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Advances in Materials Innovations in Half Metallic Heusler Alloys for Structural Magnetic and Energy Spintronic Technologies

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Abstract: Half-metallic Heusler alloys are promising materials for spintronic and thermoelectric applications. These alloys exhibit metallic conductivity in one spin direction while acting as insulators in the opposite spin direction, enabling nearly 100% spin polarization. This property is crucial for spintronic devices such as magnetic tunnel junctions (MTJs), magnetic random-access memories, and spin-based transistors. This study investigates the electronic, magnetic, and structural properties of Heusler alloys, focusing on their synthesis methods, atomic ordering, and modelling via density functional theory (DFT). DFT-based calculations serve as a key tool for predicting band structures, spin polarization, and magnetic properties. Additionally, the effects of disorder, strain, and compositional changes on material properties are analysed to explore performance optimization strategies. The potential applications of Heusler alloys in spintronic memory devices, thermoelectric energy conversion, and quantum technologies are also discussed. This work is presented as a review article and systematically compiles and interprets findings from the existing literature to provide a broad understanding of the topic. By integrating theoretical and experimental approaches, this study provides a comprehensive overview of the role of these materials in advanced technological applications.

Key words: Half-metals, Heusler alloys, spintronics, magnetic properties, density functional theory.

Malzeme Biliminde Gelişmeler Yarı Metalik Heusler Alaşımlarının Yapısal Manyetik ve Enerji Spintronik Teknolojilerindeki Yenilikler

Öz: Yarı metalik Heusler alaşımları, spintronik ve termoelektrik uygulamalar için büyük potansiyele sahip malzemelerdir. Bu alaşımlar, bir spin yönünde metalik iletkenlik gösterirken diğer spin yönünde yalıtkan gibi davranarak %100'e yakın spin kutuplaşması sağlar. Bu özellik, manyetik tünel eklemleri (MTJ'ler), manyetik rastgele erişimli bellekler ve spin bazlı transistörler gibi spintronik cihazlar için kritik öneme sahiptir. Bu çalışma, Heusler alaşımlarının elektronik, manyetik ve yapısal özelliklerini inceleyerek üretim yöntemleri, atomik düzenlenme ve yoğunluk fonksiyonel teorisi (DFT) ile modellenmesine odaklanmaktadır. DFT tabanlı hesaplamalar, bant yapıları, spin kutuplaşması ve manyetik özelliklerin tahmin edilmesinde önemli bir araçtır. Ayrıca, düzensizlik, gerilim ve bileşim değişimlerinin malzeme özellikleri üzerindeki etkisi analiz edilerek performans optimizasyonu stratejileri ele alınmaktadır. Heusler alaşımlarının spintronik bellek cihazları, termoelektrik enerji dönüşümü ve kuantum teknolojilerinde kullanım potansiyeli değerlendirilmektedir. Teorik ve deneysel yaklaşımların birleştirilmesiyle, bu malzemelerin ileri teknoloji uygulamalarındaki rolüne dair kapsamlı bir bakış sunulmaktadır.

Anahtar kelimeler: Yarı metaller, Heusler alaşımları, spintronik, manyetik özellikler, yoğunluk fonksiyonel teorisi.

1. Introduction

n half-metals, one spin channel is metallic, while the opposite is gapped (semiconducting/insulating). In the ideal, defect-free bulk at 0 K, this can yield 100% spin polarization of the density of states (DOS) at the Fermi level. However, experimental spin polarization is usually reduced by disorder, finite-temperature effects, surface and interface states, spin–orbit coupling, and measurement techniques [1-3]. Heusler alloys (X_2YZ or XYZ) are prominent examples, combining half-metallicity and ferromagnetism, where one spin channel is metallic and the other insulating. This unique property enables spin-polarized currents, making them attractive for spintronic devices such as sensors, magnetoresistance (MR) devices, and spin-based transistors [1, 2, 4-6]. For instance, MR devices utilize half-metals for precise magnetic field detection and data storage [5, 7, 8].

