

$\text{Cd}_x\text{Zn}_{1-x}\text{Se}$ Ternary Semiconductor Alloy for Emerging Quantum Computing.

Dr. Alla Srivani Ph.D., D.SC., PDF

Professor

Vasireddy Venkatadri International Tecnological Univesity (VVITU)

Abstract: The tunable band gap of the ternary semiconductor $\text{Cd}_x\text{Zn}_{1-x}\text{Se}$ has attracted a lot of interest. This can be achieved by altering the alloy's cadmium (Cd) content (x). Due to its compositional flexibility, which enables fine control over optical and electrical properties, this material holds promise for advanced photonic and opto-electronic applications. The band gap narrows with increasing Cd content, improving infrared absorption and photoluminescence properties, whereas lower Cd concentrations promote blue and ultraviolet emission. Designing solar cells, photo detectors, quantum dot lasers, and high-efficiency light-emitting diodes (LEDs) need this tunability. Moreover, $\text{Cd}_x\text{Zn}_{1-x}\text{Se}$ quantum dots and nano structures show robust quantum confinement effects, creating new avenues for photo catalysis, display technologies, and bio imaging. At the Nano scale Cd-rich compositions increase quantum confinement. This results in discrete energy levels, which are vital for quantum bit manipulation.

Keywords: Energy gap, SemiconductorAlloys, Thin film Properties.

Introduction: The solid solutions that belong to the $\text{Cd}_x\text{Zn}_{1-x}\text{Se}$ II-VI Ternary Semiconductor Band Energy Gap have been examined in the initial concept of the current work.

Cd doping in a binary semiconductor such as In fact, ZnSe and altering the dopant's composition have caused the Band Energy Gap to decrease.As a result, dopant has a wide range of applications by increasing conductivity and decreasing the Band Energy Gap. For $\text{Cd}_x\text{Zn}_{1-x}\text{Se}$ II-VI Ternary Semiconductors, the current study examines the relationship between Band Energy Gap and Electro Negativity with composition modification. The reasonable correspondence between reported and computed Band Energy Gap values The Band Energy Gaps for Ternary semiconductors are further extended in CdSe and ZnSe binary semiconductors. II–VI Ternary semiconductors are made up of different elements and have a wide range of physical properties.

In the starting concept of the present work, the solid solutions belonging to $\text{Cd}_x\text{Zn}_{1-x}\text{Se}$ II-VI Ternary Semiconductor Band Energy Gap have been investigated. Doping of Cd component in a Binary

semiconductor like ZnSe and changing the composition of do pant has actually resulted in lowering of Band Energy Gap. Thus effect of do pant increases the conductivity and decreases the Band Energy Gap and finds extensive applications.

The present investigation relates Band Energy Gap and Electro Negativity with variation of composition for $\text{Cd}_x\text{Zn}_{1-x}\text{Se}$ II-VI Ternary Semiconductor. The fair agreement between calculated and reported values of Band Energy Gaps In CdSe and ZnSe Binary semiconductors give further extension of Band Energy Gaps for Ternary semiconductors. II-VI Ternary semiconductors, which consist of various elements, have widely ranging Physical properties. They have therefore many possible applications. The physical Properties which may vary, include band gaps, crystal lattice structures, electron and Hole mobilities, optical properties and thermal conductivity.

The solid solutions that are a part of the $\text{Cd}_x\text{Zn}_{1-x}\text{Se}$ II-VI Ternary Semiconductor Band Energy Gap have been studied in the basic idea of this work. In fact, ZnSe and altering the dopant's composition have reduced the Band Energy Gap while doping a binary semiconductor with Cd. Dopants have several applications because they reduce the Band Energy Gap and boost conductivity. For $\text{Cd}_x\text{Zn}_{1-x}\text{Se}$ II-VI Ternary Semiconductors, the current study examines the link between Band Energy Gap and Electro Negativity with composition modification.

