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Original Article

First Principle Investigation of the Electronic and Optical Properties of TiCoSb: Consequences for the Photovoltaic Applications

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Abstract - *TiCoSb, a half-Heusler semiconductor, has been investigated for its electronic and optical properties using first-principles Density Functional Theory (DFT) implemented on the quantum espresso code. The structure was relaxed until the ground state was obtained. All calculations were carried out using the projector augmented wave method, the Generalized Gradient Approximation of the Perdew Burke Erzheholf (GGA-PBE). The band structure analysis reveals a moderate band gap of 1.08 eV**,** which indicates the material's ability to absorb light at lower energy. The Projected Density of States (PDOS**)** confirms strong hybridization between Ti-3d, Co-3d, and Sb-3p orbitals, influencing electronic transport properties. Optical property investigations show that TiCoSb exhibits high absorption in the visible range (1.5-5 eV**)**, comparable to conventional photovoltaic materials such as Si and GaAs. The real and imaginary dielectric functions indicate strong interband transitions, while the low reflectivity enhances light-absorption potential. The refractive index (2.5-3.5**)** supports efficient light trapping, and the energy loss function suggests moderate carrier transport, suitable for photovoltaic applications. Comparative analysis with well-established photovoltaic materials suggests TiCoSb could be a viable solar absorber since its band gap is direct and optimized for efficient charge carrier extraction.*

Keywords - *TiCoSb, Half-Heusler, First principle DFT, Optical Absorption, Photovoltaics.*

1. Introduction

The increasing demand for renewable energy has surged due to the increasing concerns over fossil fuel depletion, environmental pollution, and climate change [1, 2]. Among various sustainable energy technologies, Photovoltaic (PV) technology is an indispensable solution for clean and efficient energy conversion [3]. PV devices, commonly known as solar cells, harness sunlight and convert it directly into electricity, offering a reliable alternative to conventional energy sources. The continuous advancements in PV research aim to enhance efficiency, reduce costs, and develop materials that outperforming traditional semiconductors such as silicon and gallium arsenide [4]. One of the fundamental challenges in PV technology is the search for new materials with optimal electronic and optical properties to improve energy conversion efficiency [5]. Despite their success, traditional materials often have limitations such as high production costs, scarcity, or non-ideal band gaps [6]. Consequently, exploring novel semiconductors with suitable band gaps, strong optical absorption, and efficient charge transport properties is crucial for next-generation solar cells. Half-Heusler (HH) compounds have been found to fit due to their tunable electronic properties, structural stability, and potential for energy applications. Among these, TiCoSb, a half-Heusler semiconductor, has been envisaged to have characteristics that could make it suitable for photovoltaic applications [7]. There have been several researches on the TiCoSb material to study its electronic structural properties. Xu et al. studied the electronic structural and optical properties of TiCoSb using the first-principles calculation. They reported that the band gaps increase as the pressure increases and that the band gap increase is due to the shifting away of the Valence Band (VB) electrons of Ti 3d and Co 3d from the Fermi level. They further reported that their calculation indicates that TiCoSb has a large density of state near the Fermi level; moreover, the changes in the density of states near the Fermi level are mainly caused by Ti 3d and Co 3d under different pressures [8]. In

another work by Xu et al., they studied the electronic structure and the thermoelectric properties of TiCoSb using the first principal approach and the semi-classical Boltzmann theory. The calculation reported that the material has a large DOS near the fermi level and that the electrical conductivity rapidly increases with increased pressure [9]. In the previous works on TiCoSb, it has not been reported that it is suitable for photovoltaic applications.

Inoder to study the electronic and optical properties of TiCoSb and investigate its potential for photovoltaic applications, we carried out a first-principles calculation within the framework of the Density Functional Theory (DFT). DFT allows for a fundamental understanding of material properties at the atomic level by solving the Schrödinger equation under realistic approximations. Compared to experimental approaches, DFT simulations offer an efficient and cost-effective way to explore electronic and spectroscopic properties at the ground state or 0K [10]. The ability of DFT to model these properties with high accuracy makes it a powerful tool in the search for new and efficient photovoltaic materials. In this study, we employ first-principles DFT calculations to investigate the electronic and optical properties of TiCoSb, focusing on its potential for photovoltaic applications. The band structure, Density of States (DOS), dielectric function, optical absorption, refractive index, extinction coefficient and energy loss function were analyzed to determine its suitability as a solar absorber material. The findings of this study provide insights into the viability of TiCoSb for future PV technologies and suggest possible modifications or enhancements to improve its performance.