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The development of half-metals began with the discovery of Heusler alloys by Friedrich Heusler in 1903 [9]. Their remarkable ability to exhibit ferromagnetism, even when constituent elements are non-ferromagnetic, sparked intense research. Early examples such as Cu_2MnSn and Cu_2MnAl guided studies toward binary, ternary, and quaternary systems. In 1983, Groot and colleagues introduced the concept of half-metallic ferromagnetism, demonstrating that certain materials could conduct electrons in only one spin orientation [10, 11]. This breakthrough opened new research avenues in spintronics and materials science.

Today, Heusler alloys with high spin polarization and Curie temperatures are considered promising for advanced technologies including MR devices, thermoelectric conversion, and magnetic cooling [1, 2, 6, 12]. An important reference in this field is the book compiled by Felser and Hirohata, which provides a comprehensive overview of their theoretical foundations, structural and functional properties, and device applications [10, 13]. Topics covered include giant magnetoresistance (GMR) effects, magnetic tunnel junctions (MTJs), spin valves, and thermoelectric energy conversion [14-17].

Heusler alloys derive their versatility from adjustable composition and electronic structure. Their physical properties are strongly dependent on crystal structure and atomic arrangement [1]. Most half-metals crystallize in FCC superlattice ($L2_1$) or BCC unit cells (B2) [18], while martensitic structures such as L10, 10M, or 14M can appear at low temperatures [19, 20]. These transformations influence magnetic and thermal properties. Furthermore, controlling the valence electron concentration via atomic positioning enables tailoring for specific applications [21].

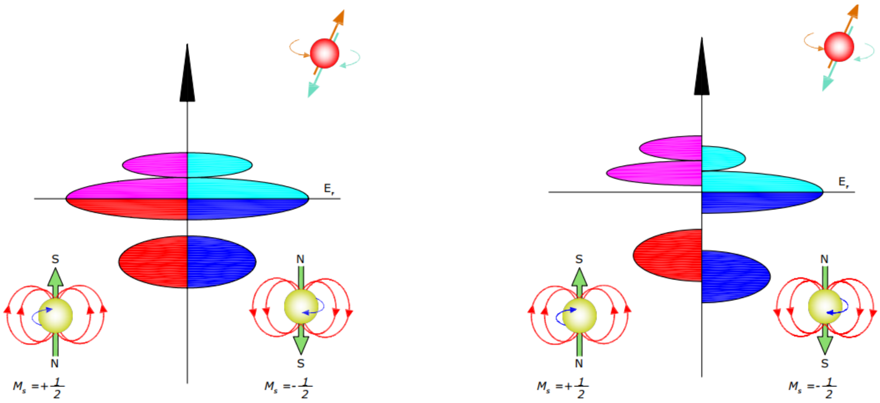
Co_2MnSi and similar alloys, with nearly 100% spin polarization, are optimal for GMR devices and MTJs, boosting sensitivity and storage performance [2, 6-8]. The DOS at the Fermi level is high for one spin channel and negligible for the other, enabling efficient spin-polarized currents. In thermoelectric, compounds like TiNiSn exhibit favorable figures of merit (ZT) by combining low thermal and high electrical conductivity. Doping or substitution strategies can further enhance the Seebeck coefficient, boosting waste heat recovery and solid-state cooling [22-24].

Overall, controlling the chemical, structural, and electronic properties of Heusler alloys remains a key research priority [21, 25]. Therefore, this study aims to evaluate the potential of these materials in spintronic, magnetic storage, and thermoelectric applications. The focus will be on their electronic, magnetic, and structural properties, complemented by an examination of production methods, structural stability, and DFT modelling. By combining theoretical and experimental approaches, this work seeks to build a solid foundation for advancing future technologies and guiding subsequent research on half-metallic alloys.

2. Half-Metallic and Magnetic Properties of Heusler Alloys

Half-metallic materials are classified by the nature of their band gap, which governs their magnetic and electronic behaviors. Three main categories exist: covalent band gaps, where magnetism and half-metallicity usually exclude each other; charge transfer band gaps, typically found in complex oxides; and d–d band gaps, originating from d-orbital interactions [26]. Heusler alloys, including semi-Heusler alloys such as NiMnSb, belong to the third group [27]. They are crucial for spintronics, existing as full Heuslers (X_2YZ, $L2_1$ structure) [5, 28] and half-Heuslers (XYZ, $C1_b$ structure) [12], with structure strongly affecting properties [1]. Half-metallicity arises from a spin-selective band gap, yielding nearly 100% spin polarization, though disorder and defects can reduce it [26, 29].

