International Academic Institute for Science and Technology

International Academic Journal of Science and Engineering
Vol. 12, No. 3, 2025, pp. 39-44.

ISSN 2454-3896

International Academic Journal of Science and Engineering

www.iaiest.com

First Principles Study of Semiconducting Heusler Alloys for High Temperature Thermoelectric Applications

Rajat Sen [a], Nikita Rane [b]

[a] *Department of Computer Science and Engineering, Quantum Logic Institute of Technology, Nashik, India.*
[b] *Department of Computer Science and Engineering, Quantum Logic Institute of Technology, Nashik, India.*

Abstract

An important topic of research pertaining to global environmental pollution and warming, energy demand, availability, and reliability is the creation of efficient alternative energy sources. In this context, thermoelectric materials can be a promising alternative energy source for power generation. Nonetheless, energy source efficiency is a constant problem, and efforts to increase it have been ongoing. To increase conversion efficiency in thermoelectric power generation, either novel materials are sought out or the properties of existing materials are adjusted. In condensed matter physics and materials research, the density functional theory (DFT) is the most used technique for examining a compound's ground state electronic structure. Density functional perturbation theory (DFPT) or the supercell and finite displacement approach (also known as the direct method) can be used to determine the phonon spectrum. Phonons are necessary to explain dynamical stability, the lattice component of thermal conductivity, thermal expansion, and other characteristics. The phonon dispersion provides information about whether a compound is dynamically stable in a certain crystal structure, which is useful when looking for novel materials. This provides an initial concept for screening a material for use.

Keywords: Shape Memory Alloys, Human Body Implants, Artificial Intelligence, Machine Learning.

DOI: 10.71086/IAJSE/V12I3/IAJSE1223
Received: 20 June 2025/Revised: 26 July 2025/Accepted: 25 August 2025/Published: 30 September 2025

Introduction

In many contemporary technology applications, energy must be transformed from one form to another. To meet these objectives, it becomes crucial to find and create appropriate materials with the required qualities. Research interests in this area include, for example, materials for battery applications, photo-voltaic materials, ferroelectric materials, piezoelectric materials, and materials for effective electricity to light conversion. One significant class of materials that allows for the conversion of heat into electricity is thermoelectric materials. An electrical potential difference is produced in these materials when a temperature gradient is applied across them. This phenomenon is known as the Seebeck effect, because it allows heat to be converted into useable power. In a similar manner, the Peltier effect—a temperature differential across the interface of materials—is produced by the current flow caused by an applied electric field gradient. This characteristic is very useful for cooling applications (Mishnaevsky Jr et al., 2014: Feng et al., 2015). Thermoelectric materials are drawn to numerous energy conversion and sensing applications due to their aforementioned characteristics. The conversion of heat to electricity is primarily being investigated for use in power generation applications (Ferraris & Spriano, 2016). The majority of heat energy is released as waste heat in many industrial operations and heat engines. Fossil fuels are also burned throughout these processes, which have an impact on the environment by raising global temperatures and causing pollution. In light of this, the use of thermoelectric materials in these fields to recover waste heat to a certain degree in the form of useful power appears to be promising. Solid-state, static heat engines are the term used to describe thermoelectric materials. Among its benefits are their reduced environmental impact, quiet operation, portability, and scalability based on application (Balazic & Kopac, 2007; Grote & Hefazi, 2021). Radioisotope thermoelectric generators (RTEGs) are a specialized and significant application of thermoelectric materials in space power sources (Teo et al., 2016). RTEGs have been successfully used in space missions including the Voyager spacecraft and the Apollo lunar missions, among others. Because of their dependability and particular need for a power source under space circumstances, thermoelectric materials have been determined to be suitable in this case (Reddy, 2017; Bird & Ross, 2014). Additional potential uses for power generation include (1) using exhaust heat in cars to increase fuel efficiency and (2) collecting waste heat from industrial activities. Additionally, they can be employed as temperature sensors, detectors, cooling optoelectronic devices, remote sensors, and small-scale solid state refrigeration.