Methodology: A variety of devices that are not achievable with silicon, the primary elemental semiconductor material, can be realized by choosing the right II-VI Ternary semiconductor materials. Therefore, it's critical to comprehend the physical characteristics of II-VI Ternary semiconductors and know how to choose the right materials for the intended uses. Specialty literature provide explanations of these features. Only a small percentage of the many II-VI Ternary Semiconductor Compounds, which are composed of more than two elements, exhibit semiconductor characteristics. According to Wilson's model, II-VI Ternary Semiconductor Compounds with semiconductor characteristics have the following characteristics. II-VI Ternary semiconductors have electronic conductivity.

By selecting the appropriate II-VI Ternary semiconductor materials, a range of devices that are not possible with silicon, the main elemental semiconductor material, can be realized. Understanding the physical properties of II-VI Ternary semiconductors and knowing how to select the appropriate materials for the planned applications are therefore essential. These characteristics are explained in specialty literature. Of the numerous II-VI Ternary Semiconductor Compounds, which are made up of more than two elements, semiconductor properties are present in just a small portion. The

following traits are present in II-VI Ternary Semiconductor Compounds with semiconductor properties, per Wilson's model.

Electronic conductivity is a feature of II-VI ternary semiconductors. It does not include ionic conductivity. As a function of temperature, pressure, dopant composition, electric and magnetic fields, and ternary conductivity, II-VI is significantly enhanced. The kind and concentration of impurities have a significant impact on II-VI Ternary Conductivity. The Ternary Semiconductor II-VI Tetrahedral bonds, which comprise both covalent and ionic bonds, are also present in the compound. For this reason, compounds are made up of many components with varying levels of electro negative. This discovery provides up a new avenue for studying the Band Energy Gap in $Cd_xZn_{1-x}Se$ II-VI ternary semiconductors.

Results: The research of ternary semiconductor materials and their alloys for use in the creation of hetero structures has received a lot of attention lately. The significance of these chemicals' physico chemical characteristics is now coming into sight. There is extensive experimental research being done on the use of these ternary semiconductor materials in optical devices. More focus is placed on the research of these substances, such as Selenide from the VI Group, Cadmium, and Zinc from the II Group.

$Cd_xZn_{1-x}Se$ is a key ternary semiconductor material, representing an arbitrary alloy of CdSe and ZnSe, with Cd composition varying from 0 to 1 at specific values of 0, 0.20, 0.27, 0.33, 0.56, and 1.00, calculated based on the composition. The results obtained showed strong agreement with both experimental and theoretical Semiconductor data from the literature. In our calculations for all five systems, we treated $Cd_xZn_{1-x}Se$ ternary Semiconductor alloys as having cubic symmetry for consistency and simplicity. We substituted one, two, and three atoms respectively to achieve the desired concentration of theoretical values. The band profiles and bandgap values align well with previous theoretical studies. The band gaps are lesser than the experimental measurements.

Objective: The main Objective of this Research paper is to calculate $Cd_xZn_{1-x}Se$ II-VI Ternary Semiconductor Band Energy Gap values. The following relation calculates band Energy Gap of $Cd_xZn_{1-x}Se$.

$$E_g(Cd_xZn_{1-x}Se) = 1-x * E_g(CdSe) + x * E_g(ZnSe) + \text{SQRT}(E_g(CdSe) * E_g(ZnSe) * x * 1-x)$$

Where: E_g = Band Energy Gap X =Cd Composition.