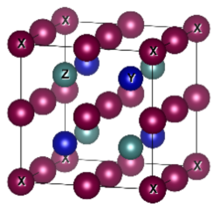
The magnetic properties of Heusler alloys are particularly noteworthy [12, 30]. These materials are typically ferromagnetic or ferrimagnetic with high Curie temperatures [14]. According to the Slater-Pauling rule, their magnetic moments are related to the number of valence electrons. For instance, YFeCrZ alloys (where Z = Al, Sb, Sn), exhibit a total magnetic moment of 2.00 μB, while Co_2TiSn shows a magnetic moment of around 1.92 μB [30, 31]. Magnetic moments and Curie temperatures are closely related to the alloy composition and atomic arrangement [14, 28]. Martensitic transformations modify crystal structure and magnetic properties, enabling effects like the magnetocaloric effect for cooling applications [21, 31]. Low magnetic damping is crucial for spintronics. In Co_2FeAl, damping decreases with higher B2 ordering due to reduced electron density at the Fermi level, while Co_2MnSi also shows low damping, suitable for high-frequency devices. Overall, classifying half-metals and examining Heusler alloys clarifies their potential in advanced applications such as spintronics and magnetic cooling [7]. Table 1 illustrates the diverse Curie temperatures and band gaps of Heusler alloys. For instance, NiMnSb has a Curie temperature of ~730 K with a band gap of ~0.5 eV, while Fe-doped CoTiSb reaches 700 K with a ~0.95 eV band gap. These variations demonstrate how composition affects their electronic and magnetic properties [32]. Martensitic transformations in some Heusler alloys modify magnetic behavior and allow magnetocaloric cooling. Moreover, low damping in alloys like Co_2FeAl and Co_2MnSi makes them suitable for spintronic devices [33]. Understanding these properties enhances their potential in spintronics, magnetic cooling, and other advanced technological applications. Spintronic devices transmit information not only through the electron’s charge but also via its spin, which can assume two values (± ½). Figure 1 schematically illustrates the concept of spin resolved. In Figure 1(a), a conventional metal is shown, where the spin-up and spin-down channels are symmetric and equally occupied. In contrast, Figure 1(b) depicts a half-metallic ferromagnet (HMF), in which one spin channel exhibits metallic conductivity while the other is separated by a band gap. This behaviour enables the realization of full spin polarization (theoretically 100%), making HMFs an ideal class of materials for spintronic applications. The N–S arrows schematically represent the magnetic moment orientations of spin-up and spin-down states [34, 35]. Due to their high Curie temperatures and wide compositional diversity, Heusler alloys are strong candidates for realizing half-metallic ferromagnetism in spintronics.



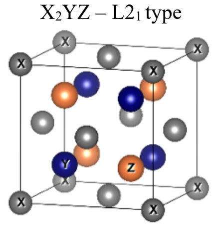
(a) (b)

Figure 1. Spin-resolved DOS: (a) in a metal, both spin channels are symmetric and equally occupied; (b) half-metallic ferromagnet [35, 36].

Table 1. Crystal structure, magnetic and electronic properties of $L2_1$ and $C1_b$ Type Heusler Alloys [23, 24, 26, 31, 34, 37-66].



X_2YZ – $L2_1$ type



XYZ – $C1_b$ type

Chemical Formula	Curie Temp. (K)	Band gap (eV)
Co_2FeAl	985-1014	~0.4
Co_2FeSi	1100	~0.094
Co_2MnSi	1000-1120	~0.8
Co_2MnGe	883	0.34-0.39
Co_2CrAl	330-340	0.475
Co_2CrGa	488	0.5
Co_2FeGe	1054	0.87-1.56
Co_2MnSn	829	0.35
Co_2MnSb	1109	0.60-1.20
NiMnSb	~730	~0.5
CoTiSb	700 (Fe addition)	~0.95
FeVSb	58-75	~0.36

Among Heusler alloys, Co_2FeSi and Co_2MnSi are distinguished by their Curie temperatures above 1000 K and high spin polarizations; however, their experimental polarization remains below the ideal values, and their thermoelectric efficiencies are quite low [13, 37, 38]. Co_2TiSn and Co_2TiGe, which have lower Curie temperatures, provide a spin polarization of around 63–64% [57]. NiMnSb has a Curie temperature of approximately 730 K and exhibits moderate thermoelectric performance [67].

