JOURNAL OF NANOSCOPE
ISSN(P): 2707-711X | ISSN(O): 2788-7456
Volume 6, Issue 1, June 2025, pp 67-85
Email: jn@wum.edu.pk | **Journal Homepage:** https://jn.wum.edu.pk

Article Title: A Theoretical Study to Investigate the physical Properties of novel Ternary Co2CuAl full Heusler Alloy

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Received: 17 December 2024 **Published:** 30 May 2025

Abstract:
The structural, thermodynamic, thermoelectric, and dielectric properties of the full Heusler alloy Co2CuAl are presented in current research work. Density functional theory (DFT) as implemented in the Wien2k simulation package, is used to perform theoretical calculations of these properties. Full Heusler alloy Co2CuAl has a cubic crystal structure and belongs to the space group $Fm\bar{3}m$ (No. 225). Co2CuAl Heusler alloy exhibits spin polarization. Calculations have been performed for thermodynamic properties at various temperatures (0–1600K) and pressures (0–100GPa). BoltzTrap2 code calculates thermoelectric properties such as thermal conductivity, electrical conductivity, seebeck coefficient, power factor, and figure of merit of Co2CuAl full Heusler alloy. The examined optical properties (i.e. the reflectivity, energy loss, absorption coefficient, optical conductivity, and dielectric constant) of Co2CuAl show isotropic characteristics throughout the investigated energy range (0–12 eV). Full Heusler alloy Co2CuAl shows excellent results in reflection. Dielectric function calculations are performed to characterize the response of these full Heusler alloys to electromagnetic radiation. The existence of a negative $\varepsilon 1(\hbar\omega)$ value supports the alloy's metallic properties. The compound exhibits its highest absorption peaks in the ultraviolet region of the electromagnetic spectrum.

Keywords: Full Heusler alloy; Spin polarization; Thermodynamic properties; Thermoelectric properties; Optical properties.

DOI Number: https://10.52700/jn.v6i1.116

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1. Introduction

Technological development is linked to the wide adoption of advanced electronics, which is significant in the rising energy demand that available resources cannot satisfy [1, 2]. A popular area of research in science and technology is the development of new, highly efficient,

environmentally friendly energy sources and the improvement of existing ones. To achieve this, we must improve the ability of the devices to convert power so that the output is as high as possible [3, 4]. This can be accomplished by creating new technologies with highly effective and reasonable materials. Additionally, by fusing theoretical and experimental research, scientists are attempting to predict new materials for novel technological uses and explore a variety of material classes to adjust the transport properties of currently available materials[5]. Numerous new material types, such as Heusler alloys (HAs)[6], double perovskites, and perovskites[5], have been produced using this method. Heusler alloys are a brand-new class of substances that satisfy every important need that applies to the circumstances in the present situation[7].

The field of computational materials science is expanding quickly and promises to find new materials with potential applications[8]. In 1903, Dr. Friedrich Heusler first time introduced Heusler alloys. Due to their remarkable application, many researchers have taken an interest in this field of solid-state physics. Generally, ternary Heusler alloy is classified into two types (i) half-Heusler alloy stoichiometric presented by XYZ, where X is a transition element and Y, Z belong to p-block element in the periodic table, and (ii) full Heusler alloy presented by X_2YZ where X, Y (for example Co, Mn, Ti, Y, Fe) transition element and Z (for example Al, Mg, Ga, In) in period table [9].

Additionally, only one research group has attempted to investigate the electronic, magnetic, and structural properties of Co_2CuAl alloy through DFT and experimental methods[10]. According to the researchers, these characteristics have promising uses in the magnetocaloric and optical domains. Over the coming century, further full Heusler alloys were found. Co-based HAs are widely synthesized experimentally and are also a focus of theoretical investigation. Cobalt-based Full Heusler alloys (Co_2YZ), Co_2MnX (X = Si, Ge, Al, Ga), Co_2YAl (Y = Cr, Mn), Co_2CrAl, Co_2NbAl and Co_2ZrAl, Co_2ZrZ (Z = Pb, Bi, As), Co_2TiSi are among them [11-17]. The literature reports on the crystallography, elemental stoichiometry, and atomic positions of Heusler alloys with an $L2_1$ structure[18]. Heusler alloy (HA), is interesting for its high Curie temperature, shape memory effect, optoelectronic, and thermoelectric properties [19-21]. Numerous intermetallic classes, including thermoelectric and thermodynamic devices, have found interesting uses for X_2YZ-type full-Heusler forms [22]. Full-Heusler compound Co_2CuAl, belonging to the second class of ternary HAs, solidifies in the cubic $L2_1$ structure with space group $Fm\bar{3}m$ (No. 225). The Wyckoff positions for the atoms

"Co_2" and "Al" are 4b (1/4, 1/4, 1/4) and 4a (0, 0, 0) respectively, whereas the atom "Cu" occupies the 4a (1/2, 1/2, 1/2).

The authors are motivated to conduct theoretical investigations because of the lack of experimental and theoretical efforts to examine the properties of Co_2CuAl full-Heusler alloy. As far as the author knows, no report has been published that examines the thermodynamic, thermoelectric, and optical properties of the full-Heusler compound Co_2CuAl. This study aims to present the findings from density functional theory (DFT) calculations examining thermodynamic, thermoelectric, and optical properties of the full-Heusler compound Co_2CuAl. Here, calculated theoretical results for Co_2CuAl alloy are presented based on First-principles calculations.

