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Original Article

A Review Zon Heusler Based Sustainable Materials and Nanotechnology: Advancements, Applications, And Future Perspectives

K. Venkanna
Department of Physics, SGA Government Degree College, Yellamanchili, Andhra Pradesh, India

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Correspondence Address:
K Venkanna
Department of Physics, SGA Government Degree College, Yellamanchili, Andhra Pradesh, India
Email: karumuri.venkanna@gmail.com

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Abstract

Heusler alloys are a class of intermetallic compounds recognized as sustainable materials for nanotechnology applications due to their tunable electrical, magnetic, and thermoelectric properties. The structure, synthesis, nano-structuring, and multifunctional uses of full-Heusler (X_2YZ) and half-Heusler (XYZ) systems are highlighted in this paper. Half-Heusler alloys like TiNiSn, ZrNiSn, HfNiSn, and NbFeSb have electrical conductivities of 10^4–10^5 S/m and Seebeck values of 150–300 µV/K in thermo-electrics. Through processes including phonon scattering and defect engineering, nano-structuring reduces thermal conductivity from 8–10 W/m·K to 2–4 W/m·K, resulting in ZT values of 1.0–1.5 at 700–900 K. Additionally, Heusler compounds display approximately 100% spin polarization, which makes spintronic devices like MRAM possible. Materials like Co_2MnSi and Co_2FeAl have Curie temperatures between 600 and 1100 K. For refrigeration, magneto-caloric alloys (Ni–Mn–In, Ni–Mn–Sn) show entropy variations of 2–10 J/kg·K, and catalytic uses include the evolution of hydrogen with over-potentials of 100–300 mV. The utilization of earth-abundant materials, recyclability above 90%, and lives exceeding 10 years are sustainability advantages that provide alternatives to Bi_2Te_3. Future methods aim for ZT > 2.0 and efficiencies above 15%, strengthening their significance in sustainable energy and electronics, despite obstacles like modest ZT, Hf element cost, and scalability.

Keywords: *Sustainable materials, nanotechnology, green synthesis, environmental remediation, circular economy, renewable energy*

Introduction

The demand for sustainable materials and energy-efficient technology has increased due to rapid industrialization, the depletion of fossil fuels, and large-scale waste heat generation. The development of innovative materials for effective energy conversion with little environmental impact is motivated by the fact that almost 60–70% of the world's energy is lost as waste heat in industrial processes, automotive systems, and power generation. Heusler alloys have become a promising class of sustainable functional materials in this regard. Through compositional and structural engineering, these intermetallic compounds, which are categorized as full-Heusler (X_2YZ) [1-2] and half-Heusler (XYZ) [3], have adjustable electrical, magnetic, and thermoelectric properties. In contrast to traditional thermoelectric materials such as Bi_2Te_3 [4], High mechanical robustness, high thermal stability (>1000 K), and the utilization of earth-abundant, non-toxic elements like Ti, Zr, and Sn are all benefits of Heusler alloys. Their performance is greatly improved by nanotechnology, which involves control at the 1–100 nm scale. Thermoelectric efficiency can be increased by optimizing phonon and electron transport by defect engineering and nano-structuring. TiNiSn [5] and other nanostructured half-Heusler systems show improved power factors of 3–5 mW/m·K². In automotive and industrial applications, its thermoelectric performance (ZT = 1.0–1.5 at 700–900 K) facilitates effective waste heat recovery. Furthermore, these materials outperform many conventional thermos-electrics by maintaining structural and chemical stability above 800 K. Lead-free compositions like ZrNiSn [6] and HfNiSn [7] lessen their environmental impact. Grain refinement, phase separation, and nanoscale precipitates are examples of nano-structuring techniques that reduce lattice thermal conductivity from 8–10 W/m·K to 2–4 W/m·K, greatly increasing efficiency.

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Heusler alloys are significant in spintronics, where their half-metallic composition allows for nearly 100% spin polarization, in addition to thermo-electrics. For spin injection devices and magnetic tunnel junctions, compounds like Co_2MnSi [8] and Co_2FeAl [9] are extensively researched. All things considered, the combination of nanotechnology and Heusler alloy design has resulted in multifunctional materials appropriate for thermoelectric generators, green electronics, waste heat recovery, and next-generation nano-engineered devices [10], making them important contributors to sustainable energy technologies.