First-Principles Study of Thermoelectric Materials

Different combinations of elements in different compositions must be synthesized in order to obtain a suitable material with the necessary thermoelectric properties through experimental procedures. It is necessary to measure each of the three transport parameters and characterize the prepared samples. Additionally, doping, alloying, or microstructure alterations are to be used to adjust the properties. However, if a lot of compounds need to be tried, this approach can be overwhelming. In this case, computational methods are superior to experimental ones for determining and forecasting the properties of the material. Computational methods are becoming the primary technique for predicting the properties of materials due to the development in modern computing power and the incorporation of first-principles theories into computer programs. A material's electronic structure, phonon spectrum, and carrier scattering mechanisms are all closely related to its transport coefficients. Classifying the material systems is made easier by the signatures in the measurement of transport properties. The electronic structure and scattering mechanisms allow for the direct derivation of the electronic transport coefficient terms S, σ, and κe. The material's κph is determined by the phonon spectrum and several phonon scattering mechanisms. Consequently, the relevant transport coefficients can be derived from first-principles after the electronic structure, phonon spectrum, and scattering mechanisms of the material have been determined. In condensed matter physics and materials research, the density functional theory (DFT) is the most used technique for examining a compound's ground state electronic structure. The two Hohenberg and Kohn theorems form the foundation of the DFT. The real ground state density is the one that minimizes the total energy in DFT, where the ground state total energy is a unique functional of the ground state electronic density. A system of non-interacting electrons in an effective potential is created by mapping the problem of a system of many interacting electrons. The self-consistent solution of a set of single particle Hamiltonians known as Kohn-Sham (KS) Hamiltonians yields the ground state energy and density. The exchange-correlation (XC) term, an unknown component of the KS Hamiltonian, is where the approximation enters. There are numerous ways to approximate this phrase, and there is a library of XC functionals for it. The most widely utilized functionals are those of the generalized gradient approximation (GGA) and local density approximation (LDA) types. The main reason for the differences between the DFT estimated results and the physical parameters of actual systems is this inadequate representation of the electron interaction effects. Functionals such as hybrid functionals, meta-GGA, or modified Becke-Johnson (mBJ) functionals are used in an effort to get around these challenges (Shahid et al., 2021).

Heusler Compounds as Thermoelectric Materials

One class of materials with intriguing and practical qualities is Heusler compounds. Fritz Heusler is the namesake of the Heusler class of chemicals. He found that an alloy with the composition Cu2MnAl possesses ferromagnetic properties in 1903. There are now several compounds in this family of materials with a wide range of characteristics. The quantity of valence electrons in a Heusler compound can be used to predict its properties. Semiconducting materials having an adjustable band gap are thought to be promising options for thermoelectric and solar cell applications. The multifunctional topological insulators have been anticipated via electronic structure calculations. Numerous Heusler materials have magnetic properties, including heavy-fermionic behaviour, antiferromagnetism, Pauli paramagnetic, and itinerant and localized magnetism. Many of the members are drawn to them as potential candidates for spintronics applications because to their half-metallic ferromagnetism (see Fig. 1).

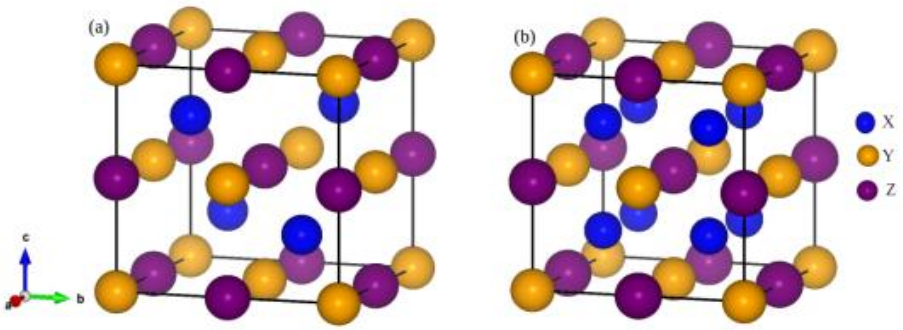


Fig. 1: The Crystal Structure of (a) Half-Heusler Compound XYZ and (b) Full-Heusler Compound X2YZ

Experiment and Evaluation

Fig. 2 illustrate the dispersion curves computed for Fe2TiSn using PBEsol and SCAN are displayed in Fig. 3. The following are the general characteristics of the compounds' band structures: At the Γ-point, the CBM is twice degenerate and the VBM is triply degenerate. Near the Fermi energy in the conduction band region, the bands are non-degenerate along the Γ-X direction and degenerate along the Γ-L direction. Along the Γ-X direction, a flat conduction band is visible. The compound is suitable for thermoelectric applications because of the flat conduction band, which raises the effective mass value. The valence and conduction bands at the Γ-point directly overlap in the PBEsol and LDA derived (not shown in the figure) dispersion curves. Additionally, the EF is being crossed by the CBM at the X-point. This trend might result from LDA and PBEsol functionals underestimating the band gap. These two functionals point to the compound's semi-metallic nature.

