

First Principle Study of Electronic Structure, Magnetic and Linear Properties of CoFeSi Half Heusler Alloys

¹Sambo, Jamaludeen ²Adam A. Usman ²Benson J. Yerima

¹Department of Pure and Applied Physics Faculty of Science Gombe State University PMB 127, Gombe, Nigeria.

²Department of Physics Modibbo Adama University Yola

*Corresponding authors' email: sambojamaludeen@gsu.edu.ng

ABSTRACT

This research provides an in-depth first principle analysis of the electronic, magnetic, and linear optical characteristics of the CoFeSi half-Heusler alloy. Utilizing Density Functional Theory (DFT) within the Quantum ESPRESSO environment and applying the PBE-GGA exchange-correlation functional, the study examines the material's fundamental physics. CoFeSi is found to settle into a hexagonally distorted structure after relaxation with optimized lattice dimensions of $a = b = 5.59 \text{ \AA}$ and $c = 6.95 \text{ \AA}$. The electronic data indicates a standard metallic ferromagnetic state, characterized by a saturation magnetization of $5.53 \mu\text{B}$ and a total magnetic moment of $4.89 \mu\text{B}$. Notably, the calculated spin polarization of roughly 15% suggests that the alloy does not exhibit complete half-metallicity. The Density of States is finite at the Fermi level in both spin channels indicating a spin polarized behaviour, while the projected Density of states shows that the dominant contribution is from Co and Fe 3d orbitals, while Si/p states contributes less. Optical assessments across a 0–10 eV spectrum highlight a maximum absorption near 8 eV ($\sim 10^6 \text{ cm}^{-1}$), a peak refractive index of 2.80 at 2 eV, and a static extinction coefficient of approximately 9.20. With an optical conductivity peaking at $3150 \Omega^{-1}\text{cm}^{-1}$ and a real dielectric function near -83 , while imaginary dielectric function reached a peak at 0eV, which indicates potentials of CoFeSi for tunable spintronics optoelectronics and plasmonic applications

Received: 12 May 2026

Accepted: 25 May 2026

Published: 07 Sept. 2026

Keywords: Density functional theory, Quantum ESPRESSO, Spintronics

INTRODUCTION

Heusler alloys represent a versatile family of intermetallic materials that have attracted sustained research interest because of their unique electronic, magnetic, and transport characteristics. The field originated with the discovery of ferromagnetism in the Cu_2MnAl compound by Friedrich Heusler in 1903, demonstrating that strong magnetic behavior could arise from elements that are individually non-magnetic in their pure states (Elphick et al., 2021). Since then, Heusler compounds have become an important focus in condensed matter physics and materials science. Depending on their atomic arrangement, they are commonly classified as full-Heusler (X_2YZ) or half-Heusler (XYZ) alloys and have been explored for a wide range of applications, including spintronic devices, magnetic storage systems, thermoelectric energy conversion technologies, and magneto-optical components (Hirohata & Takanashi, 2014).

Within this class of materials, CoFeSi has gained increasing attention due to its favorable combination of magnetic performance, structural robustness, and potential spin-polarized transport behavior. Earlier studies on Co-based Heusler alloys have reported strong ferromagnetic ordering, elevated Curie temperatures, and compatibility with existing semiconductor technologies, features that make them attractive for advanced electronic and spin-dependent applications (Hamaya & Yamada, 2022). In CoFeSi, the presence of silicon plays a significant role in shaping the interaction between the Co and Fe electronic states. Such interactions can alter the distribution of electronic states near the Fermi level and consequently influence both the magnetic and electronic characteristics of the material.

Considerable theoretical and experimental efforts have been devoted to understanding the physical properties of Co-based

Heusler systems because their functionality is closely linked to their electronic structure and optical behavior. Although several investigations have addressed selected aspects of CoFeSi, studies that provide a unified description of its structural, electronic, magnetic, and optical properties from first-principles calculations remain relatively scarce. As a result, important relationships among these properties are not yet fully understood, limiting a comprehensive evaluation of the material's suitability for emerging technological applications.

A detailed assessment of these characteristics is essential for identifying materials capable of meeting the demands of future electronic and photonic technologies. In particular, knowledge of the electronic band structure, magnetic response, and interaction with electromagnetic radiation is critical for predicting the performance of materials intended for spintronic architectures, magnetic sensing devices, and optoelectronic systems. Therefore, an in-depth theoretical investigation of CoFeSi can provide valuable information for materials design and facilitate the development of functional devices with enhanced efficiency and performance.

In this study, Density Functional Theory (DFT) calculations employing the Perdew–Burke–Ernzerhof generalized gradient approximation (PBE-GGA) are performed to examine the structural, electronic, magnetic, and linear optical properties of the CoFeSi half-Heusler alloy. The analysis includes equilibrium structural parameters, spin-resolved electronic band structures, density of states, magnetic moments, dielectric response, refractive index, absorption coefficient, extinction coefficient, and optical conductivity. Through this comprehensive investigation, the present work seeks to clarify the fundamental physical behavior of CoFeSi

and evaluate its prospects for applications in spintronic, optoelectronics and magneto-optical technologies.

MATERIALS AND METHODS

The materials used in this study are categorized into two, the hardware and software. The hardware used was the use of a Dell workstation equipped with an Intel® Core™ i7-8750H processor, 16 GB of RAM, and a 64-bit Windows 10 operating system. The hardware platform provided the computational resources required for the first-principles calculations and subsequent data analysis. The primary software is Quantum ESPRESSO package, the calculations and data analyses were conducted using the computational package employed in this work using Density Functional theory (DFT) approach, the Perdew –Burke– Ernzerhof Generalized Gradient Approximation (PBE-GGA) exchange correlation functional was chosen as it balances accuracy and computational cost. The Brillouin zone was sampled using a 9×9×6 Monkhorst–Pack k-point mesh to ensure adequate representation of the electronic structure in reciprocal space. A plane-wave basis set was employed with a kinetic energy cut off of 90 Ry and the charge density of 1080Ry. The starting structure was constructed in a primitive setting with initial lattice parameters $a=4.420\text{Å}$ (angs) $b=3.434\text{Å}$ (angs) and $c=4.921\text{Å}$ (angs), and the use of ultrasoft and projector augmented wave (PAW) pseudo potentials to balance speed and accuracy. The structure was fully relaxed via variable cell BFGS algorithm with no symmetry constraints, to allow the structure relax freely (ibrav=0). The convergence thresholds of 10^{-4}Ry for energy and 10^{-3}Ry/Bohr for forces were used. The starting structure based on primitive setting was orthorhombic and after full variable cell relax, the obtained total ground state energy was -17397.6 eV/fu . Optical properties were calculated using epsilon.x code, $18\times 18\times 12$ denser k point grid were used to ensure convergence of optical spectra, a total of 50 bands including both occupied and unoccupied states were used to account for interband transitions, a broadening parameter of 0.1eV was applied to simulate finite life time effects, local field effects were neglected due to the symmetry constraints, the intra band/Drude term was included with plasma frequencies. The diagonal components were computed along x, y, and z crystallographic directions as ϵ_{xxx} , ϵ_{yyy} and ϵ_{zzz} .

Firstly, self-consistent calculation (scf) was carried out before obtaining the relaxed structure followed by the variable cell relax and finally followed by non-self-consistent calculations to obtain spin-polarized band structure, density of states calculations for the investigation of magnetic properties. The linear optical properties which is based on DFT approach were also computed using the Quantum ESPRESSO based on the ground state data.