2. Computational Details

This article used the density functional theory implemented in the Quantum Espresso code. The Crystallographic Information File (CIF) was obtained from the Materials Project database and converted into a Quantum ESPRESSO (QE) input file using the QE input generator available on the Materials Cloud platform. Structural optimization was performed using the variable-cell relaxation (vc-relax) scheme to determine the ground-state energy and optimized lattice parameters.

The plane-wave cutoff energy was set to 150 Ry for wavefunctions and 600 Ry for the charge density. The Monkhorst-Pack k-point grid of 15×15×15 was used for Brillouin zone sampling to ensure convergence of total energy and electronic structure. The exchange-correlation function was treated within the Generalized Gradient Approximation (GGA) using the Perdew-Burke-Ernzerhof (PBE) parameterization. The Projector Augmented Wave (PAW) method accurately treated core-valence interactions [11]. After structural optimization, Self-Consistent Field (SCF) calculations were performed to obtain the converged charge density, followed by Non-Self-Consistent Field (NSCF) calculations for accurate band structure and Density of States (DOS) analysis. The optical properties, which include the dielectric function, absorption coefficient, reflectivity, refractive index, extinction coefficient and energy-loss function, were computed using the Independent Particle Approximation (IPA) as implemented in Quantum ESPRESSO. The imaginary part of the dielectric function was derived from the momentum matrix elements, while the real part was obtained using the Kramers-Kronig relations.

All calculations were conducted under periodic boundary conditions, ensuring a total energy convergence threshold of 10^{-6} Ry and a force convergence criterion of 10^{-3} Ry/Bohr. The optical spectra were analyzed to understand the material's electronic transitions and light-matter interactions.

3. Materials and Methods

3.1. Crystal Structure

The structure of TiCoSb crystallizes in the simple cubic with a space group identity of F 43 m. The relaxed structure gave rise to a lattice parameter of 5.82 angstroms. Each Co atom is tetrahedral coordinated by four Ti atoms, while four Ti atoms surround each Sb atom. This arrangement is characteristic of semiconducting Half-Heusler alloys.

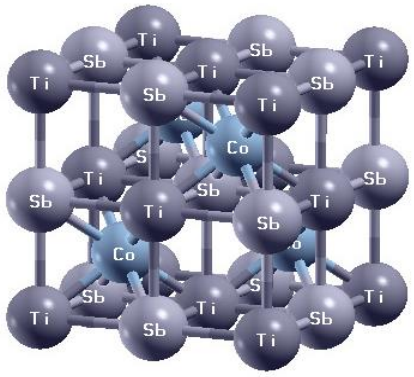

Fig. 1 Crystal structure of TiCoSb

3.2. Method and Theory

The optical properties of the studied material were investigated based on first-principles Density Functional Theory (DFT) calculations. The structural optimization was performed to obtain the equilibrium lattice parameters, which are the foundation for accurate electronic and optical property calculations. The electronic band structure and Density of States (DOS) were analyzed to determine the nature of electronic transitions contributing to the optical response.

The complex dielectric function was computed to explore the interaction of the material with incident photons according to (1) [12].

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) \quad (1)$$

The imaginary part $\varepsilon_2(\omega)$ was obtained directly from electronic transitions using Fermi's Golden Rule and the momentum matrix elements. The fundamental part, $\varepsilon_1(\omega)$, was derived from $\varepsilon_2(\omega)$ using the Kramers-Kronig relation, expressed as [12]:

$$\varepsilon_1(\omega) = 1 + \frac{2}{\pi} P \int_0^{\infty} \frac{\omega' \varepsilon_2(\omega')}{\omega'^2 - \omega^2} d\omega' \quad (2)$$

Where, P is the Cauchy principal value of the integral.This ensures that the dielectric function satisfies causality and provides insights into the material's refractive properties. The computed optical spectra, including the absorption coefficient, refractive index, reflectivity, and energy-loss function, were analyzed to understand the material's potential applications in optoelectronic and photovoltaic devices.