3. Production Methods of Half-Metals

Production methods are critical for half-metallic alloys, as controlling atomic arrangement, structure, and phases during synthesis optimizes their magnetic, electronic, and mechanical properties. Arc melting is widely used to produce high-purity, homogeneous Heusler alloys by melting components under an electric arc in inert gas, preventing oxidation. It ensures uniform composition even for complex quaternary alloys like CoFeMnZ (Z = Al, Ga, Si, Ge), with multiple remelting cycles improving homogeneity. While effective, it often yields coarse grains, requiring post-annealing to refine microstructure and optimize properties [1].

Melt spinning is widely used to produce Heusler alloys as ribbons by ejecting molten alloy onto a fast-rotating wheel, achieving cooling rates of 10^5–10^6 K/s. This rapid solidification forms metastable phases and nanocrystalline or amorphous structures, enhancing mechanical strength and magnetic softness. Ribbon thickness (10–100 µm) depends on wheel speed and melt pressure. The method is valuable for magnetic cooling applications, though internal stresses from rapid cooling often require annealing for stabilization [1, 68].

Sputtering is widely used to deposit thin films of half-metal alloys for spintronic applications. By bombarding a target with high-energy ions, atoms are ejected and deposited on a substrate, enabling epitaxial films with precise thickness and composition. It is key for fabricating multilayers in MTJs, where interface control ensures high tunnel magnetoresistance (TMR). Film properties depend on parameters like substrate temperature, gas pressure, and power, though issues such as target poisoning and non-uniform deposition require optimization [14].

Ball milling and high-pressure methods are used to tailor half-metal alloys. Ball milling refines particle size and promotes atomic-level alloying, yielding nanostructured or amorphous Heusler alloys with enhanced magnetic and mechanical properties, governed by milling time, ball-to-powder ratio, and atmosphere. High-pressure techniques (>1 GPa), such as torsion or hot pressing, enhance density, stabilize new phases, and modify electronic and magnetic behavior. While effective, both methods require careful control to avoid defects or contamination [1]. Thermal treatments, especially annealing at 500–1000 °C, optimize half-metal alloys by enhancing atomic order, controlling phase transformations, and relieving stresses. In Heusler alloys, structures like B2 and $L2_1$ critically affect properties, with $L2_1$ often giving higher spin polarization for spintronics. Precise control of annealing conditions is vital to avoid unwanted phases or grain growth, ensuring stability and performance [2]. Half-metals are of great interest in spintronics for their metallic conductivity in one spin channel and insulating behavior in the other, yielding nearly 100% spin polarization. This enables high TMR in MTJs and is frequently observed in intermetallic such as Heusler alloys [21]. The production method of half-metal alloys depends on application and desired properties; for thin films in spintronics, sputtering and MBE are preferred for precise control of thickness and composition [69, 70]. For bulk production in applications like magnetic cooling, arc melting provides high-purity alloys, while melt spinning refines microstructure and improves magnetic properties [68, 71].

As shown in Table 2, production methods such as epitaxial growth, sputtering, arc melting, melt spinning, and ball milling each uniquely influence the structural, magnetic, and electronic properties of Heusler alloys [1, 12, 21, 31, 43].

Table 2. Production methods and properties of Heusler alloys.

