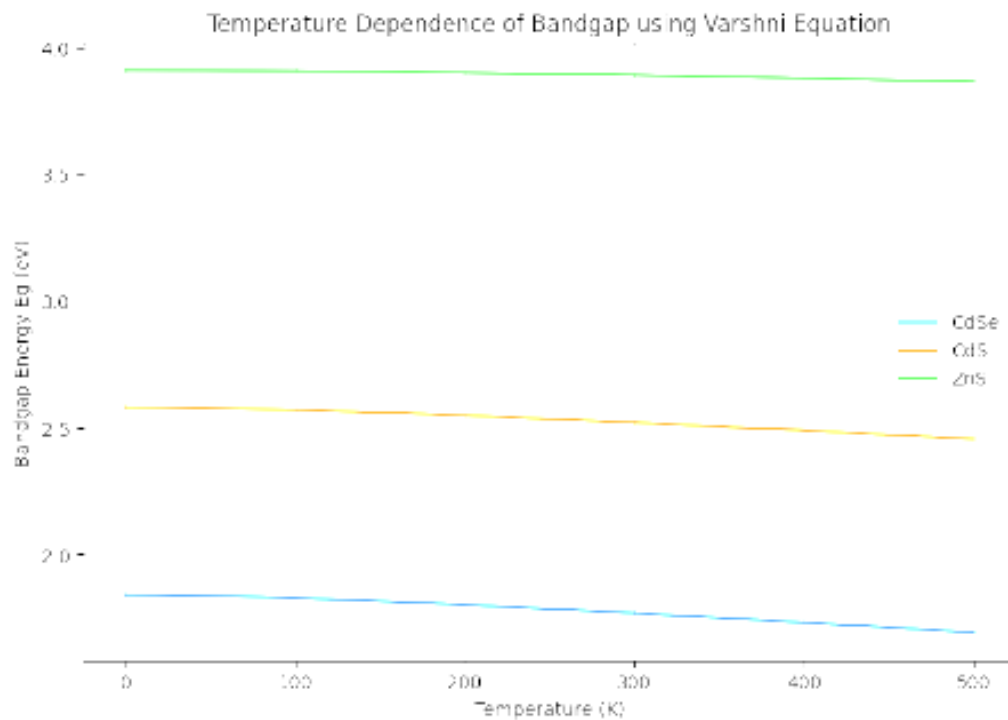


Fig. 2. Variation of bandgap energy with temperature for CdSe, CdS, and ZnS semiconductors using the Varshni model

Figure 3 depicts the temperature dependence of the bandgap for CdSe, CdS, and ZnS as evaluated with the Bose–Einstein phonon approach. Similar to the earlier model, the bandgap for each material decreases steadily as temperature increases. The downward trend reflects the growing influence of lattice vibrations on the electronic structure as thermal energy rises.

Unlike the Varshni relation, the Bose–Einstein formulation directly accounts for phonon occupancy through statistical mechanics. With increasing temperature, the number of thermally excited phonons rises in accordance with Bose–Einstein distribution, leading to shifts in the electronic energy states and a consequent narrowing of the bandgap. The comparative behavior among the materials remains consistent: CdSe undergoes the most significant reduction, CdS displays an intermediate response, and ZnS shows only a slight change. This consistency reinforces the conclusion that CdSe is more thermally sensitive, whereas ZnS maintains greater resistance to temperature-induced bandgap variation. Overall, the Bose–Einstein model offers a more physically descriptive interpretation by explicitly relating bandgap changes to quantized lattice vibrations rather than relying solely on empirical fitting parameters.

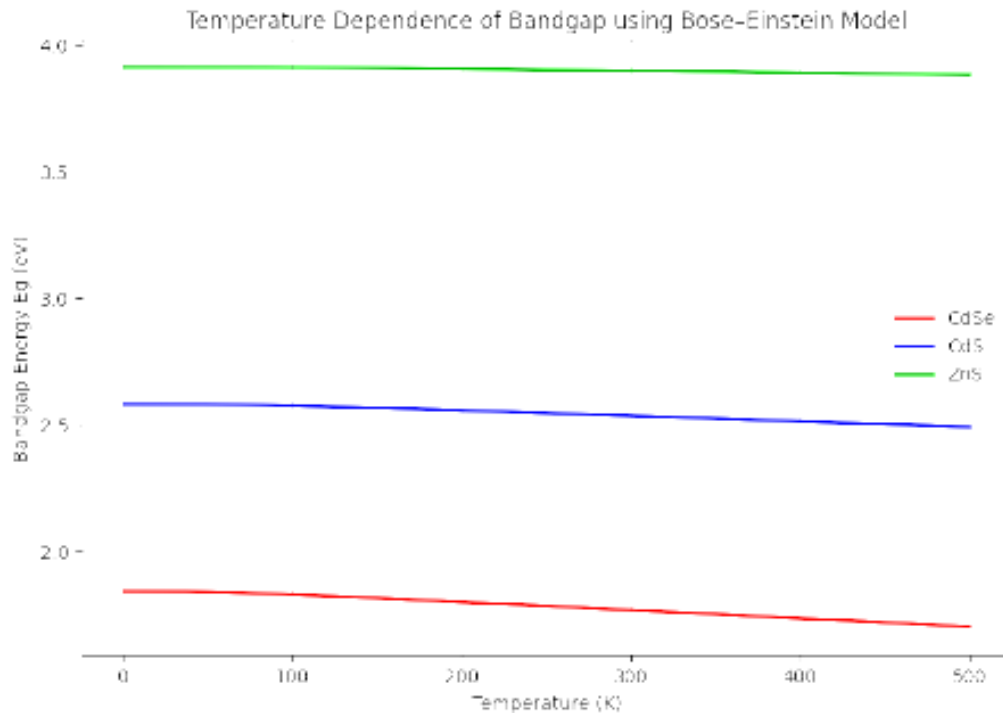


Fig. 3. Variation of bandgap energy with temperature for CdSe, CdS, and ZnS semiconductors using the Bose–Einstein phonon model

Figure 4 presents a combined plot of bandgap energy as a function of temperature for CdSe, CdS, and ZnS, incorporating results obtained from both the Varshni (solid lines) and Bose–Einstein (dashed lines) models. In all cases, the bandgap decreases in a nonlinear manner as temperature increases, indicating a consistent thermal response across the three materials regardless of the modeling approach applied.