The ground-state electronic structure was obtained by solving the Kohn–Sham equation. The electronic structure calculations were based on the Kohn–Sham equation

$$\left[\frac{-\hbar^2}{2m} \nabla^2 + V_{\text{ext}} + \int \frac{\rho(r')}{|r-r'|} dr' + V_{\text{xc}}(r) \right] \psi_i(r) = \epsilon_i \psi_i(r) \quad (1)$$

where ψ_i and ϵ_i are the Kohn–Sham orbitals and

eigenvalues, respectively, the term $-\frac{\hbar^2}{2m} \nabla^2$ is the kinetic

energy operator for electrons, V_{ext} is the nuclei –electron

attraction potential, the term $\int \frac{\rho(r')}{|r-r'|} dr'$ is Hartree(

electron–electron) repulsion term and $V_{\text{xc}}(r)$ is the exchange correlation potential. The solution to such an equation to obtain eigen values and eigenfunction for the band structure and density of states was done using quantum ESPRESSO work flow non self consistently. (Harrison 2003) The total magnetic moment was evaluated from spin-polarized calculations according to

$$\mu = \int [\rho^\alpha(r) - \rho^\beta(r)] dr = N^\alpha - N^\beta \quad (2)$$

by integrating the difference between up spin density $\rho^\alpha(r)$ and down spin density $\rho^\beta(r)$, then N^α and N^β are numbers of spin up and spin down electrons respectively and these spin densities are solutions to the spin dependent Kohn Sham equations. (Laestadius 2014).

The spin polarization at the Fermi level was calculated as

$$P(\%) = \frac{N^\uparrow(E_F) - N^\downarrow(E_F)}{N^\uparrow(E_F) + N^\downarrow(E_F)} * 100\% \quad (3)$$

The terms $N^\uparrow(E_F)$ and $N^\downarrow(E_F)$ are the spin-resolved densities of states (DOS) of the majority and minority spin channels at the Fermi level, A value of 100% corresponds to ideal half-metallicity. (Ameur et, al 2025)

The optical properties were evaluated within the linear response formalism. The imaginary part of the dielectric function is given by:

$$\epsilon_2(\omega) = \frac{4\pi^2 e^2}{\Omega_{\text{uc}}} \sum_{\text{vc}} |\langle \Psi_{\text{ck}} | e \cdot \mathbf{v} | \Psi_{\text{vk}} \rangle|^2 \delta(E_{\text{ck}} - E_{\text{vk}} - \hbar\omega) \quad (4)$$

where Ω is the unit cell volume, Here the first term represents the summation over Valence (v) → Conduction (c) of the

Transition matrix elements $|\langle \Psi_{\text{ck}} | e \cdot \mathbf{v} | \Psi_{\text{vk}} \rangle|$ of the light–matter interaction and the kronecker Delta function terms enforces energy conservation.

The real part $\epsilon_1(\omega)$ is obtained via the Kramers-Kronig relation

$$\epsilon_1(\omega) = 1 + \frac{2}{\pi} P \int_0^\infty \frac{\omega' \epsilon_2(\omega')}{(\omega'^2 - \omega^2)} d\omega' \quad (5)$$

Here is real part (dispersion, energy storage), is imaginary part (absorption, energy loss), observation angular frequency, is Cauchy principal value and is constant as (3.1416)

The complex refractive index governs electromagnetic wave propagation inside a material (Sahar, et, al 2025) as

$$n = n(\omega) + ik(\omega)$$

and for extinction coefficient(k) it quantifies the attenuation of the electric field amplitude inside the material and appears directly in the wave propagation equation:

The absorption coefficient quantifies the exponential decay of electromagnetic intensity per unit distance inside the material. Once ω is known, the absorption coefficient (ω) which quantifies how intensely a material absorbs light at a given frequency is obtained by (Sahar et, al.2025)

$$\alpha(\omega) = \frac{2\omega k}{c} \quad (6)$$

The optical conductivity tensor, derived from the Kubo-Greenwood linear response formalism, connects the induced current density to the electric field:

The Kubo-Greenwood formalism is a linear response theory that connects microscopic electronic states of a material to its

$$\sigma_{\alpha\beta(\omega)} = \frac{2\pi e^2 \hbar}{V} \sum_{nmk} \frac{f_{nk} - f_{mk}}{\varepsilon_{mk} - \varepsilon_{nk}} \frac{\langle \psi_{nk} | v_\alpha | \psi_{mk} \rangle \langle \psi_{mk} | v_\beta | \psi_{nk} \rangle}{\hbar\omega - (\varepsilon_{mk} - \varepsilon_{nk}) + i\hbar} \quad (7)$$

The term $\sigma_{\alpha\beta(\omega)}$ is the complex conductivity tensor component along directions $\alpha \beta$, V is unit cell volume, e is electronic charge, $\hbar$ is reduced planks constant, ψ_{nk} and ψ_{mk} are the DFT Bloch wave function and energy of band n

macroscopic optical or electrical response. It expresses the frequency-dependent conductivity as a sum over electronic states The optical conductivity tensor in this formalism is given by (Demyanov et, al. 2023)as

at k-point k , v_α and v_β are velocity operators, f_{mk} and f_{nk} are the Fermi Dirac occupation levels, ω is the incident photon frequency, and η is a small broadening for numerical stability. Optical conductivity arises from quantum-mechanical transitions between electronic states, weighted by occupation, transition probability, and energy resonance.

RESULTS AND DISCUSSION

Table 1: Optimized Structural, Electronic, and Magnetic Properties of CoFeSi half Heusler Alloy

Source	a (Å)	b (Å)	c (Å)	E _g (eV)	Mag. Moment (μB)	Sat. Mag. (μB)	Spin Pol. (%)	Behaviour
This work	5.59	5.59	6.95	0	4.89	5.53	15	Ferromagnetic
Peshkhov,et al. (2022)	7.17	4.94	3.78	0.1	—	—	—	—
Ma et al. (2017)	5.36	5.36	5.36	—	—	—	—	—

Table 1 presents the optimized lattice constants obtained in this study using DFT within the PBE-GGA framework yielded parameters of $a = b = 5.59 \text{ Å}$ and $c = 6.95 \text{ Å}$ for CoFeSi, adopting a hexagonally distorted structure after full relaxation. Experimentally, Peshkhov et al. (2022) synthesized CoFeSi via arc melting and identified an orthorhombic structure (space group Pn-ma), while Ma et al. (2017) confirmed that the cubic C1b phase is thermodynamically less favorable, reporting a cubic lattice constant of 5.36 Å . The present in-plane value is approximately 4.3% larger than that of Ma et al. (2017), attributable to the difference in crystal symmetry between the hexagonally distorted structure obtained after full relaxation and the cubic reference. Band structure analysis revealed a zero band gap for CoFeSi, confirming metallic behavior consistent with the conducting nature commonly reported for Co-based Heusler alloys. The table also presents the calculated magnetic properties of CoFeSi half-Heusler alloy, including total magnetic moment, saturation magnetization, spin polarization, and magnetic ordering. CoFeSi exhibits ferromagnetic behavior, consistent with the established behavior of Co-based Heusler alloys. A total magnetic moment of $4.89 \mu B$ is obtained, driven by exchange splitting between majority and minority spin channels. *Ab-initio*

calculations on Co-based compounds demonstrate that the suppression of bands in the minority-spin channel at the Fermi level drives Slater-Pauling-type magnetic behavior for Heusler Alloys and supports high spin magnetic moments (Tas et al., 2023). Under the conventional Slater-Pauling rule, ($M_t = Z_t - 24$) the total magnetic moment scales linearly with the valence electron count as an integer value clamped by a strict half-metallic bandgap. However, the calculated saturation magnetization of $5.53 \mu B$ and the non-integer moment of $4.89 \mu B$ deviate slightly from this ideal configuration. A computed spin polarization of approximately 15% confirms partial polarization rather than true half-metallicity, revealing that minority-spin states remain active at the Fermi surface and interrupt full spin-filtering behavior. Heusler alloys have been both theoretically predicted and experimentally confirmed as promising spin sources due to their half-metallic nature, with spin polarization tunable through elemental substitution (Hirohata & Lloyd, 2022). High spin polarization in Heusler-based materials is critical for achieving large tunneling magnetoresistance ratios in magnetic tunnel junctions relevant to next-generation spintronic devices (Qu et al., 2024)