Classification of Sustainable Materials

Instead of using traditional polymer-based methods, a function-oriented framework is needed for the classification of sustainable materials for Heusler compounds. Their sustainability originates from their multi-functionality, energy efficiency, and recyclability as metallic and intermetallic systems. As a result, they can be divided into advanced functional materials, nanostructured materials, hybrid systems, recyclable metallic materials, and functional energy materials. Metallic materials that are recyclable and resource-efficient make up a fundamental category. Heusler alloys, which are made up of elements like Co, Mn, Fe, Ni, Ti, and Sn, are more than 90% recyclable. Metal recycling uses 60–95% less energy than primary manufacture. Long-term applications are supported by full-Heusler (X_2YZ, such as Co_2MnSi, Co_2FeAl) and half-Heusler (XYZ, such as TiNiSn, ZrNiSn, and NbFeSb [12]) compounds, which exhibit electrical conductivities of 10^4–10^5 S/m and remain stable at 800–1200 K.

Heusler systems rely heavily on functional energy materials, particularly in thermoelectric, spintronic, and magneto-caloric applications. With Seebeck coefficients of 100–300 μV/K and thermal conductivity of 2–10 W/m·K, alloys like Hf–Zr–NiSn and NbFeSb have thermoelectric efficiency (measured by $ZT = S^2\sigma T/\kappa$) of 0.8–1.5. Heusler alloys, such as Co_2MnSi and Co_2FeSi, with Curie temperatures of 600–1100 K and nearly 100% spin polarization, making spintronic devices possible. Near ambient temperature magneto-caloric systems such as Ni–Mn–In and Ni–Mn–Sn exhibit entropy changes of 2–10 J/kg·K. By incorporating nano-inclusions, reducing grain sizes to 10–100 nm, lowering thermal conductivity by 30–70%, and increasing ZT by 20–50%, nano-structured materials dramatically improve performance. Nano-structured TiNiSn, HfZrNiSn, and Co_2MnSi [13] systems demonstrate the widespread usage of techniques such ball milling, spark plasma sintering, and thin-film deposition.

Crystal Structure and Fundamental Properties of Heusler Compounds

Heusler compounds, which are divided into full-Heusler (X_2YZ) and half-Heusler (XYZ) systems, are ordered intermetallic materials having adjustable electronic configurations. They are appropriate for sustainable applications because of their cubic symmetry and compositional flexibility, which allow control over electrical, magnetic, and thermoelectric properties.

1. **Full-Heusler Structure**

Full-Heusler compounds adopt the cubic $L2_1$ structure ($Fm\bar{3}m$) with four interpenetrating fcc sub-lattices. X atoms occupy (0, 0, 0) and (½, ½, ½), Y at (¼, ¼, ¼), and Z at (¾, ¾, ¾). Lattice parameters range from 5.6–6.0 Å. These materials show metallic conductivity with carrier concentrations 10^{21} cm^{-3} and strong magnetic behaviour. Many exhibits half-metallicity with nearly 100% spin polarization. Compounds like Co_2MnSi and Co_2FeSi show Curie temperatures of 800–1100 K.

2. Half-Heusler Structure

Half-Heusler compounds have one empty sub-lattice and crystallize in the $C1_\beta$ structure ($F\bar{4}3m$). (0,0,0), (¼, ¼, ¼), and (½, ½, ½) are occupied by X, Y, and Z, respectively. With band gaps of 0.1–0.5 eV and lattice parameters of 5.8–6.2 Å, they display semiconducting properties. It is possible to adjust carrier concentrations between 10^{11} and 10^{21} cm^{-3}. Thermo-electrics make extensive use of materials like TiNiSn, ZrNiSn, and HfNiSn.

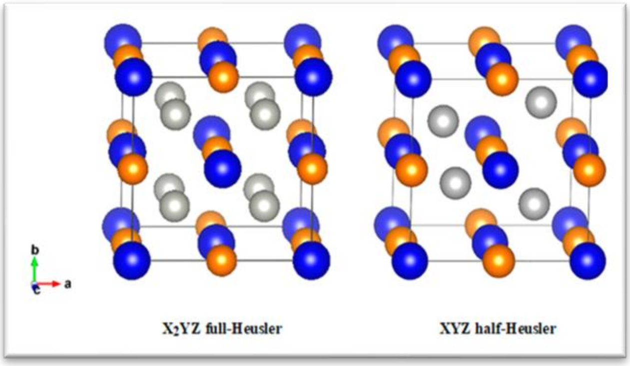

Fig.1: Crystal structure of full- and half-Heusler compounds (X atoms occupy the gray positions, Y atoms occupy the orange positions and Z atoms occupy the blue positions). (Ref: https://doi.org/10.3390/met14060688)[14]

The crystal structures of half-Heusler (XYZ) and full-Heusler (X_2YZ) compounds are compared in **Fig.1.** Two X atoms, one Y atom, and one Z atom are dispersed among interpenetrating sub-lattices in the highly symmetric cubic arrangement of the full-Heusler structure (left), where all lattice positions are occupied. The half-Heusler structure (right), on the other hand, has a similar framework but one sub-lattice is left empty, which results in a lower symmetry and a lower atomic occupancy. The gray spheres show either unique atoms or vacant/interstitial places, emphasizing the structural differences between the two alloy types, while the coloured spheres represent various atomic species.