4. Results and Discussion

4.1. Band Structure

Band structure is a deterministic parameter in the electronic properties of solids in material science, it is a representation of the allowed energy levels (bands) of electrons in a solid material as a function of their momentum (wave vector, k). It describes how electrons can move within the material. Materials with a band gap above 3eV are considered insulators, those with a band gap less than 3eV are semiconductors and materials whose bands from the conduction band cross the valence band or vice versa and exhibit metallic properties in both cases. In this case, the bands cross the Fermi level. In Figure 1, the material has a band gap of 1.08 eV, and the band's nature is direct. This means that the material can efficiently absorb light of energy greater than its band gap. The electronic band structure of TiCoSb is an indication of the material's potential in optoelectronics applications, it also means the material can perform in energy-related applications, including photovoltaics.

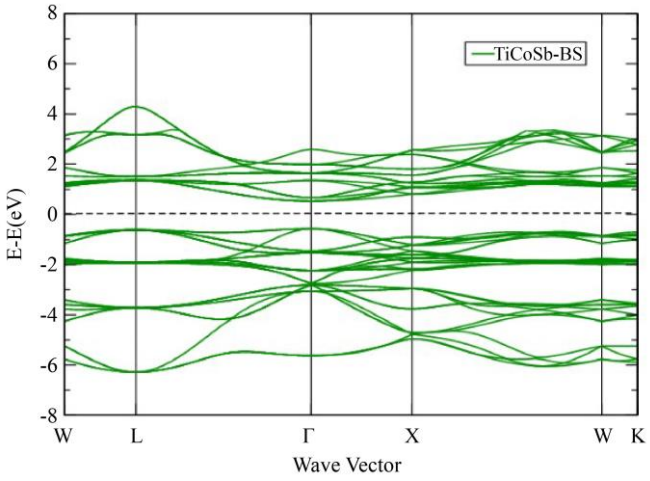

Fig. 2 Band structure

4.2. Density of State

In DFT, the Density of States (DOS) describes the number of available electronic states per unit of energy at each energy level in a material. It provides insights into how electrons are distributed across energy levels, and it also helps to determine whether a material is a metallic, insulator or a semiconductor by showing the energy separation between the Valence Band Maximum (VBM) and Conduction Band Minimum (CBM). Here, we must check the contributions of the various orbitals to the total DOS, the interest is to check those orbitals that enhance electronic transport properties around the Fermi level. In Figure 3, the high peaks observed in Ti-3d in CBM and Co-3d in the VBM indicate and enhance charge transport in the material, it is also observed that there is no peak at the Fermi level, confirming the semiconducting properties. The consequence of these enhanced electronic transport properties is that they promote photo absorption, thereby making the material fit for photovoltaic applications.