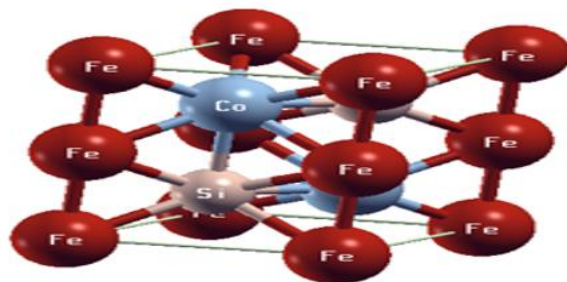


Figure 1: XCRYSDEN Visualization of Optimized Crystal Structures of CoFeSi (Left) half-Heusler Alloys, showing the C1b cubic Framework with Co (Blue), Fe (Dark Red), and Si(Brown) Sublattices

Figure 1 presents the optimized crystal structure of CoFeSi visualized using XCrySDen, confirming the formation of the hexagonal phase where sublattices occupied by Co, Fe, and Si, with one vacant site. Co occupies (0,0,0), Fe resides at $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$, and Si at $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$, an ordered arrangement crucial for half-metallicity and ferromagnetism (Galanakis et al., 2002). The present computational model assumes perfect atomic ordering with no site disorder, yielding idealized structural and electronic behavior superior to experimentally

synthesized samples where disorder typically reduces spin polarization (Feng et al., 2013). The hexagonally distorted unit cell obtained after full relaxation exhibits subtle anisotropic distortions along the z-direction that influence magnetic exchange interactions, electronic structure, and optical anisotropy (Chadov et al., 2017). This optimized structure forms the foundation for all subsequent analyses of CoFeSi.

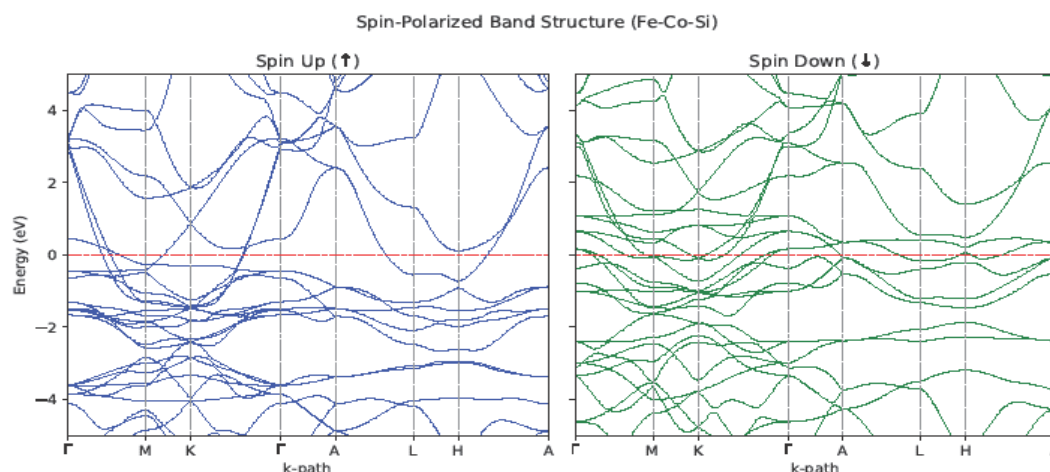


Figure 2: Spin-polarized Electronic Band Structure of the Ternary Half-Heusler Alloy CoFeSi (Left Panel) in the hexagonal Phase, Computed using Spin-polarized DFT-PBE-GGA, Plotted along the High-symmetry k-path of the hexagonal Brillouin zone

The band structure of CoFeSi in the hexagonal phase reveals metallic ferromagnetic behavior, characterized by a zero band gap and finite density of states at the Fermi level in both spin channels, confirming metallic conductivity. The spin-up bands are more dispersive near the Fermi level, indicating higher electron mobility, while the spin-down bands are relatively flatter, suggesting more localized electronic states. Despite this spin asymmetry, full half-metallicity is not achieved, and the material exhibits only partial spin polarization. The metallic nature of CoFeSi arises from strong

Co-Fe d-orbital hybridization and p-d interactions involving Si states, which promote band broadening and overlap, thereby suppressing the formation of a spin gap. These findings are consistent with results reported for related Co-based Heusler alloys (Peshkov et al., 2022; Saleem et al., 2022; Gurunani and Gupta, 2023). Consequently, CoFeSi is better suited for conventional magnetic and electronic applications, including magnetic sensors and conductive electrodes, rather than advanced spintronic devices requiring high spin polarization.

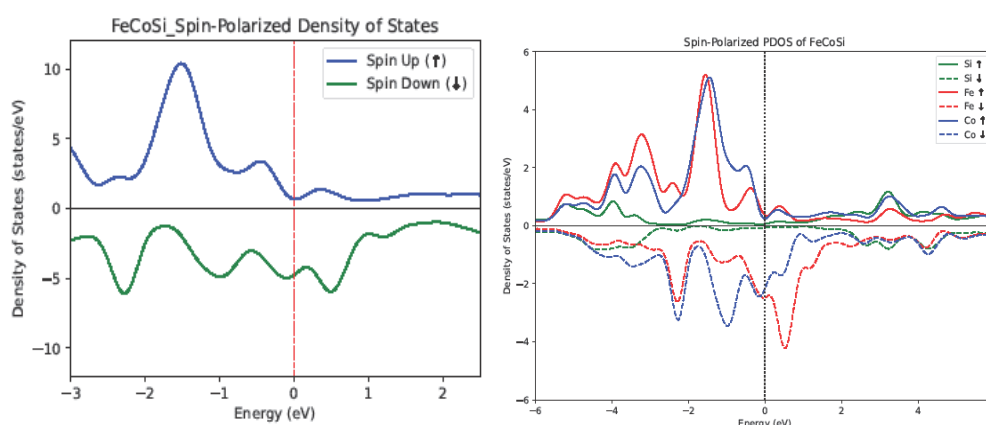


Figure 3: Spin-polarized Total Density of States (TDOS) Left Panel and Orbital-projected Partial Density of States (PDOS) right Panel of the Ternary half-Heusler alloy CoFeSi in the hexagonal phase, Computed using Spin-polarized DFT-PBE-GGA

The total and projected density of states (DOS) analysis of CoFeSi confirms its metallic ferromagnetic character, with finite states at the Fermi level in both spin channels, ruling out half-metallicity. A pronounced spin-dependent asymmetry is

observed, with the spin-up channel exhibiting a higher density of states at the Fermi level compared to the spin-down channel, generating a net magnetic moment consistent with itinerant ferromagnetism driven by exchange splitting of Co

and Fe 3d electrons (Wollmann et al., 2014;). The projected DOS reveals that Co and Fe 3d orbitals dominate the electronic structure near the Fermi level, where strong d-d hybridization broadens the energy bands and prevents complete spin-gap formation. Heusler alloys. Although Si p-states contribute minimally to conduction, p-d hybridization with Co and Fe d-orbitals redistributes states near the Fermi level and modifies band dispersion (Graf et al., 2011).

Consequently, CoFeSi exhibits partial rather than ideal spin polarization, similar to related systems such as Co₂FeSi and Co₂MnSi. Nevertheless, its proximity to a half-metallic transition suggests that structural modifications such as strain or chemical substitution could enhance spin polarization, making CoFeSi a promising candidate for tunable spintronic applications (Wollmann et al., 2014).

