First principles study on structural and electronic properties of hexagonal CdSe for improved efficiency of solar panel

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***Abstract*—Cadmium Selenide (CdSe) in hexagonal structure investigated by First Principles study with local density approximation (LDA) and generalized gradient approximation (GGA) using the SIESTA code for their structural and electronic properties. A hexagonal CdSe structure with bond length of 2.69 Å and bond angle of 109.36º was found. For calculation, electronic properties of hexagonal CdSe are obtained by k-point sampling and cut off energy, then DOS, PDOS and band structures are obtained. Results indicate different band gap values for the compounds, and the calculated values are underestimated. According to DOS calculation energy gap between the valance and the conduction band is 1.29eV same as PDOS calculation, founded smaller then experimental band gap value 1.74 eV, and it is direct band gap nature. As the band gap decreases, the efficiency of the CdSe thin films used in solar cells increases.**

***IndexTerms*—DFT, SIESTA, Electronic band gap.**

I. Introduction

In recent years, II-IV semiconductors in nano-cystalline form have experienced an enormous development owing to their interesting size dependent optical and electrical properties. In particular, nanostructures of CdSe thin films have received more attention due to its fundamental, experimental and applied interests in diverse fields such as electronic industries, solar energy utilization, space science, production of high memory computer elements, various type of sensor and other nano-scale devices.

Both cubic and hexagonal structures of compound CdSe are seen (Fig. 1(a) and (b) correspondingly). We examined the computational results of the structural and electrical properties of the hexagonal CdSe structure in this work, noting significant alterations in this phase. The Atomistic-Tool-Kit (ATK) is used by the SIESTA (Spanish Initiative for Electronic Simulation with Thousands of Atoms) code to examine structural properties utilizing Avogadro, GDIS, and other tools. LDA is used to compute the band gap, while DOS, PDOS, and electronic band structures are utilized to update the electronic characteristics of CdSe. A brief introduction is included, and the results are well-structured.

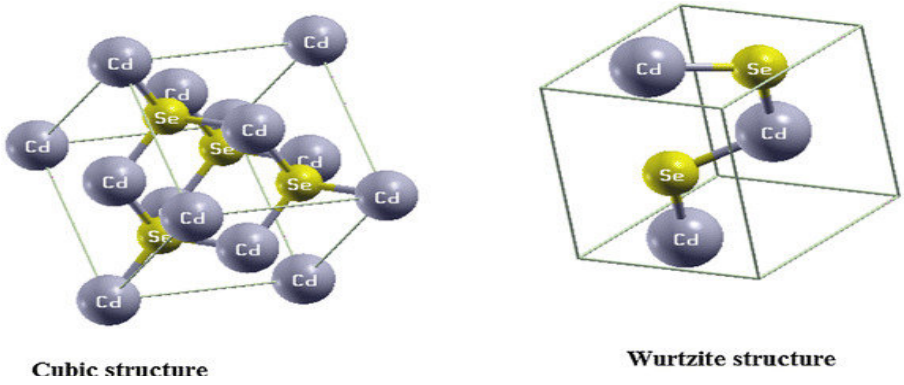


Figure1: (a) Cubic structure of CdSe, (b) Hexagonal structure of CdSe

II. Material and Methods

All calculations and optimizations are handled using the DFT-based SIESTA algorithm. The Atomistic-Tool-Kit (ATK), which includes GDIS, Avogadro, and other tools, is used by the SIESTA code to examine structural properties. LDA is used to compute the band gap, while DOS, PDOS, and electronic band structures are utilized to update the electronic characteristics of CdSe. The complete system was optimized, including all required phases like mesh-cutoff, k-point, lattice-optimization, etc. The pseudo potential technique has been used in this code to solve the Kohn Sham (K-S) equations, and the exchange and correlation energies are handled within the GGA in accordance with the PBE parameterization. The complete system was optimized after completing all required steps, including mesh-cutoff, k-point, lattice-optimization, etc. For accurate results, it is essential that every atom stay entirely calm during the optimization process.

III. Result and Discussion

1. Structural property-

Here, we discovered CdSe's Hexagonal symmetric structure. The Cd1-Se2 atoms are bound together by a 2.69Å bond length with 180˚ bond angle. The unit cell and CdSe crystal structure are shown in Fig:2(a) and (b). The pink and blue balls in the picture represent selenide and cadmium atoms, respectively.

