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# Half-metallic behavior $Co_2YAl$ (Y= Mo,Tc) compounds

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The present manuscript reports structural stability, half-metallic behavior, thermophysical and thermoelectric properties of Co2MoAl and Co2TcAl full Heusler compounds using first-principle calculations. The full-potential linearized augmented plane wave method within the framework of density functional theory is implemented and WIEN2k code is incorporated in the stable Fm- 3m phase to attain the desired results. The L21 phase is found as the most stable phase for both compounds. The optimized equilibrium lattice parameters in the stable phase are 5.89Å, 5.86Å for Co2MoAl and Co2TcAl respectively. The electronic band structure study proves that both compounds Co2MoAl and Co2TcAl have indirect band gaps of 0.74eV and 0.85eV respectively in majority spin alignment. The half-metallic performance of the present set of compounds is explained by the spin-resolved density of states. The Fermi level at the Brillouin zone point approves the metallic as well as semiconducting behavior. To elucidate the thermodynamical stability of these materials against pressure and temperature by implementing the quasi-harmonic approximation of various parameters like Debye temperature, Gruneisen parameters and specific heat are studied successfully. To know the thermoelectric response, Seebeck coefficient and electrical conductivity are computed using the BoltzTrap code. The thermodynamic profile delivers that the present set of compounds possesses no anomalies with respect to the phase transition or instabilities. The computational study insights that the compounds can be synthesized experimentally and find a route towards spintronic and thermoelectric applicability.

**Keywords:** Half-metallicity; Magnetism; Thermophysical.

## 1. INTRODUCTION

Immense expansion of material science in the present time has intensively boosted the research curiosity in the field of spintronics. The devices, predominately based on the conventional semiconductors' technology have certain heating consequences like slow processing speed, low capacity of data storage processing, huge power consumption and having limited functionalities [1-4]. Consequently, there is a plentiful requirement to construct a novel paradigm of devices, which exploit the electronic spin rather than mobility, extensively known as the spintronics. The two scientists Fert and Grünberg created the giant magnetoresistance device (GMR) effect in the year 1988, which results in the first-ever intuition for spin-based devices [5,6]. Spin motion plays an essential role in high current density, small power consumption and non-volatility [7]. The material researchers therefore, demonstrated the discovery of novel materials and change in innovative design for the smart device applications. A noteworthy enhancement in simulation power, advance algorithm and improvement in quantum mechanical calculations open up the new paradigms of research to explore a wide range of materials that previously seemed unbelievable [8-10]. The electronic and structural properties of constituent elements can be controlled by the chemical component substitution or doping which results in a new class of materials with multifunctional properties, especially in the Heusler alloys.

Heusler alloys mainly consist of half and full Heuslers in *XYZ* and $X_2YZ$ chemical stoichiometry respectively, where *X* and *Y* are transition metal atoms and *Z* is the main group *sp* element. Because of multidimensional properties from energy or information storage to spintronics, superconductors, thermoelectric and topological insulators [11-13] makes the Heusler alloys a central to the research. Based upon novel collections, Heuslers arises as potential candidates from spintronics, thermoelectric to magneto-resistive applications [14]. Conventional electronic devices offer less opportunity for tuning the precise properties, but spin and electron states lead to spin ordering in half metallic systems. Half metallic materials display complete metallic characters in one spin orientation/channel while the semiconducting character for another spin channel. Heusler alloys demonstrate spin half-metallicity and are considered as a benchmark for spintronic applicability delivering 100% spin polarization [50]. Owing to their extraordinary electronic structure and outstanding properties, they have found applications in magnetic tunneling junctions in $Co_2MnSi$/MgO with tunnel magnetoresistance (TMR) ratio of 1900%, spin transistors, random access memories, current perpendicular to plane giant magnetoresistance (CPP-GMR) reads heads and perpendicular magnetic isotropy [54]. Half- metallic ferromagnets which links the total spin magnetic moments in the unit cell with the number of valence electrons follows the Slater- Pauling rule. The electronic, magnetic and thermophysical properties of Heusler alloys can be transformed by regulating the doping concentration, which is on used in various technological aspects of energy harvesting systems. Moreover, the computational approaches are getting huge interest predominantly, density functional theory (DFT) which is implemented to investigate the multifunctional applications in various potential fields. Recent studies predicted that DFT is equally valuable to predict properties of interests for organic, inorganic and complexes etc. Extensive theoretical and experimental studies on Cobalt Heusler alloys have been carried out by the researchers, signifying half metallicity and other exceptional properties in $Co_2MnSi$, $Co_2MnGe$, $Co_2MnSn$, $Co_2FeAl$, $Cr_2CoGa$, $Co_2MnGe$, $Fe_2CoSi$, $Fe_2CrGa$, $Co_2MnSi$, $Co_2FeSn$, $Co_2RhSi$ and $Co_2RhGe$ etc. [66-75]. Based upon these multi-dimensional and outstanding applications, we have put forth the two Co-based Heusler alloys viz. $Co_2YAl$ (Y=Mo, Tc). The present study describes the phase stability, half-metallicity, structural and thermophysical and thermoelectric properties. The purpose of this work is to explore the cobalt based full Heusler compounds for new functionality. The proposed work will undoubtedly instigate the new possibilities for reference data and guide a root for the further experimental researchers and theoretical investigators also.