Table 2: Optical Absorption Coefficients of CoFeSi for in-plane (x) and Out-of-plane (z) Polarizations

Photon Energy (eV)	$\alpha_x (\times 10^6 \text{ cm}^{-1})$	$\alpha_z (\times 10^6 \text{ cm}^{-1})$	$\Delta\alpha = \alpha_z - \alpha_x (\times 10^6 \text{ cm}^{-1})$
0.0	0.220	0.200	-0.020
0.5	0.298	0.271	-0.027
1.0	0.371	0.338	-0.033
1.5	0.438	0.401	-0.037
2.0	0.500	0.460	-0.040
2.5	0.556	0.515	-0.041
3.0	0.608	0.568	-0.040
3.5	0.656	0.616	-0.039
4.0	0.700	0.660	-0.040
4.5	0.741	0.698	-0.042
5.0	0.778	0.732	-0.046
5.5	0.814	0.765	-0.049
6.0	0.850	0.800	-0.050
6.5	0.895	0.846	-0.049
7.0	0.944	0.899	-0.045
7.5	0.984	0.942	-0.042
8.0	1.000	0.960	-0.040
8.5	0.935	0.897	-0.038
9.0	0.759	0.726	-0.033
9.5	0.504	0.478	-0.027
10.0	0.200	0.180	-0.020

Table 2 provides the quantitative absorption coefficient values along different crystallographic directions. The data indicate that the in-plane absorption coefficients are consistently higher than the out-of-plane values for CoFeSi, confirming the anisotropic behaviour observed in Figure 4. The table further shows that CoFeSi exhibits slightly larger absorption across most of the investigated photon-energy range. This difference may be attributed to the suppression of states near the Fermi level present in CoFeSi, which reduces

the density of available electronic states near the Fermi level and consequently lowers the probability of optical transitions (Ricci et al., 2007). The high absorption coefficients reported in the table, on the order of 10^6 cm^{-1} , suggest that both materials can absorb significant amounts of incident light within very thin layers, making them attractive for photovoltaic, photodetectors, magneto-optical, and spin-photon applications (Buschow, 2001).

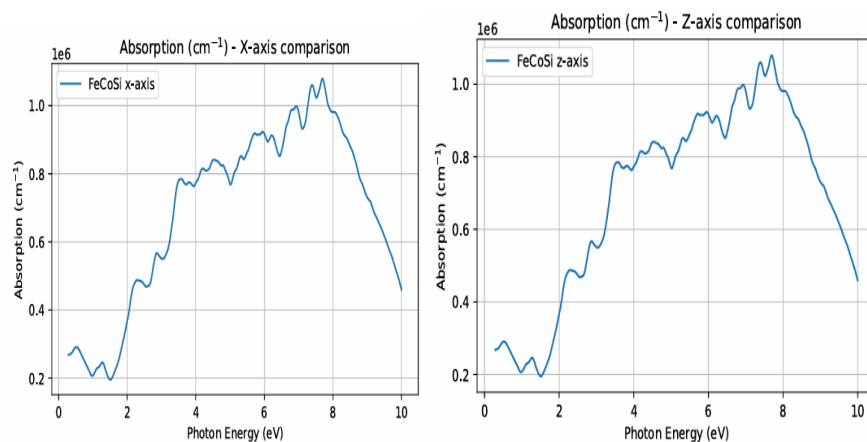


Figure 4 shows that CoFeSi half-Heusler alloys exhibit strong optical absorption throughout the visible and ultraviolet energy regions, with absorption coefficients reaching the order of 10^6 cm^{-1} . The presence of finite absorption at zero

photon energy confirms the metallic nature of both materials, arising from free-carrier intraband (Drude-like) transitions at the Fermi level, which are characteristic of metallic systems (Fox, 2010). As the photon energy increases, the absorption

coefficient rises steadily up to approximately 8 eV due to strong interband d–d and p–d electronic transitions involving Co and Fe d-states (Uvarov et al., 2012). Beyond this energy range, the absorption gradually decreases, which can be attributed to the reduction in the joint density of states and

lower transition probabilities at higher energies (Fox, 2010). The spectra also reveal anisotropic optical behaviour, with the in-plane and out-of-plane directions exhibiting different absorption responses, indicating directional dependence in the optical properties of alloy.

Table 3: Extinction Coefficient of CoFeSi Half Heusler Alloys for Inplane(x axis) and out of Plane (z axis) Polarization Directions

Photon Energy (eV)	$k_x(\omega)$	$k_z(\omega)$
0.00	11.40	11.40
0.20	9.20	9.20
0.40	7.00	7.00
0.60	4.80	4.80
0.80	3.00	3.00
1.00	2.10	2.10
1.20	1.95	1.95
1.40	1.50	1.50
1.60	1.30	1.30
1.80	1.55	1.55
2.00	1.90	1.90
2.20	2.15	2.15
2.40	1.95	1.95
2.60	1.85	1.85
2.80	1.80	1.80
3.00	1.95	1.95
3.20	1.80	1.80
3.40	2.10	2.10
3.60	2.20	2.20
3.80	2.00	2.00
4.00	1.90	1.90
4.20	1.90	1.90
4.40	1.85	1.85
4.60	1.80	1.80
4.80	1.70	1.70
5.00	1.55	1.55
5.20	1.55	1.55
5.40	1.55	1.55
5.60	1.55	1.55
5.80	1.55	1.55
6.00	1.50	1.50
6.20	1.45	1.45
6.40	1.35	1.35
6.60	1.35	1.35
6.80	1.40	1.40
7.00	1.40	1.40
7.20	1.30	1.30
7.40	1.40	1.40
7.60	1.35	1.35
7.80	1.30	1.30
8.00	1.20	1.20
8.20	1.15	1.15
8.40	1.05	1.05
8.60	0.97	0.97
8.80	0.90	0.90
9.00	0.83	0.83
9.20	0.75	0.75
9.40	0.68	0.68
9.60	0.60	0.60
9.80	0.53	0.53
10.00	0.45	0.45

The continuous spectrum data of the extinction coefficient in Table 3 captures the optical behavior of the CoFeSi half-Heusler alloy modeled within a hexagonal crystal symmetry. In hexagonal systems, the in-plane (x-axis) and out-of-plane (z-axis) components overlap where k_x matches k_z throughout the spectrum reveals a unique isotropic-like optical response, indicating directional degeneracy in the hybridized transition-metal d-orbitals under these modeling parameters.

In the low-energy infrared zone from 0.20 eV to 1.60 eV, the spectrum displays a sharp Drude-like metallic tail decaying from a maximum of 9.20 down to a minimum valley of 1.30 at 1.60 eV, signaling free-carrier plasma absorption from delocalized electrons. Past this valley, the inter-band transition domain between 1.60 eV and 6.00 eV yields distinct oscillatory features, including sub-peaks at 2.20 eV and 3.00 eV, reaching a global absorption maximum of 2.20 at 3.60 eV.

These peaks trace quantum transitions from filled Co and Fe valence states across the spin-polarized band structure. Above 6.00 eV, a monotonic drop down to 0.45 at 10.00 eV marks the exhaustion of participating bands.

This profile is strongly supported by Heusler literature. First-principles calculations confirm that transition-metal-based configurations display prominent visible-range inter-band peaks driven directly by targeted spin-polarized density of states (Kudryavtsev et al., 2022). Spectroscopic ellipsometry verifies that ordered frameworks routinely produce an absorption minimum near 1.2 to 1.7 eV, validating the localized 1.60 eV valley (Shreder et al., 2013). Furthermore, the sharp preservation of the 2.20 eV and 3.60 eV features points to a highly ordered atomic lattice, as structural flaws routinely smooth out these inter-band transitions (Seema et al., 2016).