Here is an outline of the paper's structure: Section 2 describes the computational techniques used in this work, Section 3 presents the results of the structural optical, thermoelectric, and thermodynamic properties of the newly investigated material, and Section 4 gives concluding remarks [23].

2. Methodology

2.1. Computational detail

The primary computation of this manuscript involves investigating structural properties using self-consistent Density Functional Theory (DFT) and the full potential linearized augmented plane wave (FP-LAPW) method, both integrated and implemented within Wien2k[24]. First-principles calculations are helpful to obtain exact results about the correct exchange (XC) correlation terms used in the current calculations. It is essential to remember that Wien2k is used to compute electronic structure in the Perdew-Burke-Ernzerhof (PEB) scheme using the generalized gradient approximation [24]. Monkhorst-Pack grid of special 26 × 26 × 26[25] and cut-off energy, $E_{cut\text{-}off} = -6.0$ Ry, is chosen to distinguish between the valence electron region and the ion core in Fig.3. After building the reciprocal space sample with 18,000 *k*-points, the Wien2k code generated R_{MT} values are used in the computations. To ensure the minimum energy converges, the muffin-tin radii (RMT) were set at a value preventing electron wave function overlap. The (R_{MT} x K_{max}) parameter was = 7, where K_{max} is the reciprocal lattice vector maximum value and R_{MT} is the (MT) radius of the sphere[26]. The self-consistent field (SCF) approach is used to calculate the total energy of the Heusler compound, and a value of energy equal to 10^{-6} Ry is considered. Wien2k package, Origin Pro 9.0[27], was utilized to investigate the isotropic behaviors of the optical Co_2CuAl Heusler alloy, respectively. Gibbs2 code[28] (quasi-harmonic Debye approximation (QHD)) is used to calculate the thermodynamic properties of the systems, constant volume specific heat capacities, Debye

vibrational energies, including vibrational free energies, and entropies[29]. Using the rigid band approach and semi-classical Boltzmann transport theory as implemented in the BoltzTraP2 code[30], the thermoelectric properties were computed.

3. Results and Discussion

3.1. Structure Properties

The structural optimization of the Co_2CuAl alloy was examined using PBE-GGA (exchange-correlation potentials). The transition element (having several valence electrons) in this formula occupies sites X, Y (Co and Cu), and the p block element occupies sites Z (Al). The cubic space group $Fm\bar{3}m$ (No.225) is adopted by the full Heusler alloy Co_2CuAl[4]. Initially, assume that the Co_2CuAl alloy has a lattice parameter of 5.68 Å with the $L2_1$ phase. The face-centered cubic (fcc) structure of the full-Heusler alloy has four independent Wyckoff positions for the atoms "Co_2" and "Al" are 4b (1/4, 1/4, 1/4) and 4a (0, 0, 0) respectively, whereas the atom "Cu" occupies the 4a (1/2, 1/2, 1/2) illustrates Fig. 1 [31]. Fig. 2 shows the relationship between total energy and volume is represented by the E-V curve, which is used to calculate the bulk modulus and equilibrium lattice parameters[32] by using the B.Murnaghan equation of total energy under various volumes[33]. Crystal structure data and atomic positions of Co_2CuAl are presented in Table 1.

$$E = E_o + \frac{1}{14703.6} \times \left[\frac{V \times B}{PB} \left\{ \frac{1}{1+(PB-1)\left(\frac{V_o}{V}\right)^{PB}} - \frac{V_o \times B}{PB-1} \right\} \right] \quad (1)$$

$$E = E_o + \frac{9}{16}\left(\frac{B}{14703.6}\right)V_o\left[\left(\frac{V_o}{V}\right)^{PB}\right] \quad (2)$$