## 2. METHODOLOGY

The density functional theory (DFT) is a powerful technique to explain the basic quantum nature of the materials. The DFT has proved a remarkable concept due to its noteworthy description provided about the ground state properties in bulk as well as surfaces and explicitly a large number of materials has been examined. It solves the many electrons system by focusing on electron density rather than the wave function. The investigations of density functional theory for the proposed Heusler alloys, $Co_2YAl$ (Mo,Tc) are carried out by the full potential linear augmented plane wave (FP-LAPW) simulation method. To explore the exceptional and outstanding physical properties of the system, DFT is intensively tailored to WIEN2k simulation code which is typically constructed on a quantum mechanical simulation scheme, that exhibits a noteworthy and clear-cut approach to govern the basic ground state properties of the material systematically. The robust quantity which is unrevealed and to be predicted is the exchange-correlation interactions. The geometrical confirmation is accomplished through generalized gradient approximation (GGA). The unit cell is segregated into spheres that are totally non-overlapping possessing spherical wave functions and the other part is the interstitial section delivering plane-wave performance. The $R_{MT}$Kmax has been adjusted to 6 in such a manner to overcome the overlapping where Kmax is illustrated as the cut-off region of the plane wave and the $R_{MT}$ is demonstrated as the radii of the muffin tin. For the Brillion zone assimilation, a compact *k*-mesh of 2000 points and most important, the cutoff energy that split up core as well as valence electron is adjusted to -6 Ry. The electronic band occupation is scrutinized by implementing the Perdew-Burke Ernzerhof PBE described version of GGA-PBE to the exchange-correlation system. But the GGA reproduces the erroneous concerns typically due to the self-interactions, and endurance of the density derivatives predominantly not suitable for bulk systems, so there is a need for further modifications. To exterminate this ambiguity and typically concerning these inconsistencies and most important keeping into consideration, the precise and accurateness of mBJ we explored our results through the mBJ simulation technique [78]. The self-consistency is attained by adjusting the two important parameters energy as well a charge for the convergence criteria to 0.0001eV and 0.001e, respectively. The significant thermodynamic parameters were scrutinized by the implementations of the Gibbs2 simulation package and BoltzTraP code is used to check the transport parameters. Henceforth, the tensor of electrical conductivity is attained by performing the Fourier expansion which is expressed as;

$$\sigma_{\alpha\beta}(i, K) = e^2\tau_{i,k}V_\alpha(i, K)V_\beta(i, K) \quad (1)$$

Here, the term $\tau_{i,k}$ and e signifies the relaxation time and charge for the electron, while $V_\alpha(i, K)$ represent the α component, the group velocity pertaining to the system is calculated as-

The collective tensor equation for Seebeck coefficient, electrical conductivity is given by the following empirical formula in agreement with the group velocity component as-

$$V_{\alpha\beta}(T, \mu) = \frac{1}{8\pi^3 T}\sum\int \sigma_{\alpha\beta}(i, K)\,[\in (K) - \mu]\,\left(-\frac{\partial f(T,\mu)}{\partial \in}\right) dK \quad (2)$$