Nonetheless, the band gap provided by mBJ is consistent with the experimental value. Therefore, S can be calculated using the m ∗ values that are produced if a stiff shift of bands equal to the mBJ gap is employed to establish an artificial gap in the dispersion of PBE sol, SCAN, LDA, or PBE. However, after relocating the bands, the band gaps and band positions at different k-points will differ. This suggests that all of the functionals will produce a different quantity of electrons and holes as a result of the band transition. As a result, the S derived from various functionals might not be same across all functionals. Do et al. attempted to explain the experimental data by calculating the See beck coefficient of Fe2VAl using Boltzmann transport theory. It is discovered that neither the semiconducting band structure with a band gap of 0.55 eV (GGA+U) nor the semi metallic band structure with psedudo gap can adequately explain the experimental See beck coefficient.

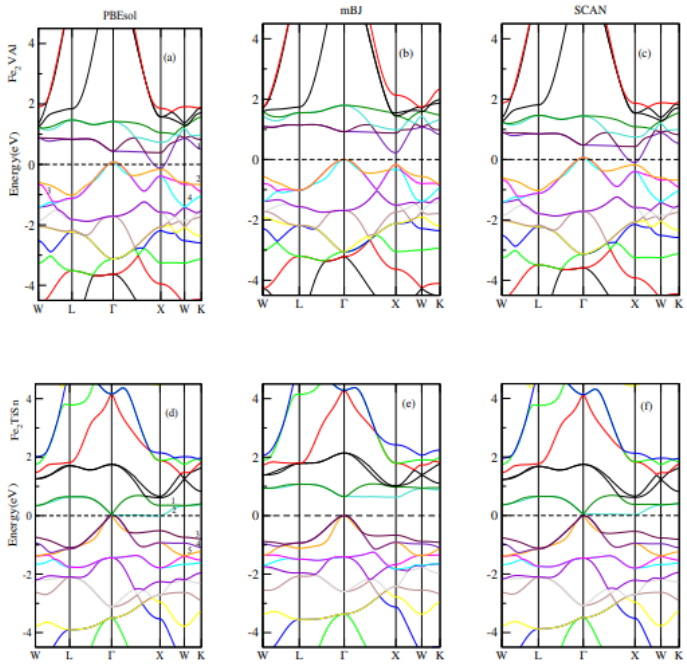


Fig. 2: Dispersion Curve

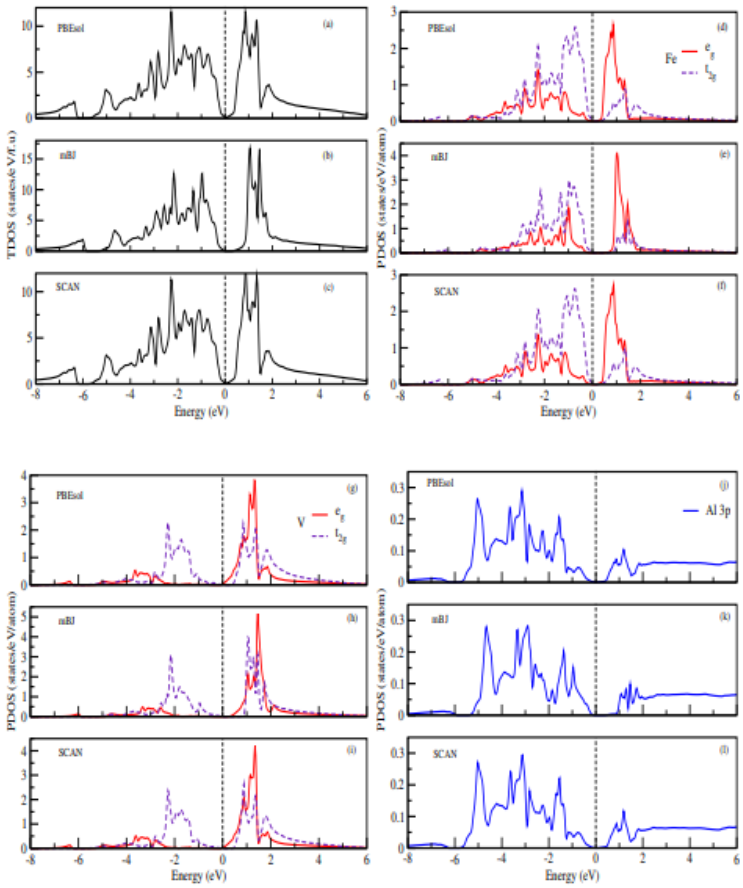


Fig. 3: Total and Partial Density of States Plots

As a result of the shift in XC functionals, the TDOS plots indicate a modest variation in the DOS (features) at the various energy positions. The PDOS plots also show the observed difference that was caused by the states of the constituent elements. When determining the chemical potential and, thus, the transport coefficients, the carrier concentration is a crucial factor. The DOS determines the carrier concentration. As a result, the transport properties computed may be marginally impacted by the XC functionals employed in the computation. These findings help to clarify that, for the two compounds, mBJ roughly represents the ground state electronic structure, but it differs significantly from the other.

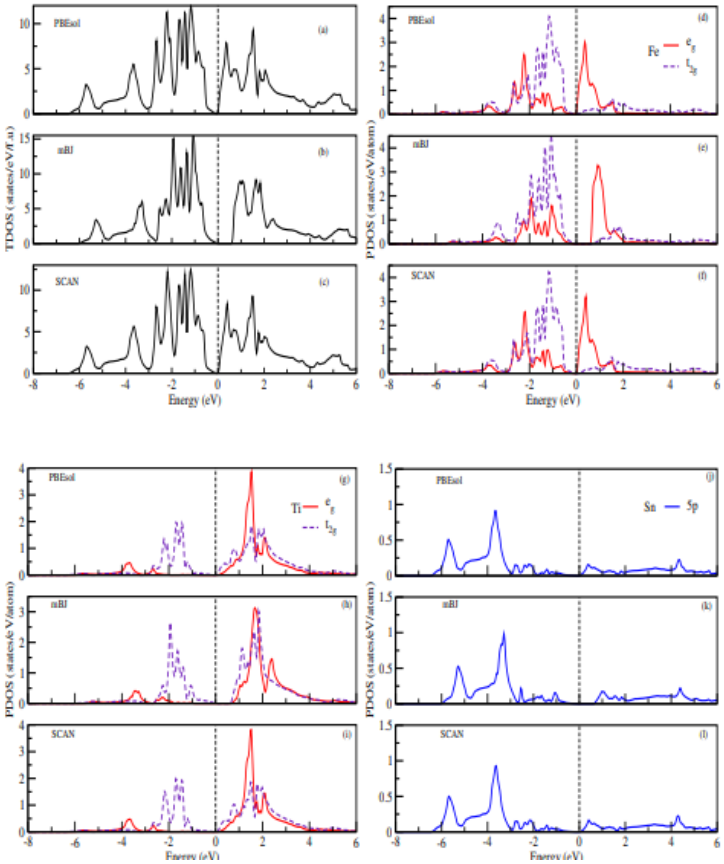


