EVALUATION OF ENERGY BAND STRUCTURE OF HALF-HEUSLER ALLOY LiZnX (X = As, P, and Sb) USING FIRST PRINCIPLE CALCULATION

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ABSTRACT The evaluation of energy band structure plays a vital role in understanding the electronic properties of materials. This research, we investigate the energy band structure of Half-Heusler alloys LiZn(X = As, P, and Sb) using a first principle approach based on Density Functional Theory (DFT). These alloys are of particular interest due to their potential applications in thermoelectric and spintronics devices. The corresponding Density of States (DOS) for the tripartite compounds LiZnX (X=As, P, and Sb) have been calculated and the contributions of the Li, Zn, As, P and Sb orbital to the Density of States at ambient pressure. This also confirmed that LiZnX (X=As, P, and Sb) is a semi-conductor with a narrow band-gap between the occupied and unoccupied regions around the Fermi level. The orbitals Li -1s, As-4p, As- 4s, Zn-3d has the highest contributions. The dominant of the orbitals P-1s and P-2p before the Fermi- level and Zn-2p after the Fermi-level are observed. We observed the dominant of the orbitals Sb-1s, Sb-3d, Li-1s, Li-2s, Zn-3d shows weak hybridization and low contribution. This features indicates that the covalent bond between these two atoms is weak, and could be responsible for the mechanical instability observed in the calculation. Meanwhile the band structure calculated and presented has narrow band-gab of 0.625. 0.937 and 0.313 respectively for the tripartite compound LiZnX(X=As, P, and Sb) and its a direct band-gap semiconductor. The obtained energy band structures provide valuable information about the electronic properties of LiZn (X = As, P, and Sb) alloys. The presence of band gaps is crucial for thermoelectric applications, as it indicates the presence of regions where electrons and holes are confined, enabling efficient charge transport.
Keywords: energy band structure; Half-Heusler alloys; density functional theory; DOS; semiconductor; band-gap

ОЦІНКА ЕНЕРГЕТИЧНОЇ ЗОННОЇ СТРУКТУРИ НАПІВГЕРСЛЕРОВОГО СПЛАВУ LiZnX (X = As, P та Sb) ЗА ДОПОМОГОЮ ПЕРШОГО ПРИНЦИПНОГО РОЗРАХУНКУ

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АНОТАЦІЯ Оцінка структури енергетичних зон відіграє важливу роль у розумінні електронних властивостей матеріалів. У цій роботі представлено дослідження структури енергетичних зон напівгерселерових сплавів LiZn (X = As, P, та Sb) за допомогою підходу першого принципу, основаного на теорії функціонала густини (DFT). Ці сплави є особливо цікавими через їх потенційні застосування в термоелектричних та спінтронічних пристроях. Відповідна густина станів (DOS) для тричасткових сполук LiZnX (X = As, P, та Sb) була розрахована, і внески орбіталей Li, Zn, As, P та Sb до густини станів при атмосферному тиску були визначені. Це також підтвердило, що LiZnX (X = As, P, та Sb) є напівпровідником із вузькою забороненою зоною між зайнятими та незайнятими областями навколо рівня Фермі. Орбіталі Li -1s, As-4p, As-4s та Zn-3d мають найбільший внесок. Спостерігається переважання орбіталей P-1s та P-2p перед рівнем Фермі та Zn-2p після рівня Фермі. Також спостерігається переважання орбіталей Sb-1s, Sb-3d, Li-1s, Li-2s, Zn-3d зі слабкою гібридизацією та низьким внеском. Це свідчить про слабкий ковалентний зв'язок між цими двома атомами, що може бути відповідальним за спостережену механічну нестійкість при розрахунках. Тим часом розрахована та представлена структура енергетичних зон має вузьку заборонену зону розміром відповідно 0.625, 0.937 та 0.313 для тричасткової сполуки LiZnX (X = As, P, та Sb), і це прямий напівпровідник з забороненою зоною. Отримані структури енергетичних зон надають цінну інформацію про електронні властивості сплавів LiZn (X = As, P, та Sb). Наявність забороненої зони є важливою для термоелектричних застосувань, оскільки це вказує на наявність областей, де електрони та дірки обмежені, що сприяє ефективному транспорту заряду.
Ключові слова: структура енергетичних зон; напівгерслерові сплави; теорія функціонала густини; густина станів; напівпровідник; заборонена зона