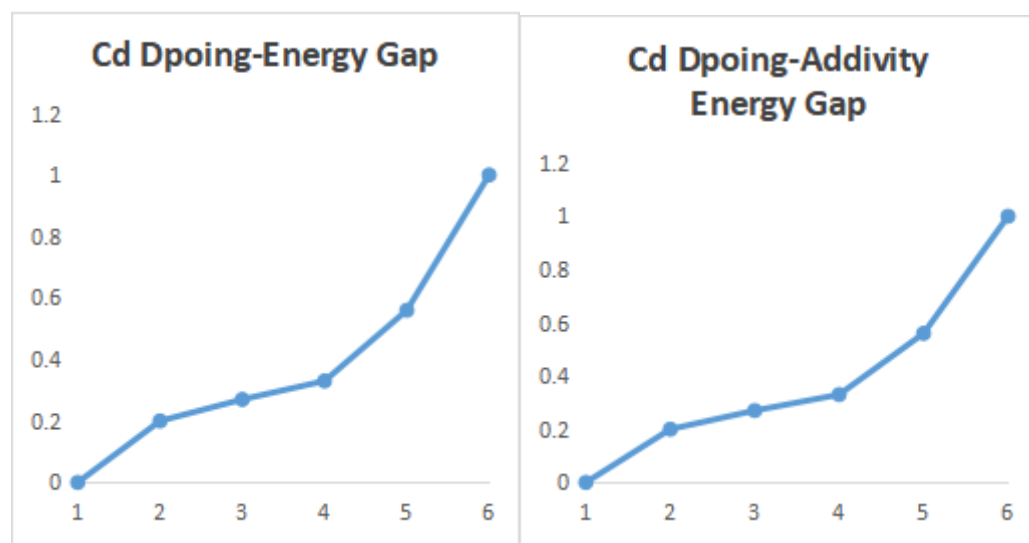
Additivity: $E_g(Cd_xZn_{1-x}Se) = X * E_g(CdSe) + (1-x) * E_g(ZnSe)$. Where: E_g =Band Energy Gap.

Sl.NO	Cd Composition	Energy gap E_g	Additivity Energy Gap (E_g)
1	0.00	2.62	2.58
2	0.20	2.40	2.41
3	0.27	2.32	2.36
4	0.33	2.28	2.31
5	0.56	2.09	2.11
6	1.00	1.71	1.74

Because they offer designed electrical, optical, and spintronic features specifically suited for quantum computing, communication, and sensing, semiconductor alloys are essential for the development and application of quantum materials. These alloys are perfect for qubit platforms, quantum dots, and quantum photonic devices because they can be adjusted at the atomic level.

Increased electron mobility enables quicker quantum gate function.
powerful quantum confinement with a low effective mass. Direct band gap for photon-based qubits for effective light emission. Lattice correspondence with InP helps create hetero structures without flaws.

Graphical representation:



This graph represents Band Energy Gap values of $Cd_xZn_{1-x}Se$. Doping of Cd component in a Binary semiconductor like ZnSe and changing the composition of dopant has actually resulted in lowering of Band Energy Gap. Thus effect of dopant increases the conductivity and decreases the Band Energy Gap

Application in Emerging Quantum Computing : The existing data set of values for $\text{Cd}_x\text{Zn}_{1-x}\text{Se}$ II-VI Ternary Semiconductors and their Band Energy Gap values incorporates the latest methods and basis sets that are still being developed. The information is also being analyzed to uncover issues with current theories and is utilized to highlight areas where further research should be conducted in the future. The significance of the ternary semiconductor alloy systems studied highlights the need to comprehend alloy broadening phenomena, as it could impact the performance of semiconductor devices.

The Energy Gap of $\text{Cd}_x\text{Zn}_{1-x}\text{Se}$ Material allows for adjustable Quantum dot Energy levels. Quantum Confinement of $\text{Cd}_x\text{Zn}_{1-x}\text{Se}$ Semiconductor enables the formation of Qubits. Exciton Binding Energy of $\text{Cd}_x\text{Zn}_{1-x}\text{Se}$ improves Optical Qubit robustness. The strain in the lattice and spin coherence of $\text{Cd}_x\text{Zn}_{1-x}\text{Se}$ allows for manipulation through strain engineering, leading to improved qubit coherence. Quantum dot qubits possess adjustable energy levels and band gaps.

Single Photon Sources improve emission using Cd-Rich Quantum Dots. Spin Qubits demonstrate tuning of spin coherence and composition.

Conclusion: This paper aims to provide a fundamental understanding of the Material physics in Quantum Computing associated with this phenomenon, regardless of the importance of ternary alloys in device applications. Cd concentration in $\text{Cd}_x\text{Zn}_{1-x}\text{Se}$ acts as an effective means for tuning the quantum and optoelectronic properties of the material. This establishes a strong foundation for various quantum computing architectures, including quantum dot-based multiple qubits, photonic systems, and spintronic devices. The Band Energy Gap of the current Semiconductor Alloy is employed for electrical conduction in semiconductors.