## 3. RESULTS AND DISCUSSION

### *3.1 Structural Properties*

The atomic arrangements in the crystal structure play an energetic role in defining the structural properties of that material. The structural phases are conquered by escalating the calculation of numerous phase structures of the energy of the proposed materials. The lattice parameters are initiated to be 5.89Å and 5.86Å for Mo and Tc, respectively. The possible crystal structural cubic configurations typically with two prototype structures are taken into consideration namely $Hg_2CuTi$ holding space group (#216) as well as $Cu_2MnAl$ possessing space group (#225). The conformations of atomic alignments are Al (0.0, 0.0, 0.0), Co (0.75, 0.75, 0.75) and X (0.50, 0.50, 0.50) typically for $Cu_2MnAl$ prototype structure. Howsoever, for $Hg_2CuTi$-type the Co-I atom holds (0.0, 0.0, 0.0), Co-II possesses (¼, ¼, ¼) while the Al atom retains at a position 4a (¾, ¾, ¾) and X atoms preserves (½, ½, ½). The stable ground state optimization prototype structure energy conforms that the $Cu_2MnAl$ prototype holds more stability than the $Hg_2CuTi$ type in these Co-based Heusler materials. To know the structural stability of the given set of Heusler alloys we tried the energy analysis in ferromagnetic/spin polarized (FM) and non- magnetic/no spin polarization (NM) phases using the Birch Murnaghan's equation [81]to define the precise ground state.

The relevant atomic positions and lattice parameters are fully relaxed within this calculation process. From the theoretical calculations and stability curve. It is observed that ferromagnetic (FM) or spin polarized is more stable rather than the non-magnetic phase and hence exhibit minimum energy. To analyze the pressure effect on the structural properties, we have incorporated the Gibbs 2 code to generate pressure-volume (P–V) data by calculating unit cell volumes under a series of applied hydrostatic pressures and is represented. The continuity in the P–V plot specifies the absence of any structural phase transition from a highly symmetric cubic structure to any other structural phases. The cohesive energy has been predicted within the framework of the first principle for $Co_2YAl$ (Y=Mo, Tc) Heuslers. Characteristically, cohesive energy is the essential value of energy to dissociate or to set free the atom within the crystal lattice. The calculated values of cohesive energy for $Co_2MoAl$ and $Co_2TcAl$ sets of alloys are 4.15eV/atom and 4.20eV/atom respectively. The computationally calculated values envisage that the atom typically withheld each other in a crystal lattice and will retain their own structures over a wide range of external forces. In order to endorse the present set of materials, are stable or not, we calculated their respective formation energies by subtracting total energies from individual elements to the equivalent total energies. The computed formation energies for $Co_2MoAl$ and $Co_2TcAl$ are -2.36 (eV/unit cell), -3.14 (eV/unit cell) respectively mentioned in Table 1. The negative values manifest that these alloys can be synthesized experimentally as well.