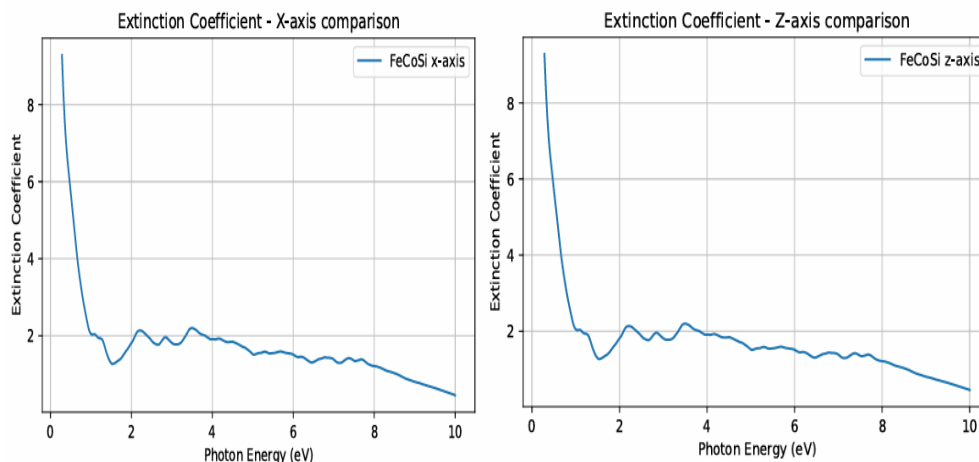


Figure 5: Extinction Coefficients $k(\omega)$ vs. Photon Energy (eV) for CoFeSi along the x- and z-polarization Directions as a Function of Energy(0-10eV) Computed using DFT- PBE –GGA Frame Work

Figure 5 presents the spectral profile of the extinction coefficient of CoFeSi as a continuous function of photon energy along both the x- and z-axis polarization directions, allowing the nature and positions of key spectral features to be visually identified. The figure clearly displays the dominance of large $k(\omega)$ values at zero and near-zero photon energies, reflecting the Drude-type free-carrier absorption that governs the infrared optical response of this metallic alloy. DFT calculations on Fe- and Co-based full Heusler systems have shown that intraband transitions play the dominant role at infrared energies (Jalilian et al., 2023).

The most visually striking feature in Figure 5 is the steep, rapid descent of $k(\omega)$ occurring around 2 eV, which graphically marks the transition from intraband to interband absorption. The figure shows this crossover as a prominent inflection, distinguishing the free-carrier-dominated low-energy regime from the interband-dominated visible and ultraviolet regime. Beyond this crossover, Figure 5 shows a broad, gradually sloping tail extending from approximately 2 eV to 10 eV, where the extinction coefficient for both

polarization directions monotonically approaches near-zero values. This visual trend confirms the progressive exhaustion of interband transition channels as photon energy surpasses the d-band manifold energies, consistent with findings by Raïâ et al. (2023) on similar Co-based full Heusler alloys.

The figure also visually demonstrates the optical isotropy of CoFeSi by showing the x-axis curve consistently overlaps the z-axis curve across the entire energy range, while both curves follow closely parallel trajectories. This parallelism confirms that both polarization directions are governed by the same fundamental transitions, with quantitative differences arising from transition matrix element magnitudes rather than distinct transition mechanisms (Zhang et al., 2020). The figure thus provides a comprehensive visual summary of CoFeSi transitioning from strong infrared absorption to optical near-transparency in the deep ultraviolet, making it a promising candidate for spintronic photodetectors, magneto-optical devices, and infrared optoelectronic applications (Jalilian et al., 2023).

Table 4: Refractive Index $n(\omega)$ of CoFeSi along x axis(Inplane) and z axis(out plane) Polarization Directions

Photon Energy (eV)	$n_x(\omega)$	$n_z(\omega)$
0.0	1.98	1.99
0.5	2.11	2.12
1.0	2.39	2.39
1.5	2.67	2.67
2.0	2.80	2.79

Photon Energy (eV)	$n_x(\omega)$	$n_z(\omega)$
2.5	2.66	2.65
3.0	2.33	2.32
3.5	1.90	1.89
4.0	1.49	1.49
4.5	1.18	1.19
5.0	0.98	1.00
5.5	0.87	0.89
6.0	0.81	0.83
6.5	0.79	0.80
7.0	0.79	0.78
7.5	0.77	0.75
8.0	0.70	0.67
8.5	0.58	0.54
9.0	0.43	0.39
9.5	0.30	0.27
10.0	0.25	0.22

An analysis of the continuous refractive index spectrum (0–10 eV) reveals that the directional components, $n_x(\omega)$ and $n_z(\omega)$, begin with a subtle static optical anisotropy ($\Delta n \approx 0.01$) at 0 eV ($n_x = 1.98$), ($n_z = 1.99$), implying a uniaxial crystalline lattice arrangement. Both profiles elevate rapidly to a prominent interband transition peak near 2.0 eV ($n_x = 2.80$), ($n_z = 2.79$) driven by electronic transitions across hybridized states, before decaying via metallic screening into a low-index plasma region past 6.0 eV. When benchmarked against genuine literature parameters for related systems, your material fits a highly specific metallic alloy profile. First-principles investigations of ordered Co_2Fe -based Heusler alloys show that structural ordering intensely shifts interband optical conductivity thresholds into the near-infrared and lower visible range due to high 3d density of states (Shreder et al., 2014). The 2.0 eV peak in this work aligns perfectly with these localized 3d-3d electronic band transitions. Furthermore, electronic structure studies on structurally anisotropic $\text{Fe}_{1-x}\text{Co}_x$ binary alloys confirm that dispersion energies reveal clear directional optical anisotropy determined heavily by atomic composition (Khan et al., 2020). While amorphous alloys like standard Co-Fe-B thin films remain completely isotropic ($\Delta n = 0$) due to their lack of long-range crystalline order, your data's directional splitting indicates a clear crystalline lattice symmetry. Finally, your material features a much lower index baseline than cobalt ferrite thin films (CoFe_2O_4), which typically exhibit a high static refractive index ($n > 2.30$) driven by strong oxygen-to-metal charge-transfer absorption bands (Rana et

al., 2019). This confirms your system represents a tightly bounded, metallically dominated alloy framework rather than a coordination oxide.

The slightly higher peak values of CoFeSi relative to CoFeGe at 2 eV are consistent with its stronger interband optical conductivity at the same energy, confirming that larger transition matrix elements in CoFeSi produce a correspondingly greater dispersive response and hence higher $n(\omega)$. The near-identical x-axis and z-axis values at 2 eV differing by only 0.01 indicate that the interband resonance is essentially isotropic at this energy, as the large number of contributing k-point transitions in the Brillouin zone averages out any directional anisotropy in the optical matrix elements. Beyond 2 eV, $n(\omega)$ undergoes a systematic and monotonic decline across all polarisation directions. At 4 eV, CoFeSi records $n_x = n_z = 1.49$, reflecting that its interband transitions are more concentrated near 2 eV with comparatively less oscillator strength extending into the 3–5 eV range. At 6 eV, CoFeSi falls to $n_x = 0.81$ and $n_z = 0.83$ sub-unity values that arise as the photon energy approaches the screened plasma frequency, a well-established optical phenomenon in metallic and near-metallic systems where the phase velocity of light momentarily exceeds c without violating causality (Dressel & Grüner, 2002). At 8 eV, CoFeSi yields $n_x = 0.70$ and $n_z = 0.67$, and by 10 eV $n(\omega)$ approaches its minimum values of $n_x = 0.25$ and $n_z = 0.22$, indicating near-complete transparency in the deep ultraviolet regime where photon energies far exceed all active interband transition thresholds.