Production Method	Advantages	Disadvantages	Material Properties
Epitaxial Growth	High-quality thin films, smooth interfaces, excellent epitaxial plane matching [1]	May be more costly and time-consuming.	MR values reach 200% at room temperature and 380% at 5 K. The $L2_1$ structure forms above 450 °C, providing high spin polarization [1]
Sputtering	Common and versatile method for thin film production.	Compared to epitaxial growth, the films may show lower quality and increased atomic disorder [12]	Giant tunnel MR of up to 330% at room temperature in Co_2FeAl/MgO/CoFe MTJs [1]. In Co_2CrAl, Cr–Al disorder maintains high spin polarization (97% in $L2_1$, 93% in B2), whereas Co–Cr disorder rapidly destroys half-metallicity [12]
Arc Melting	Suitable for the production of bulk materials [12].	It may be difficult to obtain a homogeneous structure.	Materials with high Curie temperature can be obtained [31, 43]
Melt Spinning	Metastable phases can be obtained thanks to rapid cooling [21].	Production parameters may be difficult to control [21].	Martensitic transformation and magnetic properties can be investigated in Ni-Mn based Heusler alloys [21].
High-Energy Ball Milling	It can be used to produce nanostructured materials.	Long-term milling can cause the formation of unwanted phases.	In the Fe_2CrGa alloy, an increase in magnetization due to disorder has been observed.

4. Electronic Magnetic and Thermoelectric Applications

Heusler alloys, characterized by high spin polarization, tunable magnetic properties, and structural stability, are promising candidates for advanced technologies. Half-metallic Heusler's can act as spin-polarized current sources, as they exhibit nearly 100% spin polarization of carriers at the Fermi level. Spin polarization is defined as the ratio of spin-up ($N_\uparrow$) to spin-down ($N_\downarrow$) electrons, as expressed in Equation 1 [72, 73].

$$P = \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow} \tag{1}$$

This parameter ranges from –1 to +1, describing the degree of alignment of conduction electron moments in ferromagnetic materials [74]. Such properties provide advantages in spintronic devices, including magnetoresistive random-access memory, spin-transfer torque systems, and spin-LEDs. Full Heusler alloys such as Co_2FeSi, Co_2MnSi, Co_2MnGe, and Co_2FeAl, as well as half-Heusler's like NiMnSb, are predicted to show half-metallicity [67, 75-77]. However, atomic disorder and interface defects reduce efficiency, particularly in spin injection [77].

Beyond spintronics, Heusler alloys are strongly investigated as thermoelectric materials. Half-Heusler's with 18 valence electrons follow the Slater–Pauling rule, producing a tunable band gap (0–4 eV) that depends on orbital hybridization, lattice parameters, and electronegativity differences of constituent elements. Compounds such as NiTiSn and CoTiSb exhibit semiconducting behavior with band gaps around 0.4 eV, enabling efficient charge transport [61, 78, 79]. In recent years, certain Heusler compounds, such as LuPtBi, have been found to exhibit topological insulator (TIs) properties. TIs are quantum states of matter characterized by an insulating bulk band gap and topologically protected gapless surface or edge states, driven by band inversions in their electronic structure. Notably, Heusler alloys containing rare-earth elements, such as LnPtBi (Ln = Nd, Sm, Gd, Tb, Dy), offer opportunities for multifunctional materials that combine topological properties with magnetism and, in some cases, superconductivity. For example, volumetric magnetism has been observed in compounds like LnPtBi.

These unique properties are of great importance for the development of next-generation electronic devices [80-82]. Thermoelectric performance is quantified by the dimensionless figure of merit, as given Equation 2.

$$\mathrm{ZT} = \left(\frac{S^2\sigma}{\kappa}\right) \tag{2}$$

where S is the Seebeck coefficient, σ is the electrical conductivity, κ is the thermal conductivity, and T is the absolute temperature. High ZT values, as in TaFeSb-based alloys and (Ti/Zr/Hf)NiSn systems, indicate excellent waste-heat recovery and energy conversion performance [83, 84]. Their mechanical robustness and thermal stability provide further advantages in thermoelectric generators and cooling devices.

Recent studies have revealed that certain Heusler compounds display topological insulator behavior, characterized by insulating bulk states and topologically protected surface states. Materials such as HgTe and LnPtBi (Ln = Nd, Sm, Gd, Tb, Dy) show band inversion and multifunctional properties, combining magnetism and superconductivity [82].

In energy storage, Heusler alloys are also investigated as electrode materials for lithium-ion batteries. For instance, CoMnSi gains metallic character upon lithium insertion, improving voltage and capacity, while LiMnSi reduces volume changes during cycling [85].