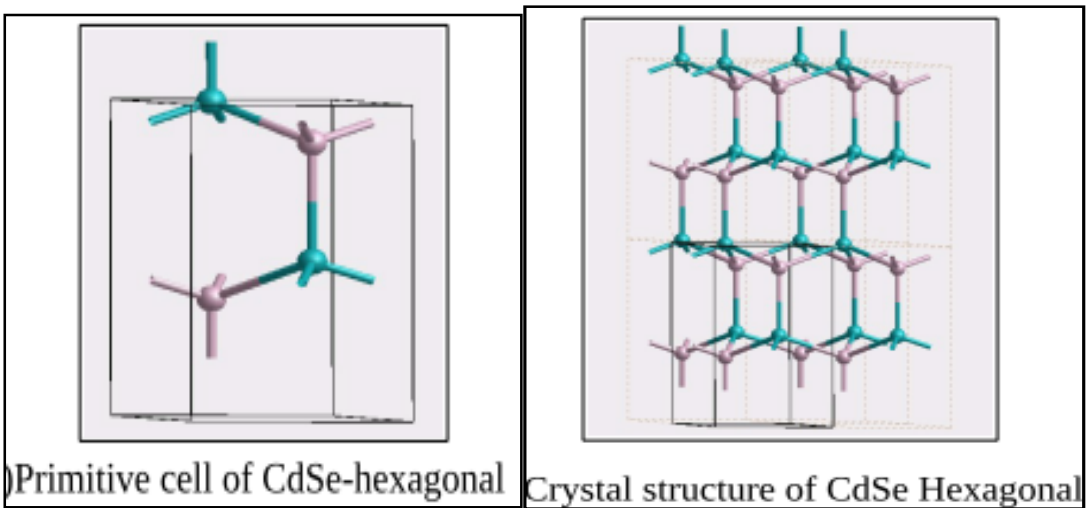


Figure: 2(a) Primitive cell of CdSe-hexagonal (b) Crystal structure of CdSe-Hexagonal

2. Electronic property-

This investigation was carried out using various GGA and LDA approximations, and it has been demonstrated that the band gap for the hexagonal structure of CdSe is direct in Γ point. Here Fig: 3 shows the CdSe Hexagonal K-Point Cutoff value.

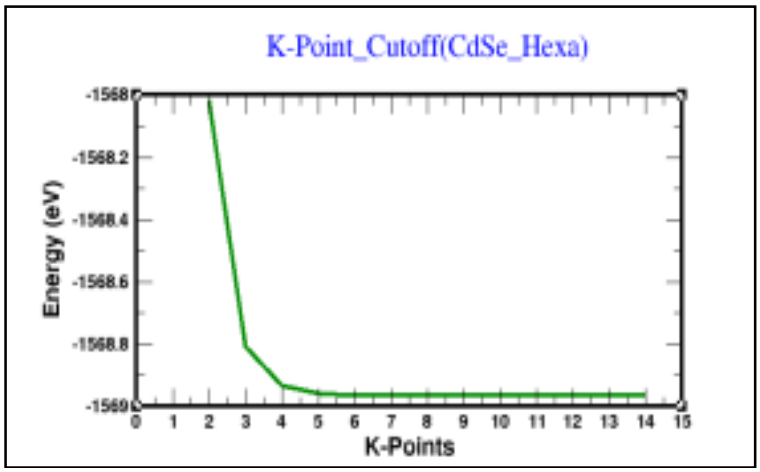


Figure: 3 K-Point_Cutoff (CdSe_Hexagonal)

Figure 4 depicts the CdSe band structure in Hexagonal complexes. Several GGA and LDA approximations were used in this inquiry, and it was shown that the gap for the ZB structure is direct in Γ point. The potential of semi-local exchange, which returns the GGA and local density approximation (LDA) to a constant electron density, is the primary reason why calculations are more accurate.

The density of state in hexagonal CdSe is depicted in Figure 5(a). We have found that the CdSe structure displays DOS with several band regions and energy levels. It is found that GGA reduces the 1.29 eV energy gap generated from the valance band and conduction band. A thorough calculation of the predicted density of states will be carried out in order to completely understand this electrical structure. The predicted density of state for CdSe is displayed in figure 5(b). There are different areas of the hexagonal structure where different energy levels are seen. The energy gap between the valance and conduction bands was found to be 1.29 eV based on PDOS calculations, which is identical to the DOS estimate.