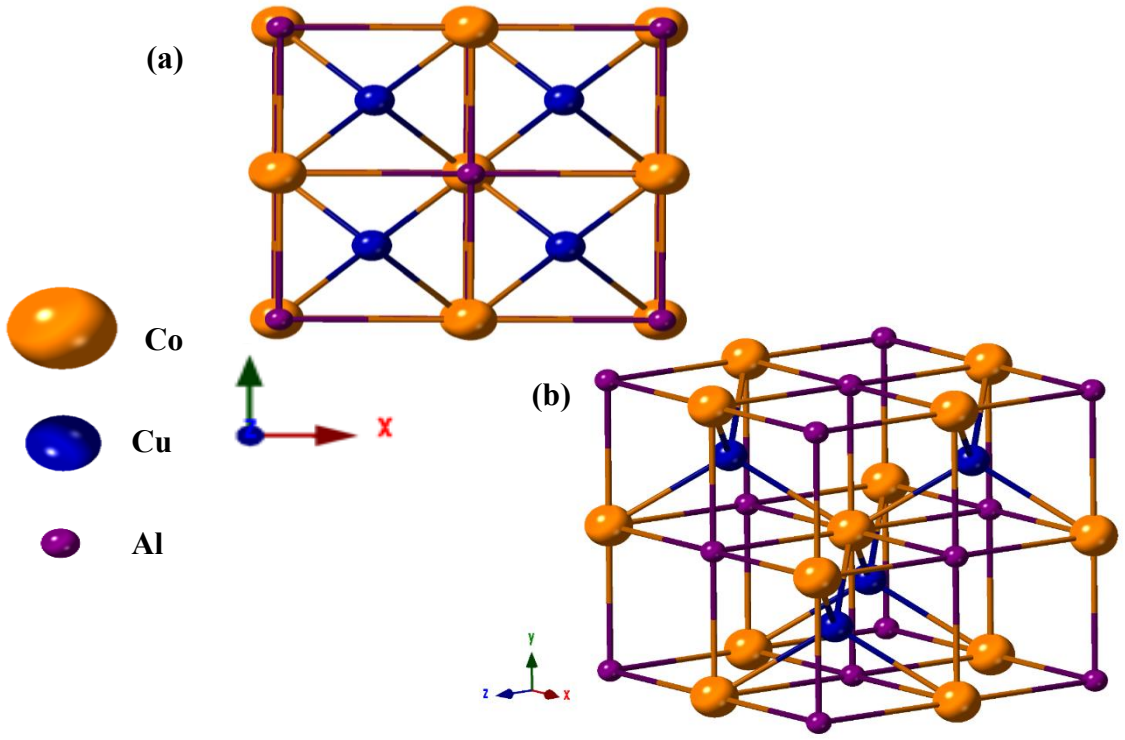

Fig. 1: Crystal structure (a) 2D view and (b) 3D view of Co_2CuAl full Heusler alloy.

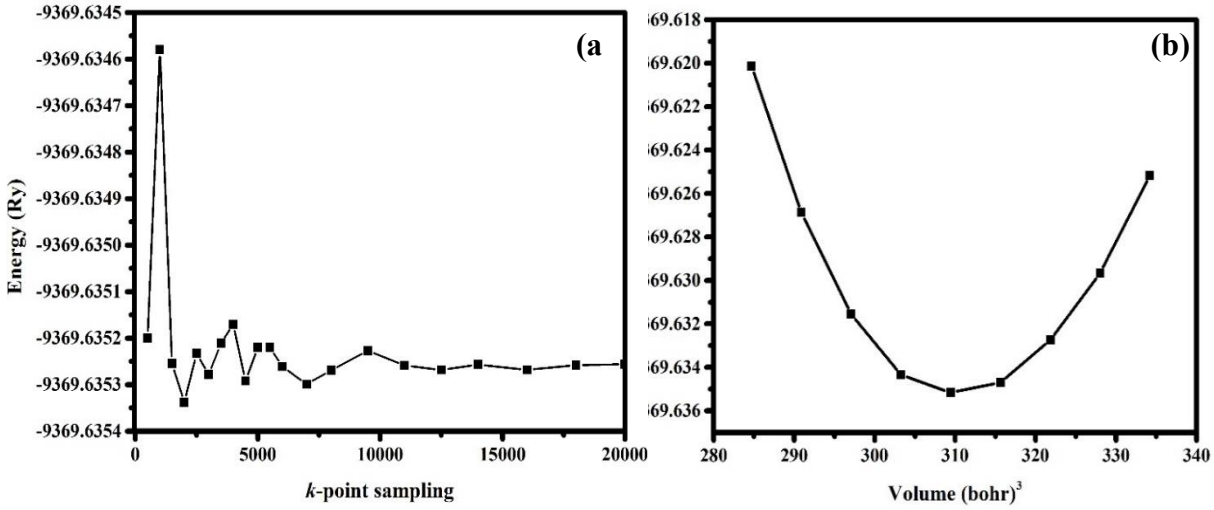

Fig. 2: (a) k-point sampling and (b) total energy as a function of unit cell volume of Co_2CuAl full Heusler alloy.

3.2. Thermodynamic Properties

Thermodynamic properties are fundamental and significant in materials science and engineering.

The QHD (quasi-harmonic Debye) model is utilized to examine the thermodynamic behavior of Co_2CuAl. The following is the Gibbs function G^* for a thermodynamic system [34].

$$G^*(V,P,T) = PV + E(V) + A_{vib}[\theta(V);T]$$

In a system with constant hydrostatic pressure, PV is the product of pressure (P) and volume (V); θ(V) provides information about the Debye temperature and characterizes the propagation of vibrations in a solid material. E(V) denotes the total energy/unit cell, which gives a measure of the overall energy of the system. [35].For Co_2CuAl full Heusler alloys, the temperature dependence of the vibrational energies, entropies, vibrational free energies, and fixed volume heat capacities C_V was determined in the temperature range of 0 to 1600 K and deformation pressure form 0 GPa to 100 GPa shown in Fig. 4(a)-4(d)[36]. A material's ability to withstand volume changes under compression is measured by a physical quantity called B. Fig. 3 (a) shows that the vibrational energy of atoms increases linearly with an increase in temperature, so bulk modulus decreases monotonically. At temperatures between 0 and 1600 K, there was a drop in the bulk modules. Different pressure settings all exhibit the same pattern. At constant temperature, there is a nearly linear relationship between the bulk modulus and pressure. As a result, compressibility and bond strength reduce with increasing temperature at constant pressure. Like this, compressibility rises with pressure while maintaining a constant temperature. In the final stages, the compound Co_2CuAl becomes less hard as temperature increases and becomes harder when compressed[36]. Fig. 3 (b) illustrates that for the full Heusler alloy Co_2CuAl, a larger volume reduction is observed at lower pressures (<40 GPa) and a larger reduction at higher pressures (40–100 GPa). At temperatures lower than 100 K, the Co_2CuAl full Heusler alloy volume stays constant[37]. Volume increases above 100 K dramatically due to thermal expansion and weak attractive force. The Debye temperature (θ_D) provides insight into the vibrational response of the material. For this purpose, determining thermophysical parameters like specific heat, thermal expansion, and vibrational entropy is essential in understanding how a material behaves at higher temperatures.