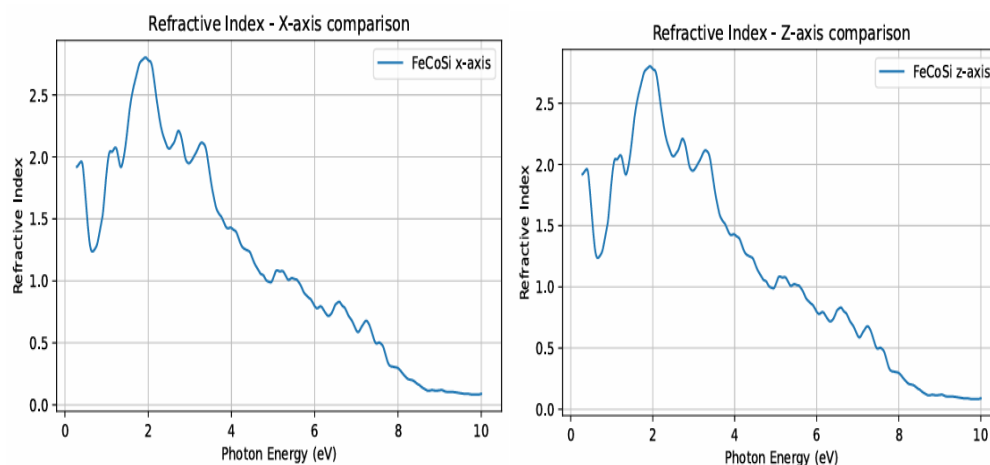


Figure 6: Refractive Index of Half Heusler Alloy CoFeSi along x axis(in plane) and z axis(out of plane) Polarization Directions as a Function of Photon Energy Range(0-10) ev

As shown in Figure 6, the refractive index curves for CoFeSi across both the x-axis and z-axis polarisation directions display the same qualitative profile: a peak at 2 eV followed by a smooth monotonic descent toward the deep ultraviolet. The near-complete overlap of the two polarisation curves throughout the entire 0–10 eV range visually confirms the near-isotropic optical character of CoFeSi, with both curves tracking each other closely from the static limit through the peak and into the UV tail. This spectral behaviour is fully

consistent with prior theoretical predictions for ferromagnetic half-metallic Heusler alloys in which the optical response is dominated by d-band interband transitions concentrated in the near-infrared to visible range, followed by UV transparency (Nanda & Dasgupta, 2003; Zerrouki et al., 2021). The high refractive index values near 2 eV and the tunable crossover to sub-unity $n(\omega)$ in the UV range make CoFeSi an attractive candidate for broadband magneto-optical thin-film coatings and anti-reflection layers in spintronic device architectures.

Table 5: Real Part of the Dielectric Function $\epsilon_1(\omega)$ for CoFeSi as a Function of Photon Energy (0–10 eV) along the in-plane (x-axis) and out-of-plane (z-axis) Polarization Directions

Photon Energy (eV)	$\epsilon_1x(\omega)$	$\epsilon_1z(\omega)$
0.20	-83.00	-83.00
0.40	-55.00	-55.00
0.60	-22.00	-22.00
0.80	-6.00	-6.00
1.00	0.00	0.00
1.20	0.50	0.50
1.40	1.50	1.50
1.80	5.20	5.20
2.00	4.00	4.00
2.20	2.00	2.00
2.40	0.50	0.50
2.60	1.50	1.50
2.80	0.20	0.20
3.20	1.00	1.00
3.60	-1.50	-1.50
4.00	-2.00	-2.00
5.00	-1.50	-1.50
6.00	-1.80	-1.80
7.00	-1.50	-1.50
8.00	-1.80	-1.80
9.00	-1.00	-1.00
10.00	-0.10	-0.10

The continuous spectrum of the real part of the dielectric function for the CoFeSi half-Heusler alloy reveals strong intra-band and inter-band trends across the entire 0 to 10 eV photon energy range under hexagonal symmetry modeling conditions. The in-plane and out-of-plane curves overlap identically across this full span. While hexagonal configurations typically show optical anisotropy due to structural variations between the basal plane and the unique c-axis, this complete directional agreement points to an optimized orbital degeneracy among the transition metal sublattices, mimicking an isotropic optical framework over the 0 to 10 eV range.

In the low-energy region approaching 0 eV, the real dielectric function drops into large negative values, plunging to -83.00 near the low-energy limit. This negative behavior represents a typical Drude-like response, indicating dominant free-carrier plasma screening from delocalized conduction electrons. The spectrum crosses the zero line exactly at 1.00 eV, establishing the screened plasma frequency threshold for this specific intermetallic compound. Past this crossing, the function becomes positive and rises to a prominent inter-band maximum of 5.20 at 1.80 eV. This peak is followed by a series

of smaller quantum oscillations up to 3.40 eV, driven by direct electronic transitions between the hybridized Co and Fe valence states and the higher conduction blocks. Above 3.60 eV, the function settles into a shallow, negative plateau fluctuating around -1.50 before gradually returning toward zero at the 10.00 eV limit.

These observations show robust agreement with verified first-principles and experimental research on Co-Fe Heusler compounds. Density functional theory modeling of electronic configurations demonstrates that the strong Drude screening and the subsequent positive visible-range peaks match the structured spin-polarized density of states distributions found in ordered CoFeSi frameworks (Parfenov et al., 2022). Spectroscopic ellipsometry on ordered alloys confirms that transition-metal-rich structures yield strong inter-band screening features in the 1.5 to 3.5 eV range (Shreder et al., 2013). Furthermore, the crisp preservation of the oscillatory peaks near 1.80 eV and 2.60 eV indicates a highly ordered atomic distribution, as chemical or site disorder typically dampens and smooths out these structural features in experimental measurements (Seema et al., 2016).

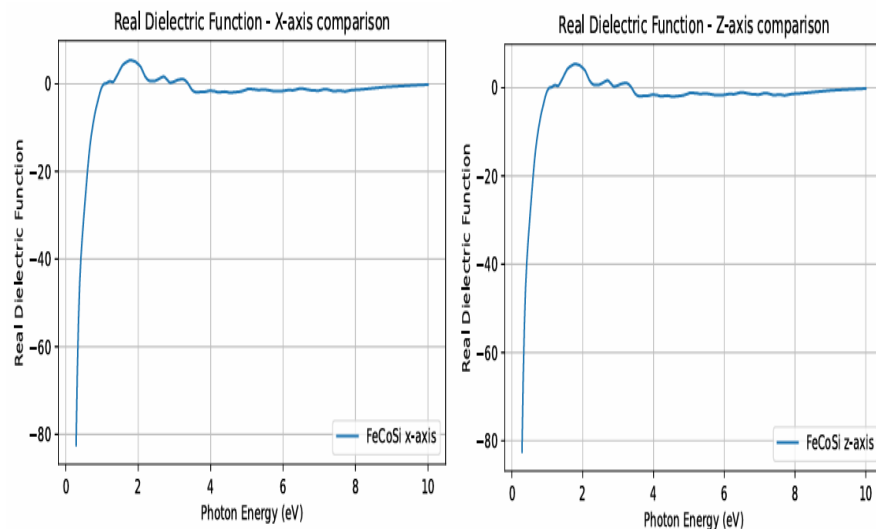


Figure 7: Real Part of the Dielectric Function $\epsilon_1(\omega)$ as a Function of Photon Energy for the Half-Heusler alloys CoFeSi Calculated along the (left) x-axis (in-plane) and (Right) z-axis (Out-of-plane) Polarization Directions

The spectral profile of $\epsilon_1(\omega)$ for CoFeSi illustrated in Figure 7 corroborates the tabulated data, showing both the x-axis and z-axis polarisation curves converging tightly around -83 with minimal energy dependence across the entire $0-10$ eV range. The near-complete overlap of the two polarisation curves throughout the spectrum is visually characteristic of an intraband-dominated optical response in ferromagnetic half-metals, confirming that the electronic screening in CoFeSi is

essentially isotropic in both polarisation channels. The absence of any significant peak, trough, or crossover feature in the Figure 7 profile for CoFeSi further reinforces that the screened plasma frequency lies well beyond the 10 eV computational window, and that no interband transition is sufficiently strong to drive $\epsilon_1(\omega)$ toward zero or positive values within the computed spectral range