3. Electronic Structure

Electronic properties depend on valence electron concentration, often following the Slater–Pauling rule ($M_t = N_v - 24$). Band engineering through doping, alloying, and band convergence enhances transport properties and improves thermoelectric performance.

4. Magnetic and Spintronic Properties

Magnetism arises from exchange interactions. Full-Heuslers are typically ferromagnetic with high Curie temperatures, while half-Heuslers vary. Their half-metallicity enables nearly 100% spin polarization, supporting spintronic devices like magnetic tunnel junctions.

5. Thermoelectric Properties

Half-Heuslers exhibit thermal conductivity of 8–10 W/m·K, reducible to 2–4 W/m·K via nanostructuring. Electrical conductivity ranges from 10^4–10^5 S/m and Seebeck coefficients from 100–300 μV/K, yielding ZT values of 1.0–1.5 at 700–900 K.

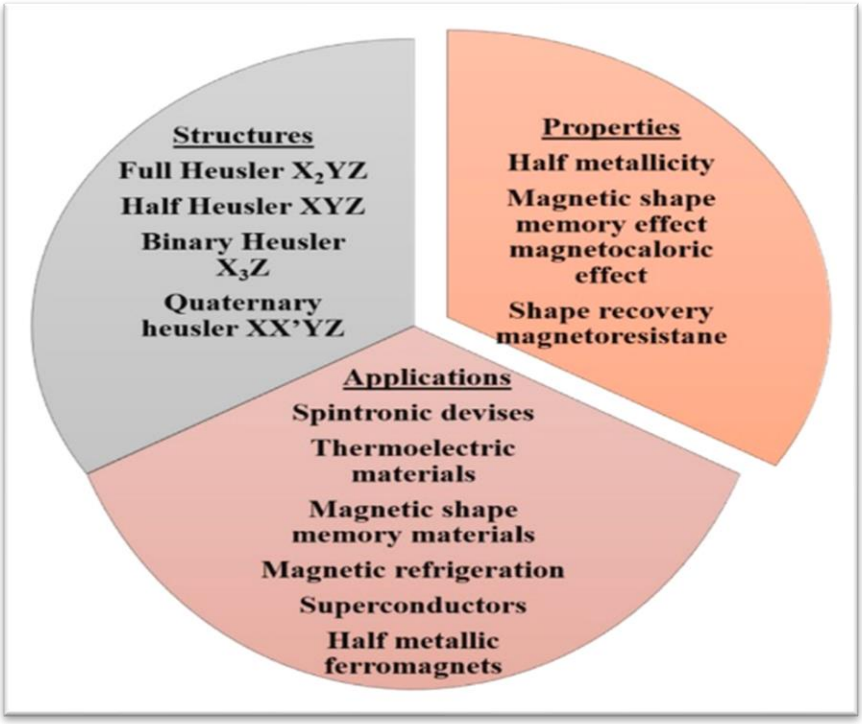

Fig.2: List of different structures, properties and possible applications of Heusler alloys. (Ref: https://doi.org/10.3390/met14060688) [15].

Heusler compounds are summarized in **Fig.2** by classifying them according to their structures, characteristics, and uses. In terms of structure, it comprises binary Heusler (X_3Z), quaternary Heusler (XX′YZ), full-Heusler (X_2YZ), and half-Heusler (XYZ). Notable characteristics of these materials include shape recovery, magneto-caloric effect, half-metallicity, magnetic shape memory behaviour, and magnetoresistance. Heusler compounds are widely used in advanced technologies such as spintronic devices, thermoelectric materials, magnetic shape memory systems, magnetic refrigeration, superconductors, and half-metallic ferromagnets because of their combination of structural versatility and functional properties.

Synthesis Methods and Fabrication Techniques of Heusler Compounds

The synthesis of Heusler compounds has a significant impact on their structure, phase purity, and functional properties. Because electronic, magnetic, and thermoelectric behavior strongly depend on microstructure, precise control over processing conditions is crucial. Bulk, nanostructured, and thin-film materials are produced using a variety of methods.

1. Bulk Synthesis Techniques

For the scalable manufacturing of high-purity alloys, bulk techniques like arc melting and induction melting are frequently employed. Arc melting entails processing temperatures exceeding 1200 °C in inert atmospheres, then repeating the melting process to achieve homogeneity. Additionally, solid-state processes are employed to produce polycrystalline materials with grain sizes of 1–10 μm by annealing at 800–1100 °C for 24–72 hours. Ordering and transport properties are enhanced by post-annealing at 700–1000 °C.