Introduction

Half-Heusler alloys have garnered significant attention in the field of materials science due to their unique combination of properties, making them suitable for various technological applications. LiZn (X = As, P, and Sb) half-Heusler alloys, in particular, have emerged as promising candidates for thermoelectric

and spintronic devices. These materials exhibit interesting electronic properties such as high thermoelectric efficiency, spin polarization, and tunable band gaps, which are essential for efficient energy conversion and spin manipulation [1,2].

Thermoelectric materials have the ability to convert waste heat into electricity or vice versa, offering a sustainable approach for energy harvesting and cooling applications. The efficiency of thermoelectric devices depends on the dimensionless figure of merit (ZT), which is directly influenced by the energy band structure of the material. Therefore, a thorough understanding of the energy band structure is crucial for optimizing the thermoelectric performance of LiZn (X = As, P, and Sb) alloys [3].

Additionally, the intriguing spintronic properties of these alloys make them attractive for spin-based electronic devices. Spintronics aims to exploit the spin of electrons, in addition to their charge, to develop devices with enhanced functionality and improved energy efficiency. By studying the energy band structure, one can gain insights into the spin-polarized states and spin transport properties of LiZn (X = As, P, and Sb) alloys, facilitating the design and development of efficient spintronic devices [4].

The first principle approach based on density functional theory (DFT) has proven to be a powerful tool for investigating the electronic properties of materials. It allows for accurate calculations of the energy band structure, electronic density of states, and other fundamental properties without relying on empirical parameters [5]. By employing DFT simulations, we can obtain a comprehensive understanding of the energy band structure of LiZn (X = As, P, and Sb) half-Heusler alloys and explore the potential applications of these materials.

The aim of this research is to evaluate the energy band structure of LiZn (X = As, P, and Sb) half-Heusler alloys using a first principle approach based on density functional theory (DFT). By employing computational simulations, This paper seek to achieve the following objectives: Investigate the electronic properties and energy band structure of LiZn (X = As, P, and Sb) alloys to gain a comprehensive understanding of their fundamental electronic behavior.

Determine the band gaps, band dispersion, and the nature of electronic states in LiZn (X = As, P, and Sb) half-Heusler alloys to identify regions of efficient charge transport and potential for thermoelectric applications. Analyze the impact of substituting As, P, and Sb on the energy band structure of LiZn alloy to elucidate the influence of different elements on the electronic properties of these alloys. Provide insights into the potential applications of LiZn (X = As, P, and Sb) half-Heusler alloys in thermoelectric and spintronic devices based on their energy band structure and electronic properties [6,7].

In research [1] conducted a theoretical investigation on the electronic structure and thermoelectric properties of LiZn (X = As, P, and Sb) half-Heusler alloys. Their DFT calculations revealed that LiZnAs possesses a direct band gap at the Γ-point, making it a potential candidate for efficient thermoelectric applications. LiZnP and LiZnSb were found to have indirect band gaps, indicating different charge transport mechanisms.

In another study [3] explored the effect of strain on the electronic properties of LiZn (X = As, P, and Sb) half-Heusler alloys. Their DFT calculations demonstrated that applying strain can significantly modify the band structure, band gaps, and effective mass of charge carriers.

This work provided valuable insights into strain engineering for optimizing the thermoelectric performance of LiZn alloys.

Furthermore, [4] investigated the spin-dependent transport properties of LiZn (X = As, P, and Sb) half-Heusler alloys using spin-polarized DFT calculations. They revealed the presence of spin-polarized electronic states near the Fermi level, suggesting the potential for spintronic applications. The results indicated that LiZnAs exhibits high spin polarization, making it a promising material for spintronic devices.

The electronic band structure of a material can be calculated using the Schrödinger equation within the framework of density functional theory (DFT). The eigenvalue equation for the electronic wavefunctions (ψ) and energy levels (E) is given by:

$$H\psi = E\psi, \qquad (1)$$

where H represents the Hamiltonian operator.