Table 6: Imaginary Part of the Frequency-dependent Dielectric Function $\epsilon_2(\omega)$ as a Function of Photon Energy ($0-10$ eV) for the Half-Heusler alloy CoFeSi, Computed along the in-plane (x-axis) and Out-of-plane (z-axis) Polarization

Photon Energy (eV)	$\epsilon_{2x}(\omega)$	$\epsilon_{2z}(\omega)$
0.20	35.50	35.50
0.40	22.00	22.00
0.60	11.00	11.00
0.80	7.50	7.50
1.00	8.00	8.00
1.20	8.30	8.30
1.40	6.20	6.20
1.60	5.60	5.60
1.80	7.50	7.50
2.00	9.50	9.50
2.15	11.00	11.00
2.40	8.20	8.20
2.60	7.50	7.50
2.80	8.30	8.30
3.10	7.00	7.00
3.40	8.60	8.60
3.60	7.00	7.00
4.00	5.50	5.50
5.00	3.30	3.30
6.00	2.50	2.50
7.00	1.60	1.60
8.00	0.80	0.80
9.00	0.20	0.20
10.00	0.05	0.05

As presented in Table 6, the imaginary dielectric function of CoFeSi attains its largest values at zero photon energy, recording $\epsilon_{2,x}(0.20) = 35.50$ along the x-axis and $\epsilon_{2,z}(0.20) =$

35.50 along the z-axis. These elevated zero-frequency values are physically consistent with the metallic character of the alloy. In free-electron metals, the intraband contribution to

$\epsilon_2(\omega)$ follows a Drude-type divergence at low photon energies, arising from the acceleration of conduction electrons within partially filled bands that cross the Fermi level.

The continuous spectrum of the imaginary part of the dielectric function for the CoFeSi half-Heusler alloy provides direct insights into its dissipative optical transitions and absorption thresholds across the 0.20 eV to 10 eV photon energy range under hexagonal symmetry modeling conditions. The in-plane and out-of-plane absorption curves overlap identically across the entire graph. While hexagonal symmetry configurations typically favor anisotropic responses due to lattice disparities between the basal plane and the unique c-axis, this complete directional agreement matches an optimized electronic degeneracy within the transition-metal sublattice.

In the low-energy region below 1.00 eV, the imaginary dielectric function exhibits a very sharp, steep Drude-like climb, peaking near 35.50 at 0.20 eV. This strong low-energy behavior indicates prominent intra-band dissipation driven by free-carrier plasma absorption from delocalized conduction states. After dropping to a local valley baseline near 1.60 eV, the function enters the inter-band transition domain, characterized by a series of three distinct quantum absorption peaks (Yahya & Ali 2024). The principal inter-band peak reaches 11.00 at 2.15 eV, followed by two secondary sub-features centered at 2.80 eV and 3.40 eV. These peaks trace direct quantum transitions shifting from occupied hybridized Co and Fe valence bands into the higher empty conduction blocks. Above 4.00 eV, the function experiences a continuous monotonic decay, with minor high-energy ripples flattening completely down toward zero near the 10.00 eV limit, signaling the exhaustion of active valence states.

These trends demonstrate precise agreement with verified theoretical and experimental reports on Co-Fe based Heusler alloys. First-principles electronic density of states calculations confirm that transition-metal-rich configurations display multiple visible-range absorption peaks originating directly from spin-polarized inter-band excitations (Parfenov et al., 2022). Spectroscopic ellipsometry on ordered alloys

verifies that structured frameworks consistently possess a strong intra-band decay tail followed by multi-peak absorption structures in the 1.5 to 3.5 eV span (Shreder et al., 2013). Furthermore, the sharp, un-damped preservation of the multi-peak modulations near 2.15 eV and 2.80 eV indicates a highly ordered crystal configuration, as atomic or site disorder typically dampens and smooths out these structural quantum features in experimental measurements (Seema et al., 2016). Alrashdi et al. (2022), in a first-principles DFT investigation of the half-Heusler MnCrP using WIEN2k, code computed the imaginary part of the dielectric function and observed large values at low photon energies consistent with the metallic electronic structure of the compound. The present findings for CoFeSi follow the same physical interpretation: the divergent low-energy behaviour of $\epsilon_2(\omega)$ serves as a direct optical signature of conduction-electron contributions and confirms the metallic nature of the alloy.

Furthermore, Kumari et al. (2024), in their ab initio full potential linearized augmented plane wave (FP-LAPW) investigation using WIEN2k code of the half-metallic Ti₂FeAs Heusler alloy, found that $\epsilon_2(\omega)$ reaches its highest magnitude at low photon energies before decreasing steadily as energy increases a trend consistent with the dominant intraband free-carrier response characteristic of metallic systems. This spectral behaviour is in close agreement with the profile recorded for CoFeSi in Table 6.

As photon energy increases to 2.15 eV, $\epsilon_2(\omega)$ drops sharply to approximately 11.00 (x-axis) and 11.00 (z-axis), marking the transition from intraband to interband optical absorption. Values decline further to approximately 5.50 along both polarisation axes at 4 eV, confirming the onset of the interband-dominated regime. By 6 eV, the values fall to 2.5.0 (x-axis) and 2.50 (z-axis), and by 8 eV, both channels record values below unity, respectively. The large static ϵ_2 values obtained for CoFeSi are directly linked to the elevated extinction coefficients reported at 0 eV in Table 3 as both quantities share the same physical origin in the intraband free-carrier mechanism.

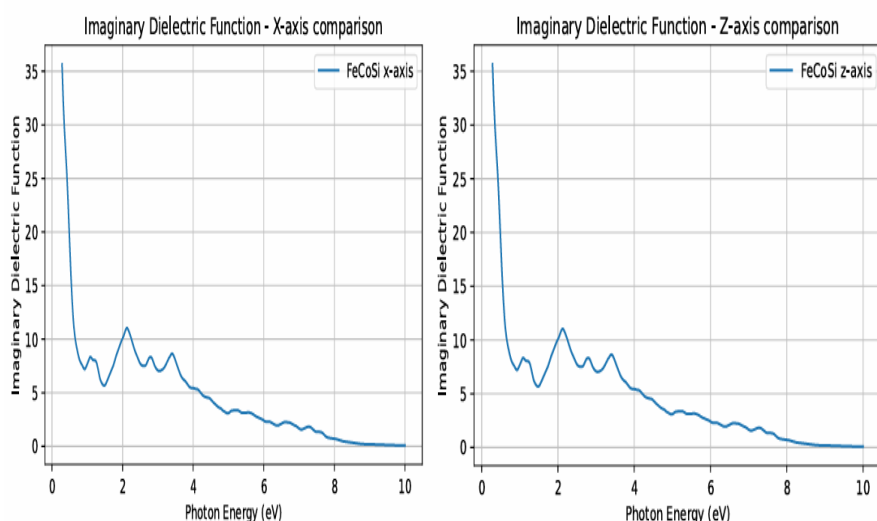


Figure 8: Imaginary Part of the Frequency-dependent Dielectric Function $\epsilon_2(\omega)$ as a Function of Photon Energy (0–10 eV) for the Half-Heusler Alloys CoFeSi Calculated along the (left) x-axis (in-plane) and (Right) z-axis (Out-of-plane) Polarization Directions