2. Mechanical Alloying and Powder Metallurgy

Through repeated deformation over a period of 10 to 50 hours, high-energy ball milling facilitates the creation of nanoscale alloys. Hot pressing or spark plasma sintering (SPS), which offers quick densification (>95%) at 800–1100 °C in 5–10 minutes while maintaining nanostructures and enhancing transport characteristics, are used to accomplish consolidation.

3. Rapid Solidification Techniques

Grain sizes of 10–100 nm are produced by melt spinning, which uses fast cooling rates of 10^5–10^6 K/s to create nano-crystalline materials. Phonon scattering is enhanced by these structures, and phase and electrical characteristics are improved after annealing.

4. Thin-Film Deposition Techniques

Spintronic applications require thin sheets. While pulsed laser deposition guarantees stoichiometric transfer, magnetron sputtering permits regulated deposition (10–500 nm). Although molecular beam epitaxy produces high-quality, flawless films, its scalability and cost are constrained. Spin valves and magnetic tunnel junctions are two examples of devices that use these films.

5. Nano-structuring and Defect Engineering

Transport properties are customized by nano-structuring methods like grain refining and nanoscale inclusions. Carrier concentration is optimized using defect engineering, such as doping with Sb, Nb, or Ta. By increasing phonon scattering, nanocomposites improve thermoelectric performance and reduce heat conductivity by 50–70%.

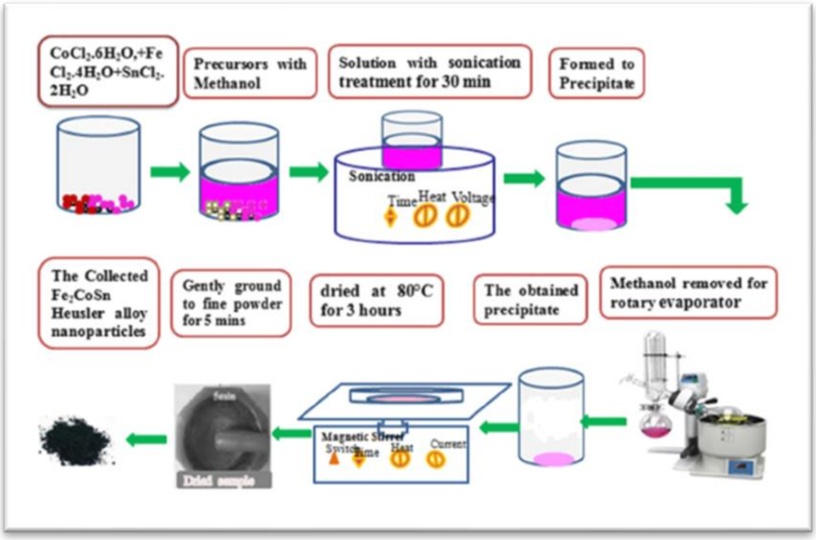

Fig.3: *Schematic diagram of synthesis of Fe_2CoSn Heusler alloy nanoparticles (Ref: DOI:10.1007/s10948-019-05292-5) [16]*

The production of Fe_2CoSn Heusler alloy nanoparticles utilizing a solution-based approach is shown in **Fig. 3.** To create a precipitate, the precursor salts ($CoCl_2·6H_2O$, $FeCl_3·4H_2O$, and $SnCl_2·2H_2O$) are first dissolved in methanol and then sonicated for 30 minutes to guarantee even mixing and reaction. A rotary evaporator is used to extract the solvent from the precipitate after it has been collected and dried at 80 °C for several hours. As seen in the final product image, the dried product is then carefully crushed into a fine powder and processed further using magnetic stirring with controlled time, heat, and current to produce consistent Fe_2CoSn nanoparticles.

6. Scalability and Industrial Considerations

While SPS and mechanical alloying provide high-performance nanostructured materials, bulk techniques are appropriate for large-scale production. Uniformity, reproducibility, and cost effectiveness are still difficult to achieve, especially with costly components like Hf. Process optimization and the creation of affordable, scalable synthesis methods are the main goals of ongoing efforts.