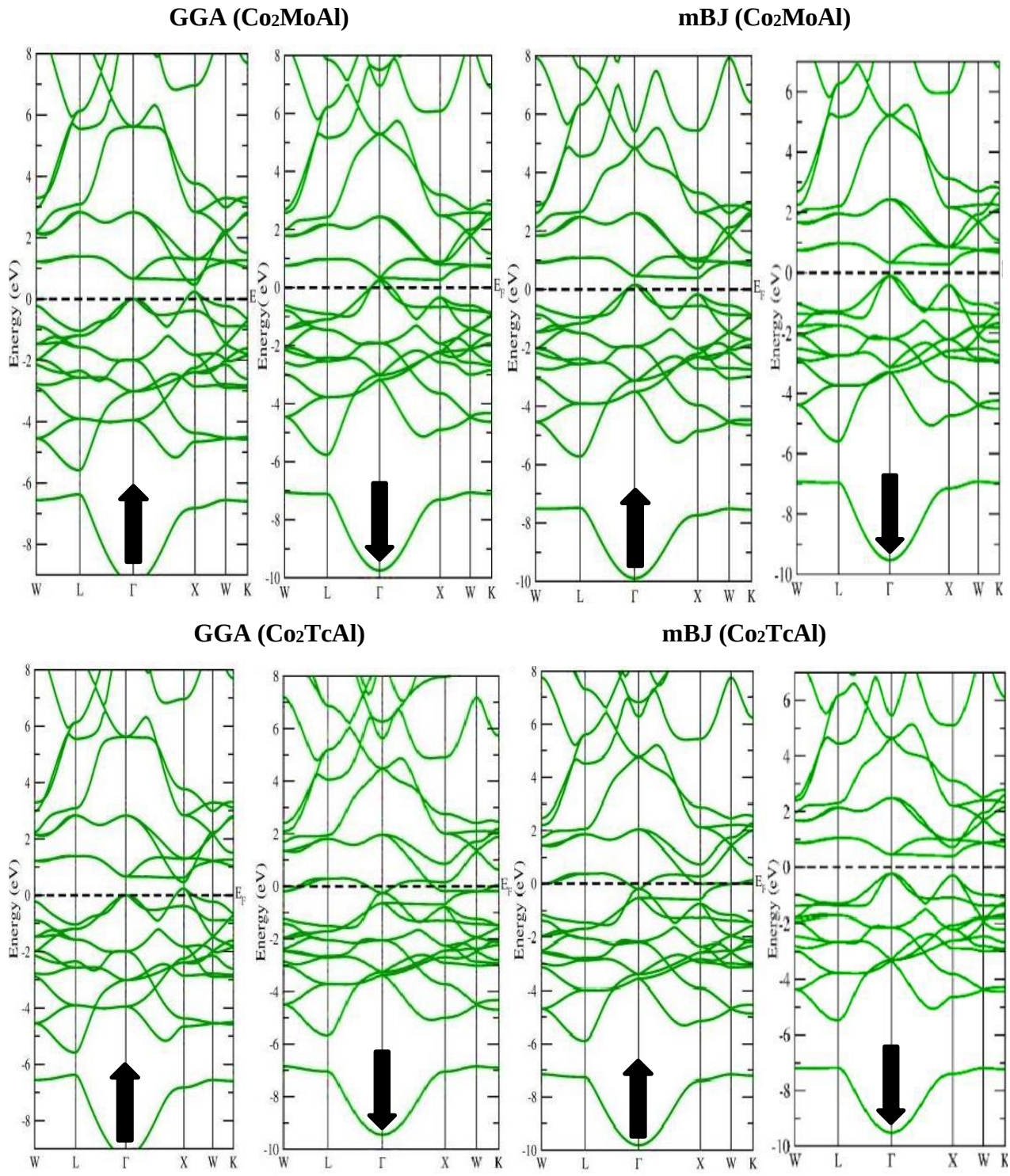


**Figure 1** Spin up and spin down channels and plots of $Co_2MoAl$ and $Co_2TcAl$ system.

### *3.2 Band Structure and Magnetism*

The electronic profile can be projected by plotting the band structure along with the symmetric points as well as the locale of the Fermi level that characteristically demonstrates its classification. The calculated bands through GGA and mBJ are presented in Figure 3. These plots convey that the in case of GGA simulation the bands demonstrate metallic presentation in both spin alignments, howsoever in mBJ the band profile portrays metallic performance in the spin minority channel and semiconducting band profile in the spin majority channel in both the materials. The valence bands typically hint the Fermi level at the Brillouin zone point and show the metallic performance while in the case of mBJ simulation scheme, exhibit a band gap of 0.74 eV and 0.85 eV in the majority spin alignment for $Co_2MoAl$ and $Co_2TcAl$ Heuslers respectively. Furthermore, the valence band maxima as well as minima do not lie at the same symmetry points confirming the Heusler materials possess indirect band gaps. To understand the band occupation, the partial density of states profile is drawn. The computed total density of states (TDOS) and partial density of states (PDOS) are summarized in Figure 4 and Figure 5 respectively for both Heusler materials. The geometrical plots, reflect the pure half-metallicity in both Heusler materials and depict semiconducting performance in spin down alignment. These plots describe that the splitting of atomic energy levels around the locale of the Fermi level is reflected to the filling of electron computation predominately in the *d*-states. In the case of the GGA simulation approach the Fermi level is exclusively occupied in spin majority as well as spin minority channels howsoever the transition metal Cobalt illustrates the majority contribution in both Heusler materials rather than the other elements which is predominately due to the *d*-state filling. Howsoever, in the case of the transition metal complex, the vital crystal field splitting takes the foremost position as main component which is typically due to the establishment of the electric field by the adjoining constituent components and through John Teller distortion to reduce the energy content of the transition metal complexes. Due to the construction of the anti-bonding ($3t_{1u}$, $2e_u$) as well as the bonding ($3t_{2g}$, $2e_g$) states for respectively atom. The typical filled bands will be laid in the valence band as well as their anti-bonding states predominately in the conduction bands. The important *d*-states are totally disproportionately dispersed which gives intensification to the magnetism of a material. The positive magnetic alignment directly hints the spin orientation of the various atoms in the same direction and displays ferromagnetic character and the negative spin alignments deliver ferrimagnetic or anti-ferro interactions. The typical integral magnetic moment possesses a noteworthy characteristic feature of the half-metallic material. Moreover, we have studied extensively the effect of pressure on the magnetic moment is illustrated. One can observe from the graphical plots that increase in the pressure considerably reduce the magnetic moment because of overlapping the states, and the electrons gets bounded into the material. It is more effective on lattice constant due to compression, which alters the physical properties of such kind of materials. Thus, the inclusive amalgamation of ferromagnetic spins establishes the net magnetism of the material in accordance with the consistent structure's alignments. Hence, the adequate magnetic moment possessing these types of Heusler materials may find a possible route typically in high spin performance predominately in the fields like spintronics, spin injection as well as shape memory alloys, etc.