Table 1: Crystal structure data and atomic positions of Co_2CuAl full Heusler alloy.

Crystal structure data	**Co2CuAl**
Crystal type	Cubic
Space group (No)	$Fm\bar{3}m$ (No.225)
Lattice Parameters	
a(Å)	5.681
b(Å)	5.681
c(Å)	5.681
α	90°

β			90°	
γ			90°	
Volume $(\text{bohr})^3$			310.262	
E_o(Ry)			-9369.635	
Formula units/unit cell			2	
Total atoms/unit cell			8	
SCF k-point			18000	
k-mesh grid			$26 \times 26 \times 26$	
Wyckoff	**Element**	**x**	**y**	**z**
Co2CuAl				
4b	Co	0.25	0.25	0.25
4a	Cu	0.5	0.5	0.5
4a	Al	0	0	0

It is evident that θ_D remained almost unchanged between 0 and 100 K and decreased linearly as temperature increased beyond 200 K. It is also demonstrated that θ_D falls with temperature and rises with pressure [38]. An indicator of how much uncertainty and disorder in a system is called entropy (S). That can evaluate the degree of disruption in materials by closely examining how variations in pressure and temperature affect the system. The relationship between entropy (S) and temperature (T) is shown in Fig. 3 (d). The graph shows that entropy increases exponentially with temperature (T) at 0 K, where pressure is also 0 GPa, indicating increased disturbance within the alloy at higher temperatures under constant pressure. On the other hand, as pressure increases, disturbance and disorder decrease, indicating that the material has a higher degree of order. Thermal vibrations are facilitated by temperature, meaning that a substance's particles vibrate more vigorously at higher temperatures. Contrarily, pressure tends to lessen these oscillations and cause the particles to move less [39].

The temperature-dependent changes in the thermal expansion coefficient of Co_2CuAl alloy are shown in Fig. 3 (e). The nature of bonding among the constituent atoms can be noticed by examining the thermal expansion coefficient against temperature. The thermal expansion coefficient and Debye temperature for Co_2CuAl full Heusler alloy rise rapidly until it reaches 300 K. However, it grows more slowly over 300 K. In addition, the thermal expansion coefficient shows a declining trend at constant temperature as pressure increases. However, this nonlinear relationship is typified by a decreasing rate of change in the thermal expansion coefficient as pressure increases.