Nano-structuring and Performance Enhancement Mechanisms

By increasing electrical transport and reducing thermal conductivity, nano-structuring is a crucial tactic for raising the thermoelectric performance of Heusler compounds. Nanoscale engineering makes it possible to partially decouple transport parameters in half-Heusler systems, which have high thermal conductivity by nature. This improves efficiency for applications like waste heat recovery. The figure of merit ($ZT = S^2\sigma T/\kappa$) governs thermoelectric performance, and the fundamental problem is still to reduce lattice heat conductivity without lowering the power factor ($S^2\sigma$). The main mechanism is phonon scattering, which lowers thermal conductivity from 8–10 W/m·K to 2–4 W/m by nanoscale grain refinement (10–100 nm) and processing techniques including ball milling and spark plasma sintering.At 700–900 K, systems like TiNiSn-based nanocomposites and $Hf_{0.5}$–$Zr_{0.5}$–Ni-Sn exhibit decreases of up to 60–70%, reaching ZT values of 1.2–1.5. As demonstrated in NbFeSb-based alloys, energy filtering further improves performance by selectively scattering low-energy carriers, raising Seebeck coefficients to 200–300 μV/K while preserving electrical conductivity of 10^5–10^6 S/m. Alloying (e.g., Hf, Ti, Sb) produces band convergence, which raises carrier effective mass and boosts power factors from 2 to 4-5 mW/m·K^2. Defect engineering improves both electrical and thermal transport by optimizing carrier concentrations in the region of 10^{19}–10^{21} cm^{-3} through doping (Sb, Ta, Nb, V) and vacancy introduction. Furthermore, multi-scale phonon scattering is introduced using nanocomposite techniques (e.g., TiNiSn–ZrNiSn, HfNiSn with full-Heusler inclusions), which further reduces thermal conductivity without sacrificing electrical characteristics. Overall, ZT values of 1.0–1.5 are made possible by the combined effects of phonon scattering, energy filtering, band convergence, and defect engineering; continued efforts aim to achieve values above 2.0, making nanostructured Heusler materials excellent options for high-efficiency sustainable energy conversion.

Applications of Heusler-Based Sustainable Materials

Heusler materials are widely explored for sustainable energy and electronic applications due to their tunable electronic structure, high thermal stability, and compatibility with nano-structuring. Their multifunctional properties enable efficient solutions to energy and environmental challenges.

1. Spintronic Applications

Heusler alloys are perfect for spintronic devices since they have almost 100% spin polarization. Curie temperatures for materials like Co_2MnSi, Co_2FeAl, Co_2FeSi, and Mn_2VAl range from 600 to 1100 K. At room temperature, they attain tunnel magnetoresistance ratios more than 200% at magnetic tunnel junctions. These characteristics improve energy-efficient data storage by enabling low-power, high-speed devices like MRAM, spin valves, and spin transistors.

2. Magneto-caloric Refrigeration

Ni–Mn–In, Ni–Mn–Sn, and Ni–Mn–Ga are examples of magnetocaloric Heusler alloys that show promise for solid-state cooling. Under 1–5 T fields, they show magnetic entropy variations of 2–10 J/kg·K (up to ~15 J/kg·K in optimal situations). They are appropriate for air conditioning and refrigeration because of their adjustable operating range (200–400 K), which offers 20–30% greater efficiency than traditional systems while getting rid of dangerous refrigerants.

3. Energy Storage and Catalysis

Because of their stability and conductivity, Heusler materials are becoming more used in batteries and catalysis. Compounds with potential for use in sodium-ion and lithium-ion batteries include Co_2FeAl and Ni_2MnGa. Heusler alloys with overpotentials of 100–300 mV and Tafel slopes of 50–120 mV/dec support HER, OER, and ORR in catalysis. For hydrogen energy systems and fuel cells, nanostructured forms increase activity and offer affordable substitutes for noble metals.

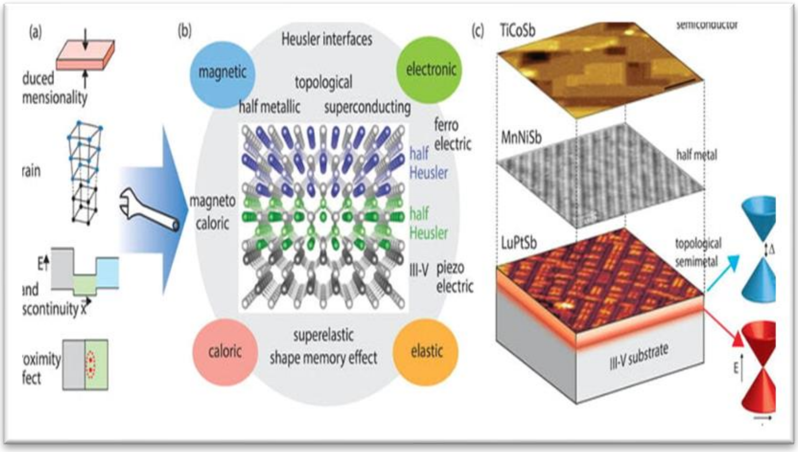

Fig.4: Emergent properties at Heusler interfaces. (a) Tuning parameters for epitaxial films and heterostructures. (b) Heusler properties, grouped into four major functionalities: magnetic, electronic, elastic, and caloric. (c) Scanning tunneling microscopy (STM) images of TiCoSb (semiconductor), MnNiSb (half metallic ferromagnet), and LuPtSb (topological semimetal). Each of these compounds can be grown on a III-V substrate. A Dirac dispersion of topological states is expected at the interface between topological semimetals and normal III-V substrates. A gapped Dirac cone and the quantum anomalous Hall effect are expected at the interface between topological materials and ferromagnets. (Ref: DOI:10.1063/1.5099576)[17]