This event is utilized in Band Gap Engineering Applications. The band structures of the alloy show features similar to those of bulk CdSe and ZnSe. Acknowledgments: CdSe has a narrower band gap (~ 1.7 eV) compared to ZnSe (~ 2.7 eV). By modifying the Cadmium Concentration (x) from 0 to 1, the band gap of $\text{Cd}_x\text{Zn}_{1-x}\text{Se}$ can be altered continuously.

Quantum dots (QDs) formed from this material with appropriate band gaps can function as quantum emitters or qubits in photonic quantum computing. At the nanoscale, especially in quantum dots

(QDs), compositions rich in Cd improve quantum confinement. This results in unique energy levels crucial for controlling quantum bits (qubits)

REFERENCES:

- [1] Smokal, V., Derkowska, B., Czaplicki, R., “Nonlinear optical properties of $\text{Zn}_{1-x}\text{Mg}_x\text{Se}$ and $\text{Cd}_{1-x}\text{Mg}_x\text{Se}$ crystals”, *Optical Materials*, 31: 518 –522 (2009).
- [2] Chen, A-B. Sher, A., “Electronic structure of pseudobinary semiconductor alloys $\text{Al}_x\text{Ga}_{1-x}\text{As}$, $\text{GaP}_x\text{As}_{1-x}$, and $\text{Ga}_x\text{In}_{1-x}\text{P}$ ” *Phys. Rev. B*, 23: 5360– 5374 (1980).
- [3] Shimomura, A., Anan, T., Sugou, S., “Growth of AlPSb and GaPSb on InP by gas-source molecular beam epitaxy”, *J. Cryst. Growth*, 162: 121-125 (1996).
- [4] Sahraoui, B., Dabos-Seignon, S., Migalska-Zalas, A., “Linear and nonlinear optical properties $\text{Zn}_{1-x}\text{Mg}_x\text{Se}$ layers grown by MBE and LPD method” *Opto-Electronics Review*, 12: (4) 405-409 (2004).
- [5] Fredj, Debbichi, M., Said, M., “Influence of the composition fluctuation and the disorder on the bowing band gap in semiconductor materials”, *Microelectronic J.*, 38: 860–870 (2007).
- [6] M. Robinson, P.D. Haynes, “Linear-scaling first-principles study of a quasicrystalline molecular Material”, *Chem. Phys. Lett.* 476: 73-77 (2009).
- [7] Kohn, W., Sham, L.J., “Self-consistent equations including exchange and correlation effects”, *Phys. Rev.*, 140: A1133–A1138 (1965).
- [8] Fischer, T H, Almlof, J., “General methods for geometry and wave function optimization”, *J. Phys. Chem.*, 96: (24) 9768–9774 (1992).
- [9] Ceperley, D.M., Alder, B.J., “Ground state of the electron gas by a stochastic method”, *Phys. Rev.Lett.* 45: 566–569 (1980).
- [10] Perdew, J.P., Zunger, A., “Self-interaction correction to density-functional approximations for many-electron systems”, *Phys. Rev. B*, 23: 5048–5079 (1981).
- [11] Troullier, N., Martins, “Efficient pseudopotentials for plane-wave calculations”, *J. Phys. Rev. B*, 43: 1993–2006 (1993).
- [12] Vurgaftmana, I., Meyer, J.R., “Band parameters for III–V compound semiconductors and their Alloys”, *J. of Appl. Phys.*, 89: 5818- 5846 (2001).
- [13] Wang, S.Q., Yes, H.Q., “Plane-wave pseudo potentials study on mechanical and electronic properties for IV and III-V crystalline.
- [14] Huheey, J. E. (1978). *Inorganic Chemistry* (2nd Edn.). New York: Harper & Row. p. 167.
- [15] Allred, A. L.; Rochow, E. G. (1958). "A scale of electronegativity based on electrostatic force". *Journal of Inorganic and Nuclear Chemistry* 5: 264..