Fig. 4: Total and Partial Density of States Plots for Fe2TiSn

Fig. 4 shows the qualitative differences between the calculated and experimental values. It is evident that the lattice constants for the two compounds deviate significantly from LDA. The experimental lattice constant (closer to the dashed line) is where the PBE-calculated values of optimized lattice constants fall. The energy-volume parabolas for the next three potentials fall between the calculated values from PBE and LDA. Additionally, the values are near to one another.

Conclusion

The dispersion curves from PBE and SCAN computations, as well as LDA and PBEsol calculations, have many general characteristics. In contrast, both compounds' mBJ-calculated electronic band structures exhibit larger alterations in relation to other functionals. The effect on the band characteristics and contributions to the Seebeck coefficient are examined by calculating the effective mass of charge carriers from the dispersion curves using the parabolic approach. It is discovered that the mBJ is appropriate for obtaining appropriate band gap values. However, when compared to other functionals, the band features defined by mBJ exhibit reasonable differences. For the Fe2VAl and Fe2TiSn compounds, phonon characteristics are investigated using a supercell method, with forces calculated using first-principles DFT. Four XC functionals—LDA, PBE, PBEsol, and SCAN—are used in the investigation. TDOS, PDOS, and phonon dispersion are computed under the harmonic approximation. Zero-point energy, Debye

temperatures, and the cv and Fph as functions of temperature are computed. PBE is determined to provide the lowest phonon energies when comparing the TDOS and phonon dispersions from various functionals, whereas LDA and SCAN provide greater values of energies.

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