The multifunctional behavior of Heusler materials and the function of interfaces in adjusting their properties are highlighted in **Fig. 4.** The electrical structure of these materials can be altered by external influences such reduced dimensionality, tension, band discontinuities, and proximity effects, as shown in panel (a). In addition to phenomena like half-metallicity, superconductivity, topological states, piezoelectricity, and shape memory effects, panel (b) summarizes the vast array of linked properties displayed by Heusler compounds, including magnetic, electronic, caloric, and elastic responses. A layered hetero structure example (such as TiCoSb/MnNiSb/LuPtSb on a III–V substrate) is shown in panel (c), illustrating how combining various Heusler phases are essential for advanced functional and spintronic applications because they can generate a variety of electronic states, including as semiconducting, half-metallic, and topological semimetal characteristics.

Sustainability Assessment and Environmental Impact

Heusler compounds are emerging as sustainable material systems due to their balance of performance, availability, and environmental compatibility. Unlike conventional thermoelectrics that rely on toxic or scarce elements, their sustainability is evaluated across the full lifecycle, including extraction, processing, operation, and end-of-life.

1. Life Cycle Assessment (LCA)

Heusler alloys are composed of relatively abundant elements such as Ti (~0.6 wt%), Fe (~5 wt%), Zr, Ni, Co, and Sn, unlike scarce elements like Te (<0.001 wt%), reducing resource depletion risks. Processing involves high temperatures of 800–1200 °C, but advanced methods like spark plasma sintering lower energy consumption by 20–40% and reduce processing time. Their long operational lifetimes of 10–20 years offset initial energy costs. Importantly, recyclability exceeds 90–95% through conventional metallurgical methods, minimizing environmental burden.

2. Environmental Benefits

Heusler alloys offer a safer alternative to conventional materials like Bi_2Te_3 and PbTe, which involve toxic elements. Lead-free systems such as TiNiSn, ZrNiSn, and NbFeSb exhibit strong thermoelectric performance and high thermal stability (>1000 K), reducing degradation and environmental risks. Their use of earth-abundant elements lowers the environmental footprint. Additionally, applications in spintronics and magnetocaloric systems enable energy savings and reduced greenhouse emissions through efficient electronics and cooling.

3. Circular Economy Aspects

With recyclability above 90% and operational lifetimes exceeding 100,000 hours, Heusler alloys align well with circular economy principles. Their metallic nature allows repeated recycling without loss of functionality. Durability in high-temperature systems reduces replacement frequency and waste. Recovery of elements like Ni, Co, and Nb further enhances sustainability. Strategies such as replacing Hf with Zr or Ti improve resource availability and reduce costs.

4. Comparison with Conventional Materials

Compared to Bi_2Te_3, which operates below 500 K and suffers from toxicity and scarcity, Heusler alloys offer superior thermal stability at 800–1000 K, lower toxicity, and more abundant raw materials. Although some compositions with Hf remain costly, overall material costs are lower. Their high-temperature stability, recyclability, and environmental safety make Heusler compounds strong candidates for large-scale, sustainable energy applications. Despite notable progress, several challenges limit the large-scale adoption of Heusler compounds in sustainable technologies. A key issue is their moderate thermoelectric efficiency. Optimized half-Heusler alloys such as $Hf_{0.5}Zr_{0.5}NiSn$, NbFeSb, and TiNiSn typically achieve ZT values of 1.0–1.5 at 700–900 K, which remain lower than advanced materials like SnSe and nanostructured chalcogenides with ZT exceeding 2.0–2.5. This indicates the need for further improvement in electronic transport and phonon scattering. Material cost is another constraint, particularly due to the use of hafnium (Hf), which can cost several hundred USD per kg. While Hf-based alloys enhance performance, their high-cost limits scalability. Alternatives such as ZrNiSn–TiNiSn solid solutions and FeNbSb systems aim to reduce reliance on Hf while maintaining competitive properties.