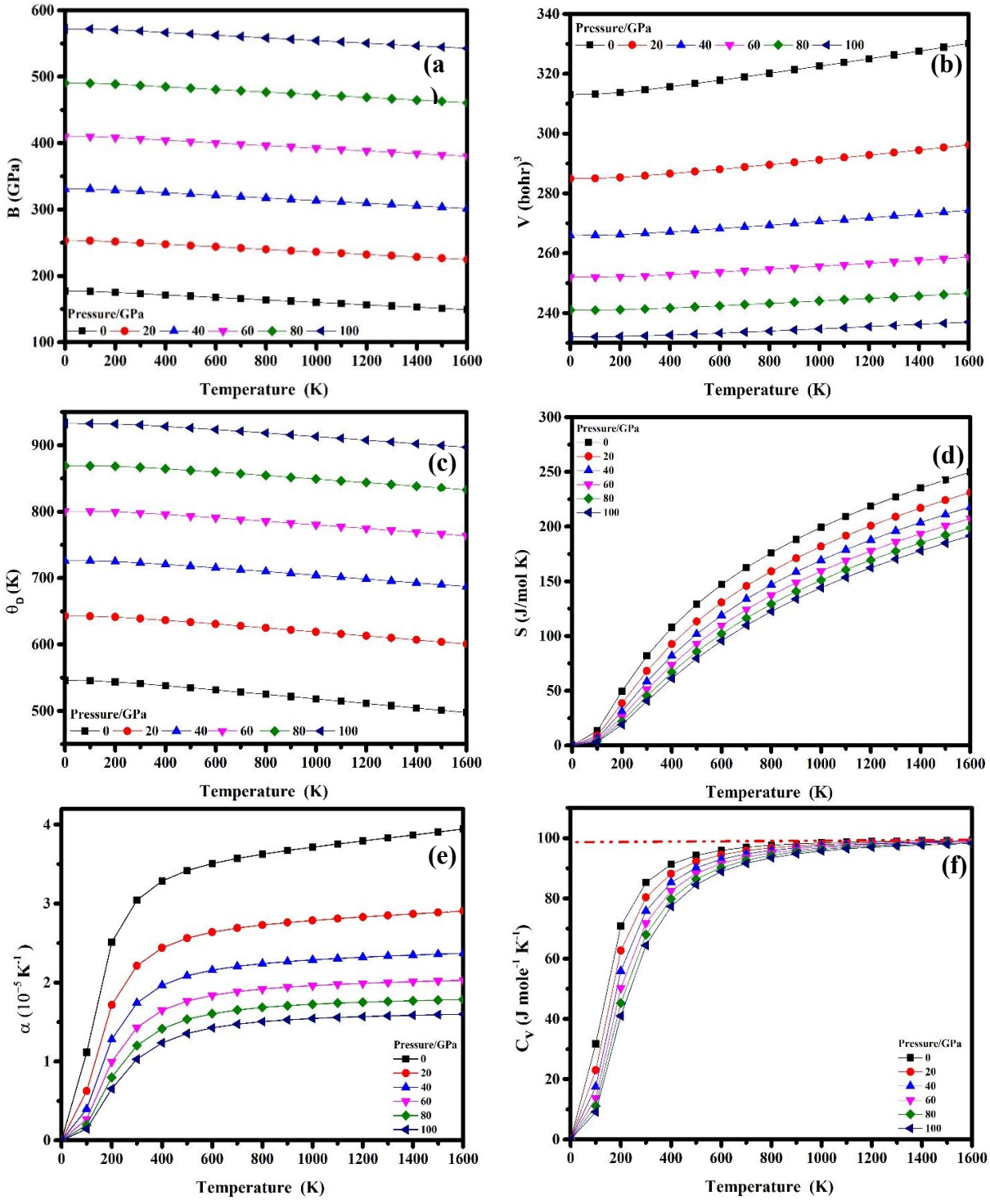

Fig. 3: Computed (a) Volume V, (b) Bulk Modulus B, (c) Debye temperature θ_D, (d) Entropy S, (e) Thermal expansion coefficient α, (f) Lattice Heat Capacity C_V for Co_2CuAl full Heusler alloy.

In Fig. 3 (f), the Dulong-Petit limit values are represented by the red dotted line. The Dulong-Petit limit value in this case is 3nR, where n is the total number of atoms in the unit cell and R

is the gas constant. Fig. 3 (f), illustrates how quickly C_V increases with temperature at very low temperatures, increasing the C_V value represented by T^3. The Cv value gets closer to 98.43 J/mol K Dulong-Petit limit values as the temperature rises. Co_2CuAl full-Heusler alloy has 16 atoms, which means that at high temperatures, their Dulong-Petit limit values are the same. Also, the Cv increases with decreasing pressure when the temperature falls below the Debye temperature. Cv reaches the limit value when the temperature far exceeds the Debye temperature, indicating that the pressure has very little effect on Cv [40].

3.3. Thermoelectric Properties

The need for energy production, conservation, and management on a worldwide scale has increased interest in more efficient power generation methods. Improvements to the current energy supply must originate from a range of sustainable energy sources, such as biomass, solar, and wind. Using thermoelectric materials to create electricity from a heat source is another possible energy source. Heat can be produced by burning fossil fuels, by sunlight, or as a byproduct of other processes (such as nuclear decay, chemical reactions, or combustion). Consequently, thermoelectric materials can potentially contribute to energy conservation and primary power generation (i.e. waste-heat harvesting) [41].

The BoltzTrap2 code is utilized to compute the thermoelectric properties of Co_2CuAl full Heusler alloy, which are investigated to explore their potential for converting heat energy to electrical energy [30].

Fig. 4 (a) shows the calculated electrical conductivity with temperature variation. A general trend for semiconductor materials is an increase in electrical conductivity with temperature. The high density of charge carriers resulting from thermal excitations of electrons from the valence band to the conduction band can be used to justify the increased value of Co_2CaAl alloy. [42]

The variation of thermal conductivity over relaxation time concerning temperature is shown in Fig. 4 (b), and for the Co_2CuAl alloy, it nearly shows a linearly increasing trend [43]. Compounds (Co_2CuAl alloy) with high thermal conductivity are typically used in situations where efficient heat transfer is essential. Heat sinks and thermal management systems, for example, are used in power plants, HVAC systems, and various industrial processes to efficiently transfer heat between fluids or gases. They are also integrated into cooling technologies such as air conditioning, refrigeration, cryogenic systems, aerospace, and automotive applications to further improve heat transfer efficiency [44].