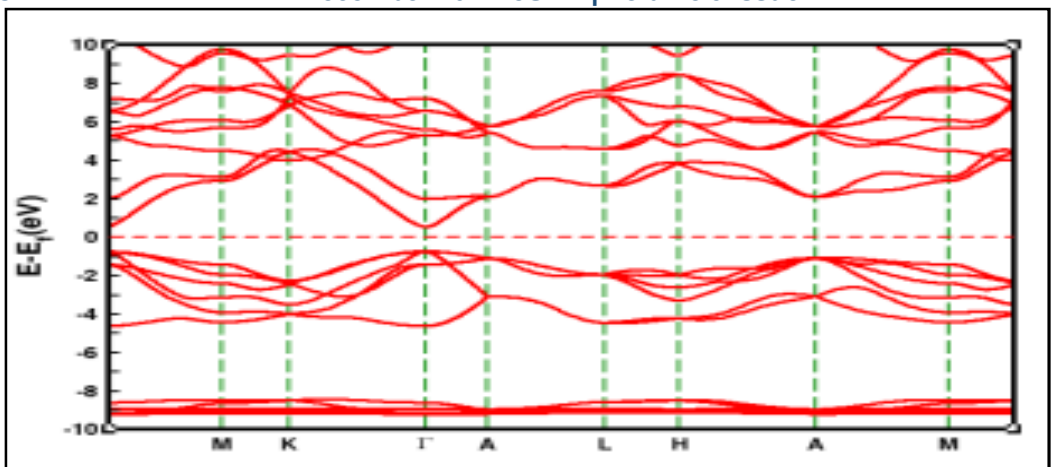


Fig: 4 Electronic Band structure of CdSe Hexagonal

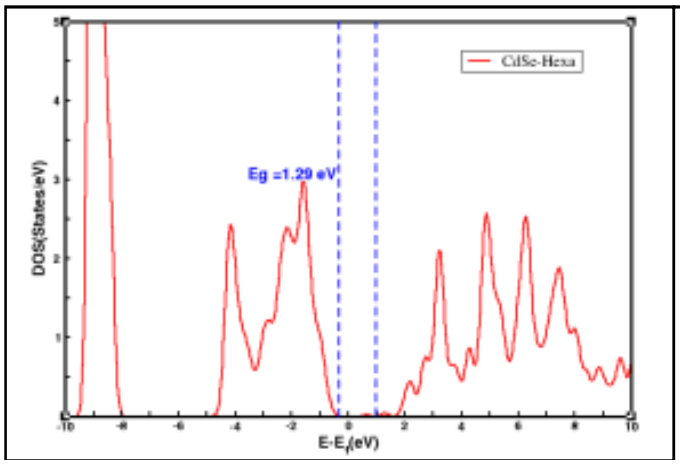
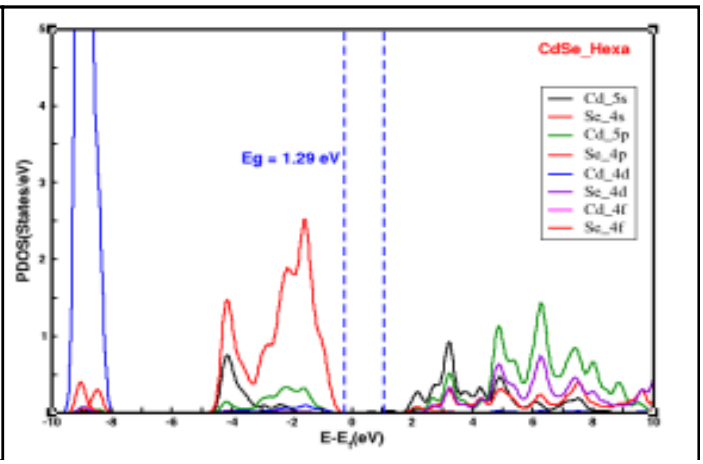


Figure:5 (a) DOS of CdSe Hexagonal



(b) PDOS of CdSe Hexagonal

IV. Conclusion

The current discoveries have been reflected in CdSe, and the LDA technique has improved the underestimation of the electrical band gaps of semiconductors based on CdSe. The electrical band structure shows that there is a 1.29 eV band gap at the Γ point. The semiconductor energy gap was calculated using the GW technique since standard DFT understates it. The atomic structure of these materials may be discovered by examining their electronic characteristics, which is crucial for creating new technological uses. CdSe is sometimes used to create photo resistors and thin layers for infrared lighting devices since it is transparent to infrared light.

Because of its high absorption coefficient, high photosensitivity, and technical applications such as gamma-ray detectors, infrared windows for solar cells, LEDs, and sensors, it is considered a promising material that has been extensively studied over the past few decades.

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