Scalability and manufacturing also present challenges. Techniques like spark plasma sintering (SPS), melt spinning, and molecular beam epitaxy (MBE) offer precise control but are expensive and difficult to scale. SPS, for example, is typically limited to small sample sizes (centimeter scale) and requires strict control conditions, making large-scale production difficult. Phase stability and compositional control are critical concerns. Heusler alloys are sensitive to antisite defects, secondary phases, and stoichiometric deviations, which can degrade performance. In TiNiSn systems, excess Ni or unwanted phases can reduce efficiency. Long-term stability at >800 K over 10,000–100,000 hours is also essential for reliable operation. Finally, intrinsic trade-offs between electrical conductivity and Seebeck coefficient complicate optimization. Increasing carrier concentration improves conductivity but reduces the Seebeck coefficient. Although approaches like band convergence and energy filtering help, achieving a major breakthrough in ZT remains a challenge.

Future Perspectives

The future development of Heusler compounds will be driven by advanced design strategies and emerging technologies to overcome current limitations and enhance performance. Artificial intelligence (AI) and machine learning (ML) are playing a key role in accelerating materials discovery by enabling rapid screening of compositions based on electronic structure, stability, and transport properties. These approaches can predict optimal doping, band structures, and thermoelectric behavior, reducing experimental effort. High-entropy Heusler alloys are another promising direction, incorporating multiple elements to increase configurational entropy and stabilize complex structures. Systems such as (Ti,Zr,Hf) (Ni,Co)Sn show reduced thermal conductivity below 2 W/m·K due to enhanced phonon scattering, with potential to achieve ZT values near or above 2.0.

Flexible and wearable thermoelectric devices are also emerging, where Heusler nanoparticles or thin films are integrated with polymers like polyimide or PDMS. Current performance remains modest (ZT ~0.3–0.8), but improvements in interface and composite design aim to enhance efficiency while maintaining flexibility. Integration with renewable energy systems is gaining interest. Half-Heusler-based thermoelectric generators can be combined with solar thermal or waste heat sources, and hybrid photovoltaic–thermoelectric systems may reach overall efficiencies of 15–20%. Future efforts target ZT > 2.0 and device efficiencies above 15% through combined optimization of composition, nano-structuring, and device design. Replacing costly elements like Hf and Co with abundant alternatives such as Ti and Fe will be critical for scalability. Additionally, advances in additive manufacturing and large-scale fabrication are expected to enable complex device architectures and accelerate real-world deployment of Heusler-based technologies.

The **Fig.5** illustrates the integration of machine learning (ML) in the lifecycle of nanoparticle development, forming a closed-loop workflow.

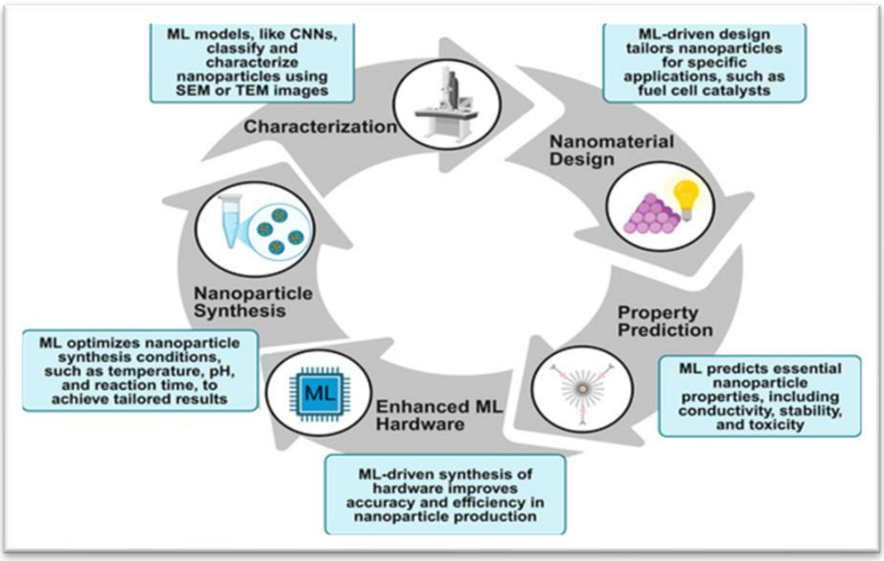

Fig.5: A cartoon depicting convergence and collaboration between ML and nanotechnology. (Ref: https://doi.org/10.3390/ijms252212368) [13].

It shows how ML contributes to key stages, including nanomaterial design, property prediction, synthesis, characterization, and hardware optimization. ML models, such as convolutional neural networks (CNNs), assist in analysing SEM/TEM images for accurate characterization, while predictive algorithms estimate properties like conductivity, stability, and toxicity. Additionally, ML optimizes synthesis parameters (e.g., temperature, pH, and reaction time) and supports the development of advanced hardware to improve production efficiency. This iterative ML-driven approach enables faster; more precise design and fabrication of nanoparticles tailored for specific applications.