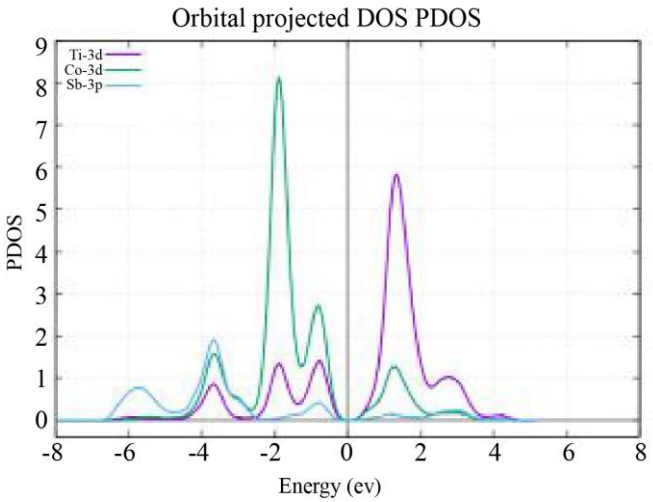

Fig. 3 Projected density of state

4.3. Dielectric Properties

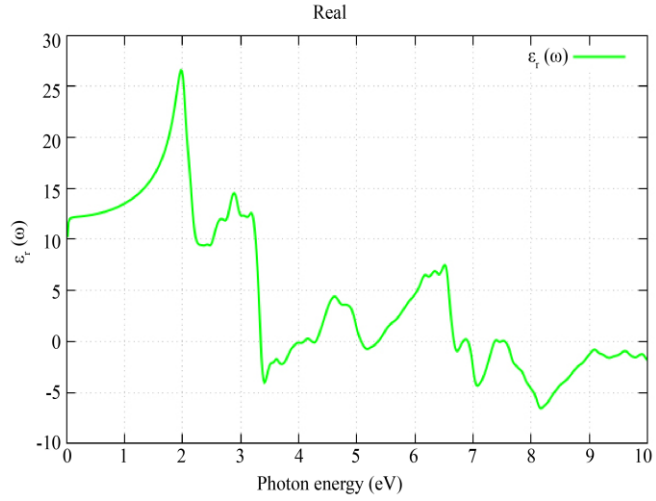

Fig. 4 Real dielectric function

Dielectric is a complex function comprising the real and imaginary parts. Generally, dielectric is the ability of a material to polarize in response to an electromagnetic field, the fundamental part of the dielectric describes how a material can store energy from an electric field, while the imaginary part describes the absorption of the energy from an electric field.

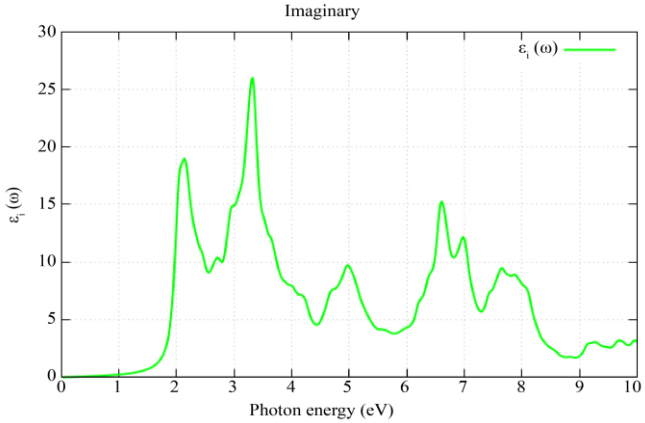

Fig. 5 Imaginary dielectric function

Studies reported by [15] show that an ideal photovoltaic material has a dielectric with a sharp peak between the ranges of 1.5 eV to 3.5 eV, corresponding to the visible range. In the case of TiCoSb in this present study, it is obvious from Figures 4 and 5 that there are sharp peaks between 2 and 3.5 eV, making the material suitable for energy conversion.

4.4. Absorption Coefficient

The absorption coefficient primarily deals with light absorption into the material again, this also ensures a depth of penetration of this light before its being absorbed by the material; this property has an inverse relationship with the wavelength of the material, which means that light of lower wavelength gives a high absorption, the point of interest here is a high absorption at the visible spectrum of at least 10^5. In Figure 6, a sharp peak of 1.3 x10^6 was observed. This result is consistent with the general consideration for solar applications.

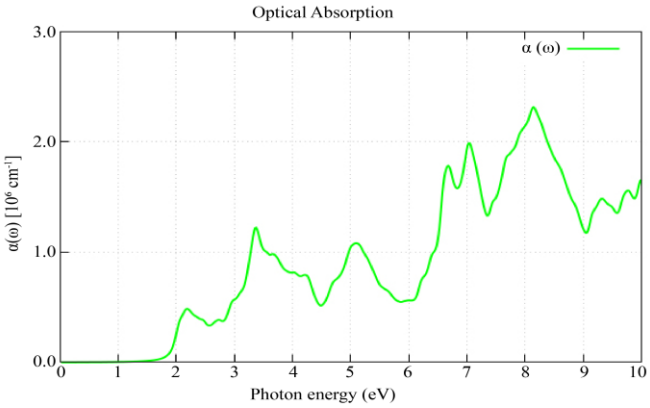

Fig. 6 Absorption coefficient

The material starts to absorb significantly above 1.08 eV, which aligns with the bandgap. Beyond 2 eV, the absorption coefficient rises sharply, indicating that TiCoSb effectively absorbs light in the visible and near-UV regions.