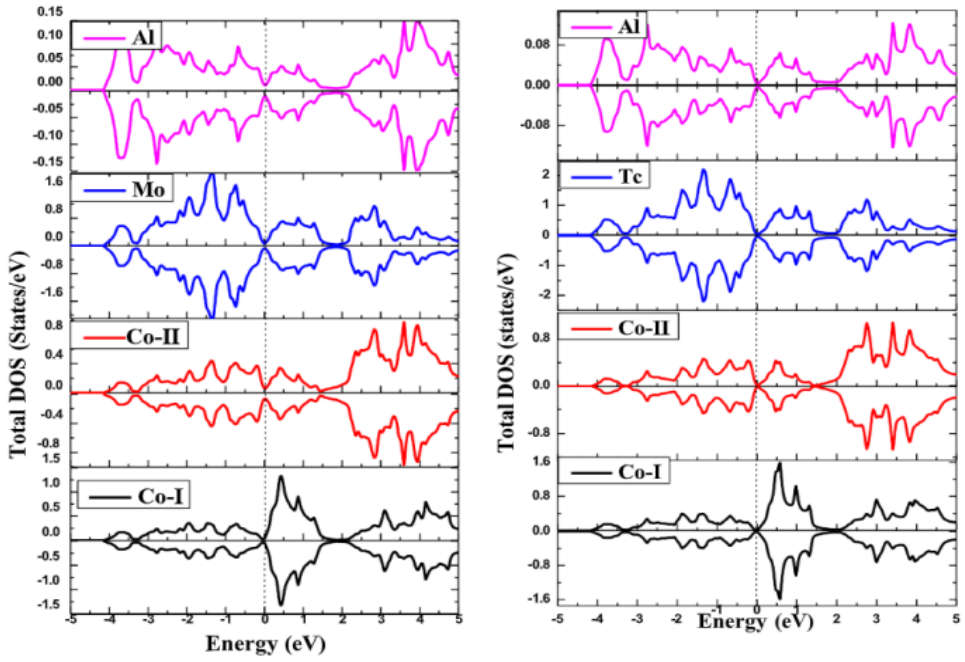


**Figure 2** Total density of states (TDOS) plots for $Co_2MoAl$ and $Co_2TcAl$. Alloys. The vertical dotted line represents the Fermi level.