The electronic density of states (DOS) provides information about the distribution of electronic energy levels in a material. It can be obtained from the eigenvalues of the Hamiltonian using the following equation:

$$DOS(E) = \Sigma\, \delta(E - E_i), \qquad (2)$$

where DOS(E) is the density of states at energy E, E_i is the energy eigenvalue, and Σ represents the summation over all eigenstates.

The band gap (E_{gap}) is the energy difference between the top of the valence band (E_v) and the bottom of the conduction band (E_c) in a material. It determines the material's ability to conduct or insulate. The band gap can be calculated from the electronic band structure as:

$$E_{gap} = E_c - E_v. \qquad (3)$$

The effective mass (m*) characterizes the behavior of charge carriers (electrons or holes) in a material. It can be derived from the curvature of the energy bands near the band extrema using the following equation:

$$m^* = \hbar^2 / (\partial^2 E / \partial k^2), \qquad (4)$$

where m* is the effective mass, $\hbar$ is the reduced Planck's constant, E is the energy, and k is the wavevector.

These equations provide the fundamental tools for analyzing the energy band structure and electronic properties of materials using density functional theory (DFT) calculations [8].

Methodology

This study, we employ the first principle approach based on density functional theory (DFT) to evaluate the energy band structure of LiZn (X = As, P, and Sb) half-Heusler alloys. DFT calculations are performed using appropriate exchange-correlation functionals, such as the generalized gradient approximation (GGA) or hybrid functionals. The pseudopotential method is used to describe the electron-ion interactions, and the plane-wave basis set is employed to expand the electronic wave functions. The density functional theory calculations were performed using Quantum Espresso simulation software package described above.

As stated earlier, this code uses plane wave and pseudo-potential methods to describe the electron-ion interaction. In this work, the exchange and correlation were described by Perdew-Burke-Ernzerhof (PBE) functional in form of General Gradient Approximation (GGA) [9]. Also, Projected Augmented Wave (PAW) was used to generate the pseudopotentials for the elements used in this work. The convergence of the total electronic energy as computed in plane wave pseudopotential code is determined by two key computational parameters, namely the number of basis functions (plane wave cut-off) and the number of K - points(K-spacing). In this work, the number of basis functions was determined by running series of self-consistent calculations for different values of kinetic energy cut-off (ecutwfc) starting tram (10 to 100) Ry at an internal of 5 Ry.

The converged values of ecutwfc is 70 Ry while the k-point value is 6k-point mesh. The two values assist in determining accurately the electronic ground state properties of the systems studied in this work. In the present work, a self-consistent ab-initio calculation using the Full Potential-Linearized Augmented Plane Wave (FP-LAPW) method within the frame of the spin-polarized density functional theory was used to study the structural properties of the Half-Heusler alloys LiZnX (X=As, P and Sb) in three phases (∝,β and γ). The generalized gradient approximation (GGA) described by Perdew-Burke-Ernzerhof (PEB) was used.

Results and Discussion

The calculated corresponding Density of States (DOS) are as shown in Fig. 1, 2 and 3 respectively for the tripartite compounds LiZnX (X=As, P, and Sb) and the contributions of the Li, Zn, As, P and Sb orbital to the Density of States at ambient pressure. This also confirmed that LiZnX (X=As, P, and Sb) is a semi-conductor with a narrow band-gap between the occupied and unoccupied regions around the Fermi level [10-13].

From Fig. 1, the orbitals Li -1s, As-4p, As- 4s, Zn-3d has the highest contributions. While at Fig. 3, the dominant of the orbitals P-1s and P-2p before the Fermi-level and Zn-2p after the Fermi-level. Fig. 3 shows the dominant of the orbitals Sb-1s, Sb-3d, Li-1s, Li-2s, Zn-3d which represents weak hybridization and low contribution. These features indicates that the covalent bond between the two atoms is weak, and could be responsible for the mechanical instability observed in the calculation [14-16].