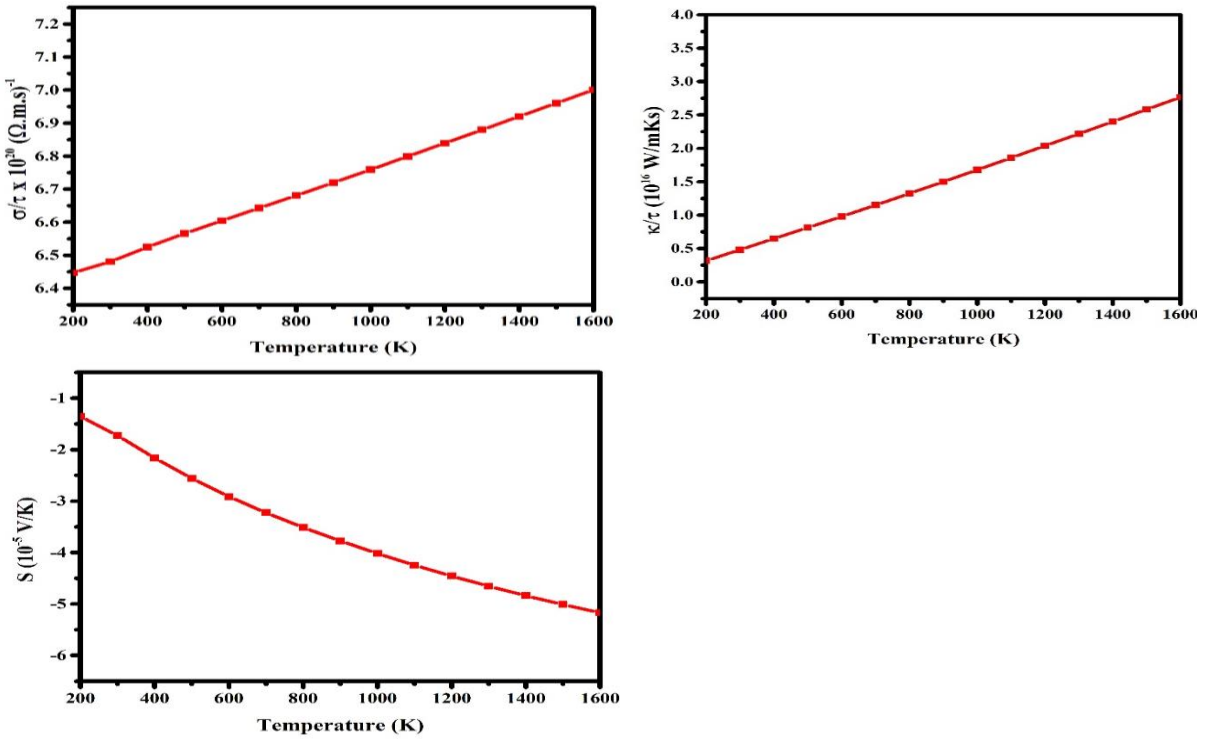

Fig. 4: Calculated (a) Electrical Conductivity (b) Thermal Conductivity and (c) Seebeck coefficient for Co_2CuAl full Heusler alloy.

Fig. 4 (c) shows the seebeck coefficient plot for Co_2CuAl full Heusler alloy. The intermetallics compound exhibits high negative charge carriers at room temperature. In the case of a negative seebeck coefficient, the electrons are majority carriers. For Co_2CuAl compounds, the seebeck coefficient decreases with increasing temperature. When bipolar transport begins, there is a decrease in the seebeck coefficient. This fall results from the opposing currents that holes and electrons generate in response to the temperature gradient[43]. The seebeck coefficient, connected to other thermoelectric parameters like electrical and electronic thermal conductivity, is directly correlated with the electronic energy band. A thermoelectric material's efficiency is determined by its figure-of-merit (ZT). ZT is calculable and depends on S, σ, k, and temperature T. The ZT plot of Co_2CuAl full Heusler alloy is 0.1 at high temperatures, as seen

$$ZT = \frac{S^2 \sigma T}{\kappa} \qquad (3)$$

in Fig. 5 (a). ZT values for Co_2CuAl full Heusler alloy is greater than those for other materials that have been documented in the literature [45]. These findings imply that full Hesuler alloy may have a combination of optical qualities and make good thermoelectric materials.

Fig. 5 (b). Shows the plot of the thermal power of Co_2CuAl full Heusler alloy. Since thermal power ($S^2\sigma$) rises with temperature, it has proven suitable for thermoelectric materials. $S^2\sigma$ for Co_2CuAl at high temperature is 1.872×10^{12} W/mK^2.

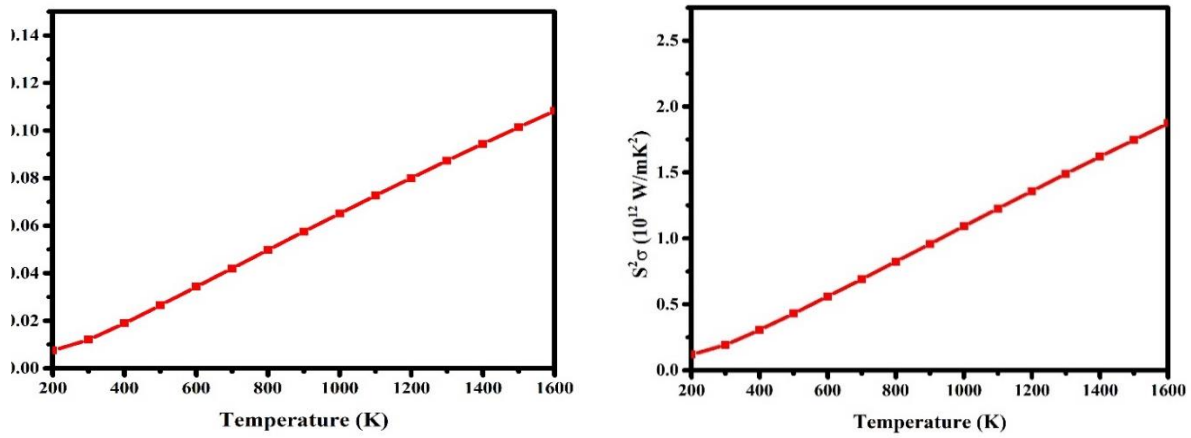

Fig. 5: Calculated (a) Figure of merit ZT (b) Power factor of Co_2CuAl full Heusler alloy.