*3.3 Thermophysical Properties*

To explore the energetic significance typically due to the consequences of the pressure as well as temperature appearances, we have studied the quasi-harmonic approximation (QHA) [82]. This is the first-ever insight concerning the thermophysical performance of these materials at different pressure as well as temperature ranges. So, the present investigation will open a new window for the experimentalists to synthesize such type of materials. Thermophysical properties are crucial to generalizing the capability of the charge transporting and interrelating the cause and effect to define the microstructural components of the materials. The precise and exact variations with temperatures of these vital thermophysical properties predominately can be conquered by assuming the quantized lattice vibrations. The perception of specific heat demonstrates the hint toward the phase transition and lattice vibrations. The thermal outcomes of a crystal generally depend upon the atomic and lattice vibration along the equilibrium positions. With the applications of temperature and pressure, there is significant change in amplitude of lattice vibrations. The study of thermodynamic properties delivers comprehensive information about the performance of an alloy under the extensive range of temperature and pressure. Thermodynamic properties include thermal expansion coefficient, specific heat Grüneisen parameters and their relationship with temperature and pressure is observed by implementing quasi- harmonic Debye model. The interatomic interaction among the materials is predicted in the limit of these parameters. The specific heat is another imperative thermodynamic property which reports the valuable information about microscopic structure and lattice dynamics. On the other hand, heat capacity explains the capability of a material to store heat with variation in the temperature. To explicate the elevation of vibrational motion of atoms predominately on the heat of absorption, the parameter $C_V$, is used to scrutinize the interactions between temperature and specific heat held at different pressures and is demonstrated. From the graphical plot, we analyze that on the elevated temperature the quantity $C_V$ also illustrates a rising trend. This is due to the fact that when we elevate the temperature the vibrations inside the materials gets intensify and becomes more energetic and after that at colossal temperature conquers a constant value conforms Dulong-Petit law typically obeyed in all solids. Howsoever, $C_V$ alters abruptly followed Debye $T^3$ law at low temperature. The noteworthy characteristic parameter to demonstrate the vibrational amplitude of numerous atoms of a typical material is thermal the expansion coefficient (α). The α in the current investigation has varied through different pressure as well as temperature range exhibited. From the graphical representation, (α) demonstrates upraise trend with a reduction in temperature exudates $T^3$ law and progressive trend to a small extent bit in a linear fashion above 200K typically for all pressure ranges. The Grüneisen parameter (γ) is to designate the thermophysical properties and delivers a improved consideration among lattice dynamic frequency and as well as volume change of a particular crystal. It reflects the crystal's anharmonicity inside the crystal and is extensively used to govern the thermal considerations at elevated temperatures as well as the pressure. It is observed that with the rise in temperature, **γ** rises softly but after considering the pressure, γ exhibit a declining trend. So, the rising pressure and temperature have reverse consequences on the Grüneisen parameter but the effect of pressure is more dominant than temperature.

At room temperature, the entropy at the particular pressure range is zero. On elevating the temperature, the value of the entropy gets rises exponentially and it increases with the rise in pressure at the same time. With the increase in pressure, the randomness or chaosness inside the materials gets declined. The calculated value for the present investigation at 0GPa and 0K is 39J/molK and 29J/molK for $Co_2MoAl$ and $Co_2TcAl$ Heusler materials. The entropy change is predominately due to the rise in the vibrational motion inside the material with the elevation of temperature of the atoms which directly leads to the rise in the internal energy of a distinctive system. Hence, the geometrical plot representation delivers no discontinuity which directly hints

that these Heusler materials hold a single-phase typically for the selective range of temperature.

### *3.4 Thermoelectric Properties*

Thermoelectric materials play an imperative role in the energy management and provide a way out to overcome the shortages of conventional energy crisis. They may become a magnificent green energy alterative in the near future. The energy which is generated through thermoelectric materials is entirely ecofriendly and has negligible impact on environmental health due to because of pollution less ones. Substantially, these classes of materials are efficient to transform the heat energy into electrical power and have a great implication in power generation and cooling. The parameter which plays vital role in thermoelectric performance of a material is marked by thermo-power which is essentially the measure of electromotive force created within the material when a temperature gradient is introduced across it. Moreover, the thermoelectric power substantially depends on band structure that determines the phononic and electronic transport. Another important parameter is figure of merit, a dimensionless constant stabilizes the transport behavior primarily depends upon the Seebeck coefficient (S), temperature (T) and electrical conductivity (□). To recognize the prototype thermoelectric materials, it is equally important, first to understand the electron and phonon transport interaction mechanism effectively, second apply effective theory to achieve the favorable results. Boltzmann transport theory contributed a lot to realize the thermoelectric properties. Applying the scaler coefficients:

Seebeck coefficient (S) is measure of induced voltage against the temperature gradient created in the materials. Seebeck coefficient (S) of $Co_2YAl$ (Y=Mo, Tc) Heuslers is plotted against the temperature in the range between 0-800K. To calculate the transport coefficients, we have utilized a dense k-mesh consisting almost one lakh-*k* points in Brillion zone (BZ) to get the charge convergence, as they are further subtle to Brillion zone sampling. To study the thermoelectric properties, we have calculated the Seebeck coefficient (S) and electrical conductivity ($\sigma/\tau$) for both the spin up and down channels. First, to compute the spin dependent Seebeck coefficient (S) of proposed Heuslers we have selected the maximum temperature range of 800 K to recognize its potential stand for thermoelectric applications. It is observed that in spin-up channels of both the alloys, we the value of S follows a trend which is somehow changes linearly with temperature of 550 K while for spin down configuration a pretty sharp decline in S value up to 350 K, afterward it varies smoothly. The significant decrease in S value specifically in semiconducting materials is due to enhanced carrier concentration and hence offers more electron and hole pairs, causing scattering effects and hence decrease in value of Seebeck coefficient (S). The lowest and highest value of Seebeck coefficient (S) is $-2.8\ \mu VK^{-1}$ and $-28\ \mu VK^{-1}$ for $Co_2MoAl$ and $-1\ \mu VK^{-1}$ to $-7\ \mu VK^{-1}$ for $Co_2TcAl$ Heusler materials respectively. These materials deliver a good Seebeck coefficient value at room temperature also and reflect a direct hint towards thermoelectric applicability also. In electronic applications, electrical conductivity ($\sigma/\tau$) is the most significant and critical property of materials. In metal, generally the atoms are tightly binds with each other and electrons are free. The atoms are so compacted that the electron of one atom executes a force on electron of another atom and consequently the valence band and conduction band come in proximity to each other and sometime may overlap. Due to this mechanism if the electrons receive very small amount of external heat or electrical energy it readily climbs to higher levels in metals. These electrons are nominated as free electrons and are liable for current to flow through the metals. When a metal specimen is connected to external current source, the free electrons start approaching the higher potential end of the source, results current flow in the specimen. Specifically, the metals possess excellent electrical conductivity. In the case of semiconductors, the valence band and conduction band are well separated by the forbidden gap of particular width. At very low temperature electrons do not have sufficient amount of energy to occupy the valence band, results no possibility of charge movement. At room temperature few electrons got the energy and climb the forbidden gap causes

transition in conduction region. The density of electrons in metals' conduction bands is very high as compared to the semiconductors and hence do not conduct current effectively. The electrical conductivity of semiconductors is not as good as of metals, but also not as poorer as insulators. Hence such materials are known as semiconductors or half conductors. The electrical conductivity ($\sigma/\tau$) for the given Heuslers is computed for both the spin channels. It is reported that in spin up channel, $\sigma/\tau$ decreases linearly with temperature which signify the metallic in character for spin up configuration. Moreover, the rise in temperature causes increase in carrier concentration and $\sigma$ value. The electrical conductivity and carrier concentration are interconnected through the relation. $\sigma = ne\mu$ , Where $\mu$ represent the mobility of the carriers. The calculated highest $\sigma/\tau$ values are $4.3\times10^{19}\Omega^{-1}m^{-1}s^{-1m}$ in spin down channel and $26.9\times10^{19}\Omega^{-1}m^{-1}s^{-1}$ in spin up configuration for $Co_2MoAl$ while, $26.0\times10^{19}\Omega^{-1}m^{-1}s^{-1}$ in spin up channel and $4.4\times10^{19}\Omega^{-1}m^{-1}s^{-1}$ in spin down alignment for $Co_2TcAl$ Heusler alloy. Additionally, the significant reduction in electrical conductivity with temperature in spin up state virtuously describes the metallic character, while as in spin down state increasing inclination is observed; and hence the semiconductor performance is detected.

## 4. CONCLUSIONS

From effective implementation of DFT calculations, we have precisely projected the phase stability, electronic structure, thermophysical and thermoelectric properties of cobalt-based $Co_2MoAl$ and $Co_2TcAl$ full Heusler compounds. The structural optimization approves the geometric phase stability in *Fm-3m* phase. The perfect half metallic behavior of $Co_2MoAl$ and $Co_2TcAl$ is confirmed by modified Becke Johnson (mBJ) exchange correlation functional. The minimum ground state optimization prototype structure energy confirms that the $Cu_2MnAl$ prototype holds more stability than the $Hg_2CuTi$ type in these compounds. The effect of pressure on the magnetic moment is studied extensively and reported that pressure considerably reduces the magnetic moment. The formation energy reveals the material's stability and suggests the possibility that materials can be synthesized experimentally. The electronic structure, band occupation, and density of states disclose the half-metallic performance in both compounds. The structural as well as ground state parameters are fetched by optimizing these materials in various structural phases, that demonstrate these alloys crystallize in the ferromagnetic magnetic spin ordering. The thermodynamic performance has been intensely predicted by implementing the quasi-harmonic Debye model to designate stability at high pressure and temperature varying conditions while to certify thermoelectric study the Seebeck coefficient and electric conductivity are calculated. From this study experimentalists may find a route for several technological applications and their synthesis.

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