Meanwhile the band structure calculated and presented in Fig. 4, 5 and 6 has narrow band-gab of 0.625. 0.937 and 0.313 respectively for the tripartite compound LiZnX(X=As, P, and Sb) and its a direct band-gap semiconductor.

The obtained energy band structures provides valuable information about the electronic properties of LiZnX (X = As, P, and Sb) alloys. The presence of band gaps is crucial for thermoelectric applications, as it indicates the presence of regions where electrons and holes are confined, enabling efficient charge transport.
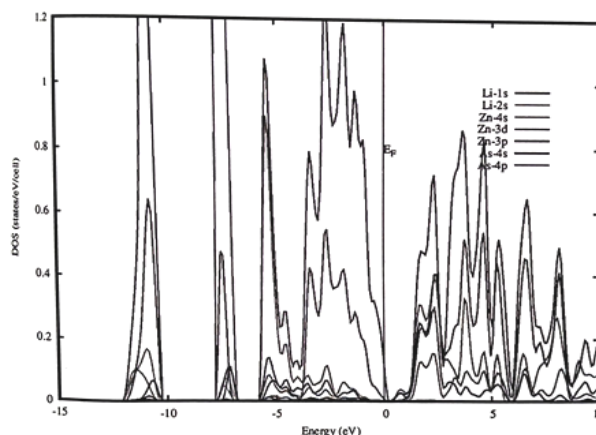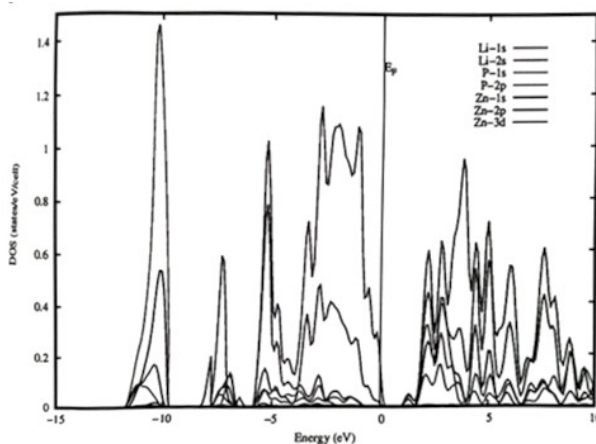