The Varshni curves represent the temperature dependence through an empirical description that reflects the influence of thermal expansion on the crystal lattice. In contrast, the Bose–Einstein curves relate the observed bandgap reduction to changes in phonon population and the interaction between lattice vibrations and electronic states. Despite differences in formulation, both models produce closely aligned trends, supporting the reliability of the predicted temperature behavior.

The comparison further reveals a clear ordering in temperature sensitivity among the materials, showing a systematic variation in how strongly each semiconductor responds to increasing thermal conditions:

$$\text{CdSe} > \text{CdS} > \text{ZnS}$$

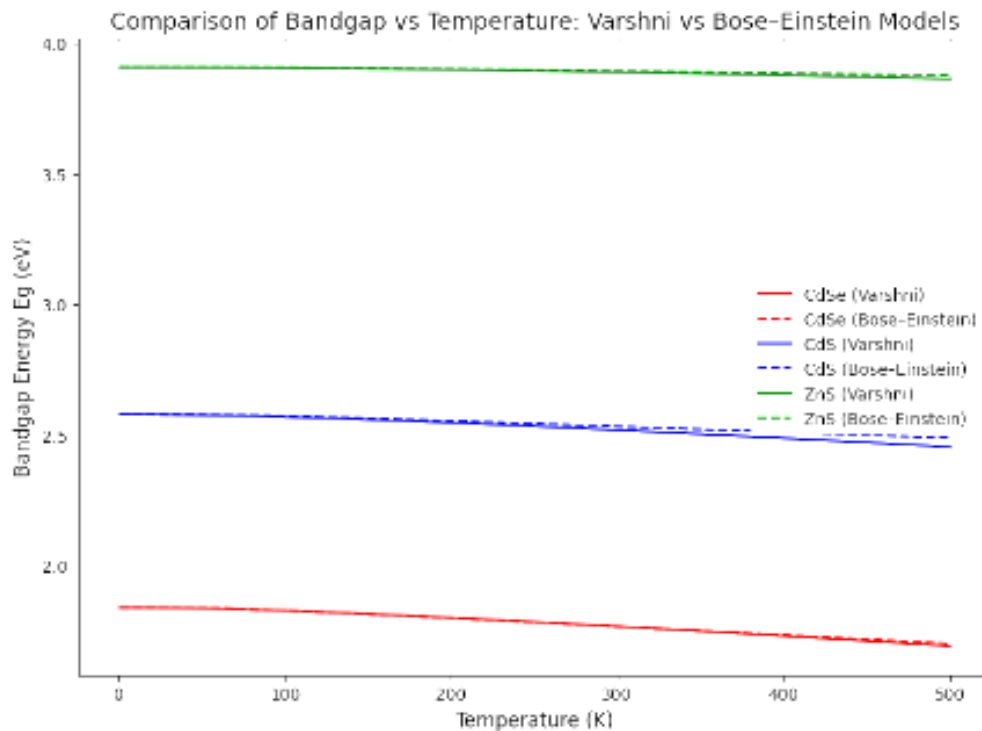


Fig. 4. Unified visualization of bandgap energy versus temperature for CdSe, CdS, and ZnS

This combined representation illustrates that the two models complement each other, offering a more complete picture of how bandgap energies respond to temperature. It provides valuable insight for selecting materials and designing devices that must maintain reliable performance under varying thermal conditions in optoelectronic applications.

In general, CdSe exhibits high thermal sensitivity, which may limit its use in devices exposed to elevated temperatures but enables tunable emission for temperature-sensitive photonic applications. CdS demonstrates moderate thermal response, making it well-suited for general-purpose LEDs and photodetectors with reliable and predictable performance. ZnS shows excellent thermal stability, supporting its use in high-temperature LEDs, UV detectors, and laser devices.

5. CONCLUSION

This study provides a theoretical analysis of how temperature affects the bandgap energies of Cadmium Selenide (CdSe), Cadmium Sulfide (CdS), and Zinc Sulfide (ZnS) using both the Varshni equation and the Bose–Einstein phonon model. The findings indicate that the bandgap of each material decreases nonlinearly with rising temperature, driven by lattice expansion and electron–phonon interactions. Among the three, CdSe shows the greatest thermal sensitivity, with the largest reduction in bandgap due to its relatively soft lattice and strong electron–phonon coupling. CdS exhibits intermediate thermal response, reflecting a balance between lattice stiffness and phonon effects, while ZnS demonstrates the highest thermal stability, with only minor bandgap variation, owing to its rigid ionic lattice and weaker phonon interaction. Both theoretical models consistently reproduce this trend in temperature sensitivity. By combining the Varshni and Bose–Einstein approaches, the study establishes a unified framework for predicting temperature-dependent bandgap behavior, providing both empirical and physical insights. These results are essential for guiding the selection and design of optoelectronic devices with high thermal stability, offering valuable insight for applications where temperature fluctuations can impact performance, efficiency, and spectral reliability.

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