3.4. Optical Properties

Many phenomena are produced when photons interact with materials. For example, photons can absorb energy from materials, cause materials to eject photons with the same energy as incident photons or transmit photons without interacting with the material's structure and experience a change in velocity (refraction). Each interaction can be seen and reveals a material's optical behavior. In addition, a wide range of other phenomena, including localized defects, magnetic excitations, lattice vibrations, and excitations, can be caused by optical properties. Optical characteristics are purely based on the electronic transition[46]. Dielectric function ε ($\hbar\omega$) is based on two parts $\varepsilon_1(\hbar\omega)$ one is real, and the other one is imaginary part $\varepsilon_2(\hbar\omega)$ both relate to each other.

$$\varepsilon(\hbar\omega) = \varepsilon_1(\hbar\omega) + i\varepsilon_2(\hbar\omega) \quad (4)$$

In this equation the real part $\varepsilon_1(\omega)$ gives a detailed explanation and information about polarization when an electric field is applied to the material and the imaginary part $\varepsilon_2(\omega)$ gives about the absorption feature of the material.

This relation is used to calculate the $\varepsilon_2(\omega)$ [47].

$$\varepsilon_2(\omega) = \frac{e^2 h}{\pi m^2 \omega^2} \sum \int |M_{cv}(k)|^2 \, \delta\,[\omega_{cv}(k) - \omega]\; dk^3 \quad (5)$$

$\varepsilon_1(\omega)$ dielectric function can be found by using Kramers-Kroning relations[48].

$$\varepsilon_1(\omega) = 1 + \frac{2}{\pi} p \int_0^{\infty} \frac{\omega' \varepsilon_2(\omega')}{\omega'^2 - \omega^2} d\omega' \quad (6)$$

Where ω is the angular frequency and P is the Cauchy Principal value.

It can be observed from the $\varepsilon_1(\omega)$ versus energy plots (Fig. 6 (a)) that according to the Drude model, Co_2CuAl full Heusler alloy exhibits metallic behavior due to its static dielectric function $\varepsilon_1(\omega)$ is negative. Co_2CuAl full Heusler alloy shows isotopic behavior whole energy range (0-

12 eV). The high availability of free-charge carriers in these metallic systems is indicated by the non-zero value of $\varepsilon_1(\omega)$. The highest peak in the spectrum for polarization occurs between 3.46 and 6.38 eV of incident photon energy[49].

Fig. 6 (b) displays the imaginary part of the dielectric function $\varepsilon_2(\omega)$. It describes the loss factor or energy absorbed by the material and is always positive. It is associated with dielectric loss. For Co_2CuAl polarization, the imaginary part of the dielectric function approaches zero from above. It is additional evidence that the Co_2CuAl full Heusler alloy is metallic[50].

The absorption coefficient gives information about a material capacity to transform solar energy into other beneficial forms and measures how well it absorbs incident radiation across a spectral range. Fig. 6 (c) illustrates the absorption coefficient of the Co_2CuAl full Heusler alloy, where the metallic nature of the compounds under study causes the spectra to rise from zero photon energy. In the visible and ultraviolet energy ranges, this kind of material is frequently utilized in optical and UV detectors, UV photodetectors, and UV filters[50].

Maximum reflection is shown at zero photon energy (Fig. 6 (d)). For the Co_2CuAl full Heusler alloy, the reflection is 0.59 at 0.0 eV. The value of reflection demonstrates that this compound can absorb light from the ultraviolet to the far ultraviolet spectrum. This indicates that the Co_2CuAl alloy is highly reflective of far ultraviolet light and may find use in solar reflectors and optical shielding devices[37].

When there is an alternating electric field present, optical conductivity is an essential measurement that indicates electrical conductivity. The materials photoconductivity can be accurately estimated from optical conductivity[51]. Fig. 6 (e) displays the Co_2CuAl full Heusler alloy's optical conductivity. The Co2CuAl full Heusler alloy can be identified by a sharp peak in the optical conductivity spectrum close to the zero frequency (Optical conductivity peaks at low photon energy region). Rapid decrease in optical conductivity confirms the conduction nature. The amount of energy lost by fast electrons moving through a material is described by the energy loss function (Fig. 6 (f)). The highest point represents the plasma oscillation at 24.15 eV, which is influenced by the real and imaginary parts of dielectric functions in a complex way. The corresponding material shows a sharp decline in its reflectivity