4.5. Refractive Index

The refractive index of a material is a quantity that measures how deep a light penetrates a material compared to its speed in a vacuum. Light travels faster in a vacuum than any other media, meaning the level of light penetration will depend on the type of material. For instance, the work reported by [14, 15] shows that a refractive index within the range of 2 to 4 is crucial for energy applications, the value may also depend on the materials.

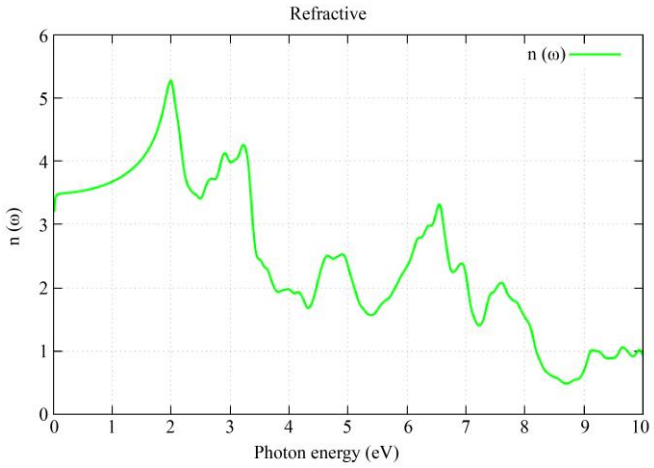

Fig. 7 Refractive index

The studies reported by [16] opined that titanium oxide has a tunable refractive index, hence its versatility. Half-Heusler semiconductors possess high refractive indices in the near-infrared region, which is why they are suitable for light control [17]. In Figure 7, it is observed that the refractive is above 3.5 within the visible spectrum, which is consistent with the result reported [18]. This article has validated the performance of TiCoSb half-Heusler semiconductor for photovoltaic applications through its refractive index since this result is consistent with other literatures.

4.6. Reflectivity

This is the ability of a material to reflect light or electromagnetic radiation incident on it. It is the ratio of the intensity of the reflected light to that of the incident light, this is related to the extinction coefficient and refractive index of a material [19]. High values of reflectivity reported in this work, around 0.3 to 0.4 at near-infrared in Figure 8, suggested that the absorbable incident light is more than the reflected, this is good in this case because if a greater percentage of the light is reflected away, the performance of the material for PV will be compromised which is bad. This result agrees with a study by Das et al. [20] on the reflectivity of HH materials.

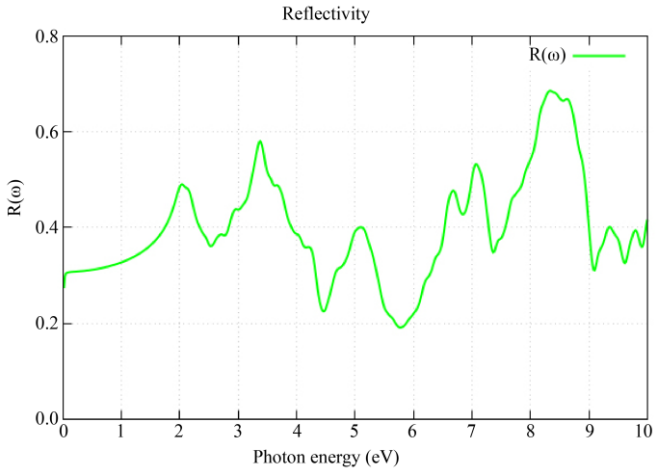

Fig. 8 Reflectivity

4.7. Extinction Coefficient

The extinction coefficient tells us how much light a material absorbs at various photon energies. From Figure. 9, we can see that K(*w*) starts low at very low photon energies but then rises sharply, showing peaks around 2-3 eV, 5 eV, and 7-8 eV. The 2-3 eV peak indicates strong absorption in the visible spectrum, which is excellent for Photovoltaic (PV) applications since most solar energy falls between 1.5-3 eV. The higher energy peaks (around 5-8 eV) relate to interband transitions, suggesting absorption in the Ultraviolet (UV) range. The implication is that absorption happens in the visible range (1.5-3 eV), making TiCoSb effectively capture sunlight. The extinction coefficient describes how light is absorbed when it travels through a material. It is directly related to the absorption coefficient. A high extinction coefficient indicates a strong absorption; a weak value indicates poor absorption; a zero value indicates that the material is dielectric; consequently, it is transparent.