Furthermore, Ni–Mn-based Heusler alloys can undergo martensitic transformations, enabling both shape memory behavior and significant magnetocaloric effects, making them attractive for solid-state magnetic cooling [1, 6, 7, 21]. Alloys such as Co_2MnGe and Co_2FeSi exhibit high Curie temperatures and low damping, which are advantageous for high-frequency spintronic devices [86]. However, atomic disorder remains a critical limitation: in Co_2MnSi and Co_2MnAl, Co antisite defects drastically reduce spin polarization, while Mn–Si mixing has a milder effect. In Co_2FeSi, B2 and $D0_3$ disorder identified by XRD measurements strongly influence surface spin polarization [5, 12, 67, 87].

Overall, Heusler alloys combine half-metallicity, adjustable electronic structures, martensitic transformations, and durability, making them versatile candidates for spintronics, thermoelectric, magnetic cooling, shape memory, and energy storage. Ongoing research focuses on reducing structural disorder, designing new compositions, and optimizing thermoelectric efficiency to enable next-generation energy-efficient devices [1, 82, 87, 88].

5. Density Functional Theory in the Modelling of Half-Metallic Alloys

DFT is a key quantum mechanical method for calculating ground-state properties from electron density and is widely used to study half-metals. These materials show metallic behavior in one spin channel and insulation in the other, leading to 100% spin polarization ideal for spintronic devices [86, 87, 89-91]. DFT assumes that a system's total energy is a functional of electron density, enabling a simpler density-based approach instead of solving many-electron equations. The Kohn–Sham equations are solved to obtain the electron density and electronic structure, with the exchange-correlation functional approximating electron–electron interactions [89-91]. In some cases, the Hubbard U correction is applied to better model electron interactions in the d and f orbitals of transition metals and f-elements [86, 92]. DFT calculations are a powerful tool for analyzing material properties, particularly structural stability, by comparing the total energies of different crystal structures [89]. For example, it has been shown that $MAlO_3$ (M=Ce, Pr) perovskites are more stable in the cubic structure [91], XCrSb (X=Ti, Zr, Hf) half-Heusler alloys are more stable in the ferromagnetic (FM) phase [89], and the stable structures of Mn_2ScZ (Z=Si, Ge, Sn) Heusler alloys have been optimized [92]. Such structural analyses provide important insights into the durability and application potential of materials [89]. DFT reveals electronic and magnetic properties of half-metals through band structures and DOS. In half-Heusler alloys such as XCrSb (X = Ti, Zr, Hf) and XCaB (X = Li, Na, K, Rb), the spin-up channel is metallic while the spin-down channel is semiconducting, resulting in nearly 100% spin polarization. DFT also predicts magnetic moments that vary with structure and composition—for instance, ~3 μB in XCrSb and ~2 μB in XCaB, consistent with the Slater–Pauling rule, which links magnetic moments to valence electron counts. Additionally, other material classes, such as cubic perovskites like $CeAlO_3$ (~1 μB) and $PrAlO_3$ (~2 μB), exhibit similar half-metallic behavior, though their structural and chemical properties differ significantly from Heusler alloys [87, 89-91]. As shown in Table 3, DFT has been widely applied to study the spin-resolved band structures of Heusler alloys such as XCrSb (X = Ti, Zr, Hf), Mn_2ScSi, and Co_2YZ (Z = P, As, Sb, Bi), confirming their half-metallic and ferromagnetic properties [86, 87, 89].

Table 3. Spin-up and spin-down band structures of Heusler alloys obtained by DFT modelling.