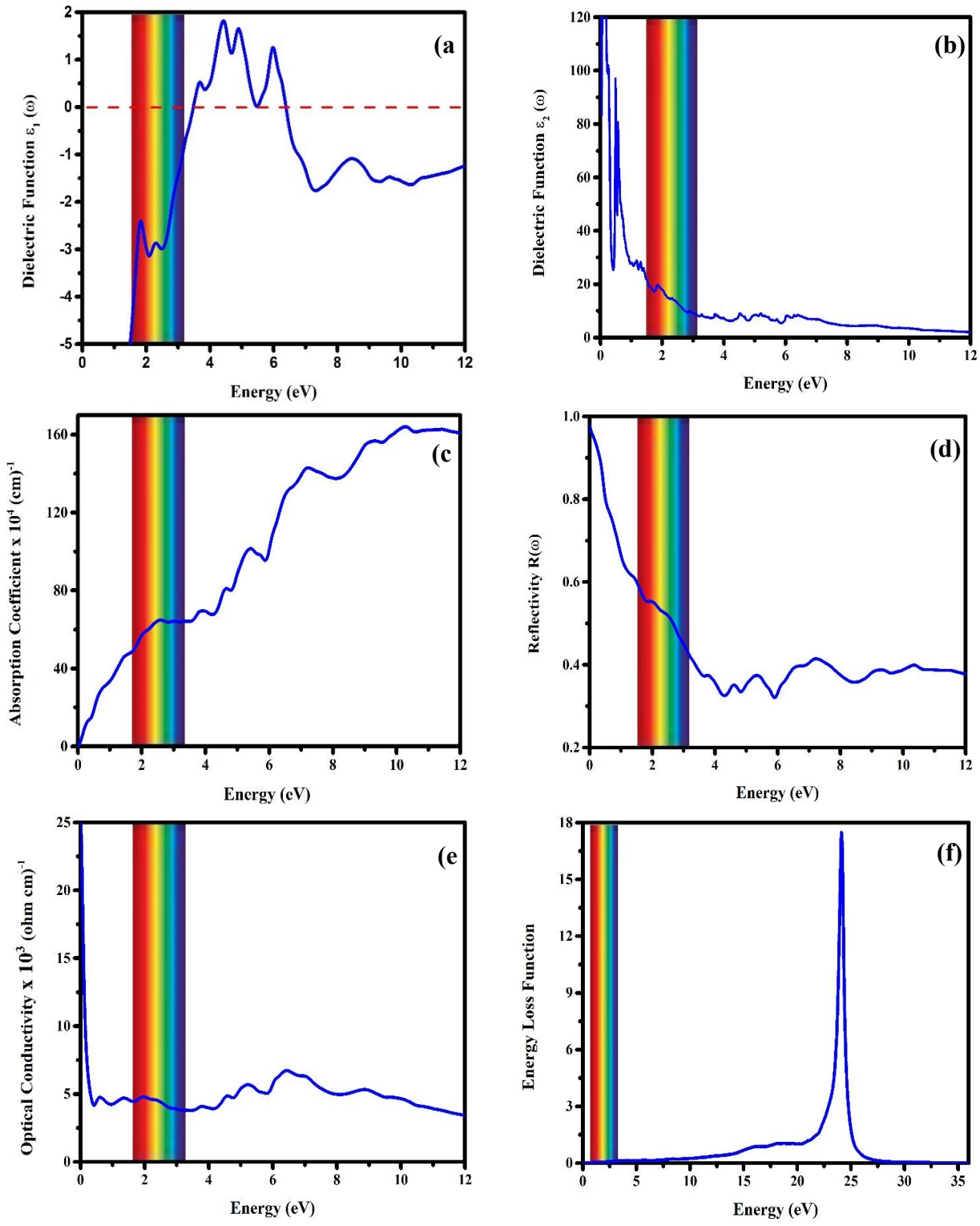

Fig. 6: Calculated Optical parameters of Co_2CuAl full Heusler alloy.

spectrum at this frequency and transitions from a metallic to a dielectric response. Additionally, the dielectric function real part $\varepsilon_1(\omega)$ drops to zero at this frequency. Due to the large imaginary part of the dielectric function $\varepsilon_2(\omega)$. , the energy loss spectrum does not exhibit a peak in the

energy range of 0 to 22 eV[52]. The material exhibits metallic properties [$\varepsilon_1(\omega) < 0$] below this frequency, and dielectric behavior [$\varepsilon_2(\omega) > 0$] above it[53].

4. Conclusions

The thermodynamic, thermoelectric, and dielectric properties of the full Heusler alloy Co2CuAl are determined theoretically using the DFT-based Wien2k simulation package. Co2CuAl crystallizes in space group $Fm\bar{3}m$ with a space group number of 225. Two formula units make up the unit cell of the compound Co2CuAl. There is a total of eight atoms per unit cell. The chosen k-mesh grid for SCF calculations was 26× 26 ×26. To the best of my knowledge, there is currently no documentation available that provides the k-sampling calculations for Co2CuAl full Hesuler alloys. The full Heusler alloy Co2CuAl is found to be thermodynamically stable within the investigated temperature range (0-1600K).

The thermoelectric behavior of Co2CuAl alloy in the temperature range of 200–1600K has been studied. The calculated ZT value of Co2CuAl at high temperatures is ~0.1, indicating its possible use in different devices such as TEGs. The value of the Seebeck coefficient (-5.723× 10^{-5}V/K) at higher temperatures indicates electrons as charge carriers in the studied material. The results suggest that Co2CuAl alloy may be a good replacement for thermoelectric systems in a variety of applications.

Full Heusler alloy Co2CuAl exhibits isotropic behavior in the energy range (0-12eV), according to optical properties. From optical results, it is revealed that Co2CuAl alloy absorbs most light in the ultraviolet (UV) region of the e.m. spectrum.

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