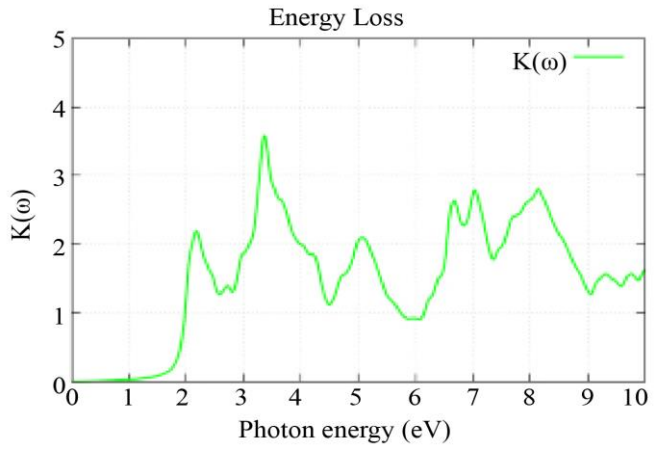

Fig. 9 Extinction coefficient

For the HH materials, it was reported that a band gap value in the range of 0.94 - 2.04 eV Das et al. [20] is suitable for PV applications, which is consistent with this result.

4.8. Energy Loss

The energy loss function shows the energy lost due to the interaction of photons with the material, particularly through plasmons (collective electron oscillations). The peaks in L(w), especially around 8-9 eV, indicate plasmon resonance energy, meaning TiCoSb experiences significant electron excitation at these levels. A low loss function in the visible range suggests minimal energy dissipation, a plus for PV applications since less energy is wasted on electronic scattering.

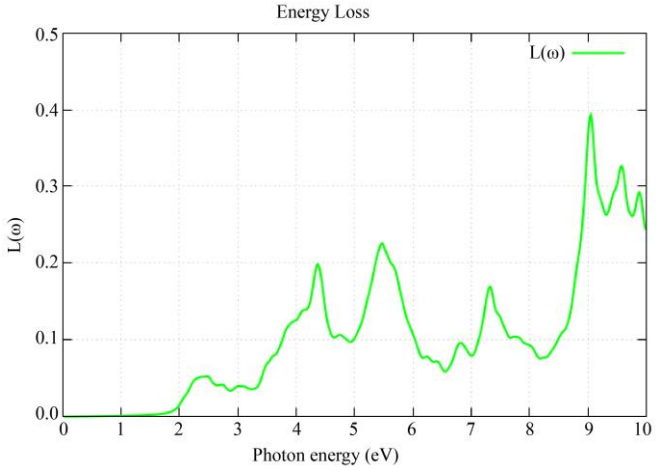

Fig. 10 Energy loss function

A material with a high energy loss function in the visible range is not ideal for PV because it indicates energy loss rather than efficient conversion into electricity. Since Figure 10 shows relatively low energy loss below about 5 eV, TiCoSb could be quite effective at utilizing visible light with minimal losses.

5. Conclusion

The band structure analysis suggests TiCoSb is a semiconductor with an estimated band gap of 1.08 eV. This range is within the optimal window for Photovoltaic (PV) applications, allowing for efficient solar absorption. Furthermore, the nature of the band gap is direct, which is good for effective light absorption. Direct band gap materials typically exhibit higher radiative recombination efficiency, making them preferable for PV applications. If a material has an indirect band gap, further optimization, such as doping or alloying, may be required to enhance its photovoltaic efficiency. The contributions of Co-3d, Ti-3d, and Sb-3p orbitals, as seen in the partial DOS in the conduction and valence bands around the Fermi level, indicate the potential for good charge transport properties, which are critical for efficient solar energy conversion. TiCoSb exhibits strong optical absorption, low reflectivity, and a suitable band gap of 1.08 eV, making it a good material for photovoltaic applications. The optical properties revealed that this material is a potential photovoltaic material. Further studies on carrier lifetimes, defect tolerance, the effect of strain on the electron and hole effective masses, and stability may be necessary to confirm its viability for real-world solar cell applications.

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