Alloy	Method	Spin-Up Band Structure	Spin-Down Band Structure	Results
XCrSb (X=Ti,Zr,Hf)	Spin-polarized DFT (GGA)	Exhibits half-metallic character [1, 26, 30]	Has narrow energy ranges	XCrSb (X = Hf, Ti, Zr) half-Heusler alloys show mechanical and thermodynamic stability with ~3 μB magnetic moments, making them promising for spintronic applications [89].
Mn_2ScSi	DFT + U or SCAN [31]	Majority-spin bands show a gap at EF, whereas minority-spin bands display multiple crossings at the Fermi level	Transition from metallic to half-metallic behaviour is observed	Mn_2ScSi exhibits a low-magnetic half-metallic state at small lattice volumes and a high-magnetic metallic state at larger volumes [30]
Co_2YZ (Z = P, As, Sb, Bi)	FP-LAPW+lo (GGA+U) [86]	Exhibits half-metallic ferrimagnetism in the stable ferromagnetic phase [86].	Exhibits half-metallic ferrimagnetism in the stable ferromagnetic phase [86].	Co_2YZ alloys (Z = P, As, Sb, Bi) show half-metallic ferrimagnetism in the stable ferromagnetic phase [30].
CoYCrZ (Z = Si and Ge)	(DFT, GGA) [87]	Exhibits half-metallic (HM) behavior for structure type II [87]	Exhibits half-metallic (HM) behaviour for structure type II [87]	CoYCrZ (Z = Si, Ge) alloys exhibit type-II half-metallicity with 100% spin polarization [30]
NiMnSb	FSKKR [40]	An energy gap is observed for the majority spin channel [31]	Several band crossings are found at the energy level (EF) for the minority spin channel [31, 40]	In a calculation involving the spin polarization of NiMnSb, the density contributions in the Ni region are specified [26].
Co_2FeSi	LDA+U [77]	In the $L2_1$ phase, the majority sub-band shows finite density at the Fermi level [77]	In the $L2_1$ phase, the minority sub-band has no states at the Fermi level, indicating half-metallicity [77]	DOS for the $L2_1$ and B_2 phases of Co_2FeSi is shown. It is stated that the $L2_1$ phase is a half-metal [26]
Co_2MnAl, Co_2MnGa, Co_2MnSi, Co_2MnGe	FSKKR [40]	The spin-up density shows a large peak just below the Fermi level [40]	It has an indirect band gap, with the valence band maximum at Γ and the conduction band minimum at another k-point [40]	Spin-resolved densities show that Co_2MnAl, Co_2MnGa, Co_2MnSi, and Co_2MnGe are half-metals with small spin-down gaps [5].

According to DFT studies, Co_2FeSi has an energy gap in the spin-down channel while exhibiting conductivity in the spin-up channel. This gap has been calculated to be in the range of approximately 0.4–0.6 eV, and the total magnetic moment is approximately 6 μB [38, 43]. Although a 100% spin polarization is theoretically predicted, a lower value has been reported in experimental data due to surface disorders and thermal effects [37].

Co_2TiGe and Co_2TiSn alloys exhibit half-metallic or semiconductor-like properties, with narrow band gaps observed in the spin-down channel. The magnetic moments of these alloys are approximately 1.8–2.0 μB, while their experimental spin polarizations have been found to be at levels of ~0.63–0.64 [57]. In general, full Heusler alloys with an ideal crystal structure exhibit high spin polarization and half-metallic behavior.

6. Conclusions

This study examines half-metallic materials, particularly Heusler alloys, which combine high spin polarization and Curie temperatures for spintronic and thermoelectric uses. Their spin-dependent conductivity enables MTJs, magnetic storage, and energy conversion. Processing methods such as arc melting, sputtering, and ball milling affect atomic order, while disorder reduces half-metallicity.

This review highlights relationships how production methods (arc melting, melt spinning, sputtering) affect the structural and electronic properties of Heusler alloys. By combining DFT modelling with experimental insights, it links spin polarization, Curie temperature, and band gap to structure–property–performance correlations. Comparative analyses of alloys like NiMnSb, Co_2FeSi, and high-ZT half-Heusler's (e.g., NiTiSn, TaFeSb) provide new perspectives for multifunctional material design, underscoring the potential of Heusler alloys for advanced applications. Future research should optimize Heusler alloys like Co_2FeSi and NiMnSb for spintronics via improved semiconductor interfaces and enhance half-Heuslers such as NiTiSn and TaFeSb through doping to increase ZT for waste heat recovery. Ni–Mn-based alloys merit further study for magnetocaloric and shape memory uses, while quaternary (CoFeMnZ) and rare-earth Heuslers (LnPtBi) hold promise for multifunctional applications. Combining DFT with experimental validation will advance tailored, energy-efficient Heusler alloys

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