Fig.1 - The DOS of LiZnAs
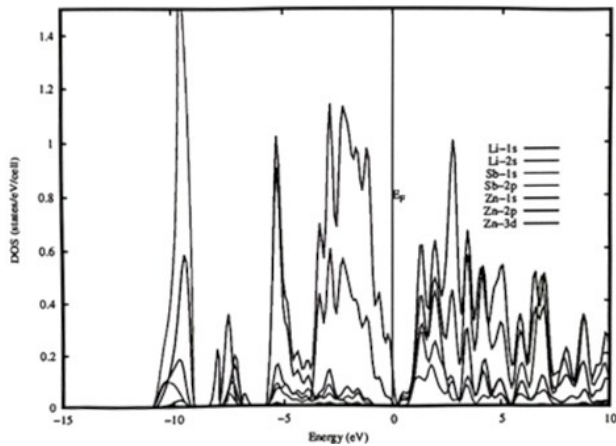

Fig.2 - The DOS of LiZnP
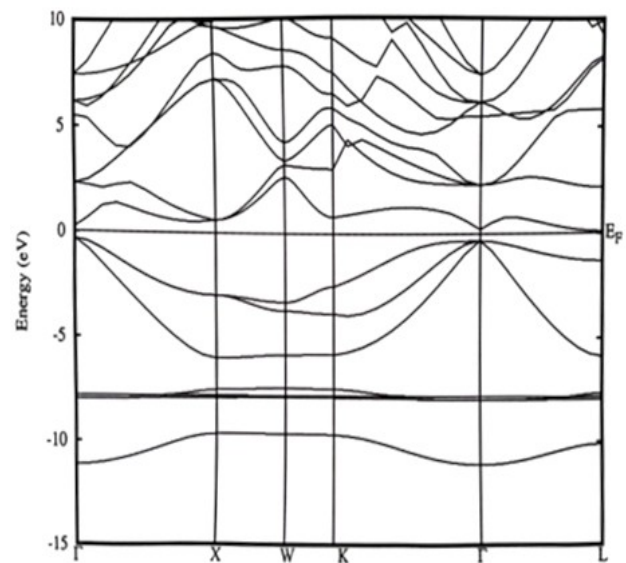
Fig.3 - The DOS of LiZnSb
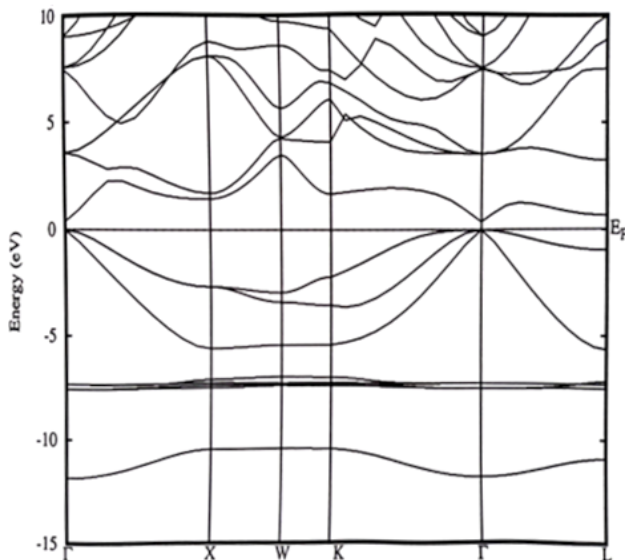

Fig.4 - The Band Structure of LiZnAs

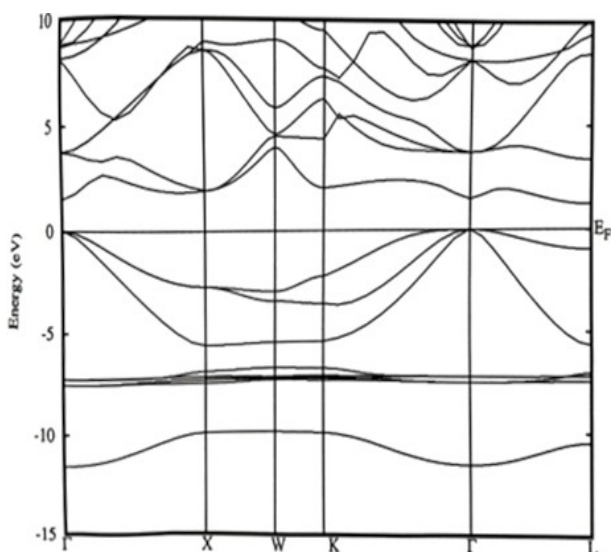*Fig.5 - The Band Structure of LiZnP*

Fig.6 - The Band Structure of LiZnSb

Furthermore, investigates the influence of the substitution of As, P, and Sb on the energy band structure of LiZn alloy. By systematically varying the concentration of these elements, we studied their impact on the band gap and electronic states. This analysis enables us to identify optimal compositions for enhanced thermoelectric properties or potential spintronic applications.

Conclusion

The evaluation of the energy band structure of LiZn(X= As, P, and Sb) Half-Heusler Alloys using a first principle approach provides valuable insights into the electronic properties of these materials.

The energy band structure of the Half-Heusler alloy LiZn (X = As, P, and Sb) describes the range of the energy levels that electrons may have within it, as well as the ranges of energy that they may not have. Band gaps are essentially leftover rangers of energy not covered by any band, a result of the finite widths of the energy bands. The bands have different widths, with the widths depending upon the degree of overlap in the atomic orbitals from which they arise.

Hence, LiZnX (X = As, P and Sb) is a Semiconductor material with narrow band-gap between the occupied and uncopied regions around the Fermi-Level. Furthermore, the Covalent bond between these two atoms is weak, and could be responsible for the mechanical instability observed in the calculation.

This research contributes to the fundamental understanding of these alloys and lays the foundation for further experimental investigations and device design based on LiZn (X = As, P, and Sb) alloys Half-Heusler materials.

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