Conclusion

Heusler compounds are highlighted in this review as a promising class of environmentally friendly materials with a wide range of uses in electronics, energy, and environmental technology. High thermal stability (>1000 K), mechanical robustness, compositional tunability, and the utilization of common, non-toxic elements like Ti, Zr, Fe, and Sn are some of its main features. Their lengthy lifespan (>10–20 years) and high recyclability (>90%) further bolster their sustainability and conformity to the principles of the circular economy. A key factor in improving their performance is nanotechnology. ZT values of 1.0–1.5 are made possible by techniques including band convergence, nanoscale inclusions, defect engineering, and grain refinement that lower lattice thermal conductivity from 8–10 to 2–4 W/m·K while preserving strong electrical characteristics. These enhancements show how nanoscale engineering may maximize energy conversion. Heusler compounds are also multifunctional, with uses in magneto-caloric refrigeration, thermos-electrics, spintronics (near 100% spin polarization), and new fields including energy storage and catalysis. Environmentally friendly and energy-efficient technology is supported by these characteristics. There are still challenges with scalability, phase stability, high costs of components like Hf, and moderate ZT in comparison to advanced materials. However, ZT > 2.0 and efficiencies above 15% are the goals of future approaches like AI-driven design, high-entropy systems, adaptable thermos-electrics, and renewable energy integration. Heusler compounds are positioned as essential materials for next-generation energy systems due to the integration of material design, nanotechnology, and sustainability; nevertheless, further study is required for large-scale deployment.

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Conflicts of interest
The authors declare that there are no conflicts of interest regarding the publication of this paper.

References

1. G. Rogl and P. Rogl, "How nanostructuring and alloying improve the thermoelectric performance of half-Heusler compounds," **Acta Mater.**, vol. 131, pp. 336–348, 2022.
2. G. J. Snyder and E. S. Toberer, "Complex thermoelectric materials," **Nat. Mater.**, vol. 7, no. 2, pp. 105–114, 2021.
3. H. Zhu *et al.*, "Half-Heusler alloys for high-performance thermoelectric cooling," **Nat. Commun.**, vol. 14, Art. no. 38446, 2023.
4. C. Fu, T. Zhu, Y. Liu, H. Xie, and X. Zhao, "Band engineering of high-performance p-type FeNbSb based half-Heusler thermoelectric materials," **Energy Environ. Sci.**, vol. 8, pp. 216–220, 2022.
5. S. Chen and Z. Ren, "Recent progress of half-Heusler for moderate temperature thermoelectric applications," **Mater. Today**, vol. 16, no. 10, pp. 387–395, 2021.
6. B. Balke, G. H. Fecher, and C. Felser, "Spintronics with Heusler compounds," **Appl. Phys. Lett.**, vol. 90, no. 15, p. 152504, 2022.
7. T. Graf, C. Felser, and S. S. P. Parkin, "Simple rules for the understanding of Heusler compounds," **Prog. Solid State Chem.**, vol. 39, no. 1, pp. 1–50, 2021.
8. B. Gurunani and D. C. Gupta, "Electronic structure and magnetic properties of Heusler alloys: A DFT study," **Sci. Rep.**, vol. 13, Art. no. 48316, 2023.
9. S. Sharma and D. C. Gupta, "Inverse Heusler alloys for spintronic applications," **Sci. Rep.**, vol. 14, Art. no. 72305, 2024.
10. T. Bachagha and J. J. Suñol, "Recent advances in all-d-metal Heusler alloys," **Metals**, vol. 13, no. 1, p. 111, 2023.
11. C. Fu *et al.*, "Realizing high figure of merit in heavy-band p-type half-Heusler thermoelectric materials," **Nat. Commun.**, vol. 6, Art. no. 8144, 2022.
12. S. Yin *et al.*, "Enhanced thermoelectric performance in $TiFeCu_xSb$ half-Heusler alloys," **J. Materiomics**, vol. 10, 2024.
13. Y. Pei, H. Wang, and G. J. Snyder, "Band engineering of thermoelectric materials," **Adv. Mater.**, vol. 24, no. 46, pp. 6125–6135, 2021.
14. "Enhanced thermoelectric performance in $Mg_{1-x}Ti_xNiSb$ quaternary half-Heusler alloys," **ACS Appl. Energy Mater.**, vol. 7, 2024.
15. R. He *et al.*, "Achieving high thermoelectric performance in n-type half-Heusler materials through nanostructuring," **Adv. Energy Mater.**, vol. 11, no. 15, 2022.
16. "Entropy-stabilized half-Heusler alloys for thermoelectric applications," **Phys. Chem. Chem. Phys. (PCCP)**, 2025.
17. "Electronic and thermoelectric properties of ZrPtSn half-Heusler compound," **J. Mater. Res.**, 2025.