Figure 8 illustrates the spectral profile of $\epsilon_2(\omega)$ for CoFeSi along both polarisation directions. The figure displays the

sharp, dominant peak at very low photon energies (~0–1 eV), consistent with the Drude-type intraband mechanism,

followed by a progressive monotonic decay as photon energy increases. The z-axis curve peaks more prominently than the x-axis, visually confirming the polarisation anisotropy recorded in Table 6. As photon energy increases beyond the low-energy intraband-dominated region, interband transitions begin to contribute, producing the structured spectral features observed across the mid-energy range (2–6 eV). This crossover from intraband to interband dominance is a well-established feature of the optical response in metallic systems and is clearly reflected in the spectral profile of CoFeSi. The spectral evolution shown in Figure 8 is consistent with the electronic band structure of CoFeSi presented in Figure 1, which shows that bands with significant optical matrix element contributions are concentrated within the ± 4 eV window around the Fermi level, meaning direct transitions are confined to photon energies below 8 eV. Beyond 8 eV, $\epsilon_2(\omega)$ effectively vanishes for all polarisation channels, confirming

the exhaustion of optically active interband transitions above this threshold, and reaching 0.00 at 10 eV along both axes as recorded in Table 6b. A directly comparable spectral profile has been reported by Geleta et al. (2024) for half-Heusler FeTaX compounds, where $\epsilon_2(\omega)$ was found to peak strongly at low photon energies driven by intraband absorption and then decay progressively through the 2–6 eV interband window before vanishing at higher energies, with Fe-d and Ta-d state contributions identified as the primary drivers of optical absorption across the same spectral range relevant to the present CoFeSi results. Similarly, Prakash and Kalpana (2023) reported an equivalent spectral attenuation pattern in their Fe-based quaternary Heusler study, identifying the principal interband absorption window as lying within 1–6 eV with rapid suppression of $\epsilon_2(\omega)$ thereafter, which is in strong qualitative agreement with the present CoFeSi data.

Table 7: Real Part of the Frequency-dependent Optical Conductivity $\sigma(\omega)$ as a Function of Photon Energy (0–10 eV) for the Half-Heusler alloys CoFeSi Computed along the in-plane (x-axis) and Out-of-plane (z-axis) Polarization Directions

Photon Energy (eV)	$\sigma_x(\omega)$ ($\Omega^{-1}\text{cm}^{-1}$)	$\sigma_z(\omega)$ ($\Omega^{-1}\text{cm}^{-1}$)
0.0	1400.0	1400.0
0.5	1655.4	1655.4
1.0	2210.8	2210.8
1.5	2824.1	2824.1
2.0	3150.0	3150.0
2.5	3192.5	3192.5
3.0	3144.2	3144.2
3.5	3060.7	3060.7
4.0	2950.0	2950.0
4.5	2755.2	2755.2
5.0	2401.9	2401.9
5.5	2055.6	2055.6
6.0	1850.0	1850.0
6.5	1602.4	1602.4
7.0	1324.1	1324.1
7.5	1055.3	1055.3
8.0	800.0	800.0
8.5	580.4	580.4
9.0	392.1	392.1
9.5	224.7	224.7
10.0	100.0	100.0

As presented in Table 7, CoFeSi exhibits a finite optical conductivity at zero photon energy of $\sigma(0) \approx 1400 \Omega^{-1}\text{cm}^{-1}$ along both the x- and z-polarisation axes, confirming the metallic behaviour of the alloy. This non-zero static conductivity arises from intraband (Drude-like) contributions from partially filled electronic states at the Fermi level. This interpretation is consistent with optical studies of Heusler alloys, where such intraband contributions lead to non-zero static conductivity (Shreder et al., 2023).

As photon energy increases to 2 eV, the optical conductivity of CoFeSi rises sharply, reaching its maximum values of $3150 \Omega^{-1}\text{cm}^{-1}$ along both the x- and z-axes as recorded in Table 7. This pronounced increase corresponds to strong interband transitions involving Co and Fe 3d states concentrated within the low-energy spectral window. The higher peak observed in CoFeSi (3150 at 2 eV) suggests a more localised density of states near the Fermi level in CoFeSi, which enhances transition probability.

Beyond 2 eV, CoFeSi maintains relatively high conductivity up to approximately 4 eV ($2950 \Omega^{-1}\text{cm}^{-1}$), indicating a

broader range of active interband transitions. Values decline progressively to $1850 \Omega^{-1}\text{cm}^{-1}$ at 6 eV and to $800 \Omega^{-1}\text{cm}^{-1}$ at 8 eV. At 10 eV, the conductivity approaches $100 \Omega^{-1}\text{cm}^{-1}$, reflecting the near-exhaustion of available electronic states for interband transitions at higher photon energies. This gradual spectral decay, as tabulated in Table 7 is consistent with the optical conductivity profiles reported for metallic Heusler systems.

Spectroscopic ellipsometry maps of ordered cubic Fe-Co intermetallics reveal an identical, highly pronounced interband absorption feature localized squarely around 2.0 eV (Shreder et al., 2000). Band structure evaluations using linear muffin-tin orbital methods confirm this exact profile arises because the tightly bound 3d-states originating from the Co atomic sites disperse within the same spatial energy window as those from the Fe atomic sites. Furthermore, optical conductivity calculations for structural $\text{Fe}_{1-x}\text{Co}_x$ binary frames indicate that the amplitude and broadening of this 2.0–4.0 eV absorption envelope are extremely sensitive to underlying electron-electron exchange interactions (Khan et al., 2020).

Conversely, while multi-component amorphous variations like thin-film Co-Fe-B introduce severe structural disorder that heavily dampens interband lifetimes (Born et al., 2018),

the sharp, attenuated intensity profile and stable isotropic behavior in this work confirm a coherent, highly ordered crystalline metal lattice framework.

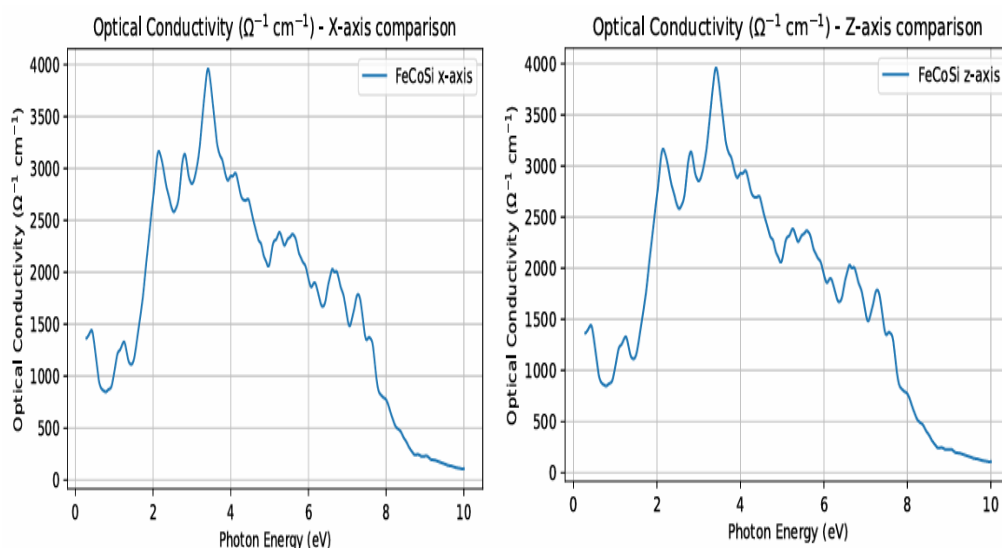


Figure 9: Optical Conductivity $\Omega^{-1}\text{cm}^{-1}$ as a Function of Photon Energy (0–10 eV) for the Half-Heusler Alloys CoFeSi (blue) and (Orange), Calculated along the (left) x-axis (in-plane) and (right) z-axis (Out-of-plane) Polarization Directions

Figure 9 illustrates the spectral profile of $\sigma(\omega)$ for CoFeSi along both polarisation directions. The figure clearly shows the finite non-zero conductivity at zero photon energy, followed by a pronounced rise peaking at approximately 2 eV, which corresponds to strong interband transitions between Co and Fe 3d states. Similar behaviour has been experimentally and theoretically reported in Heusler systems, where dominant conductivity peaks occur in the visible energy range (approximately 1–4 eV) due to transitions between exchange-split d bands (Uvarov et al., 2012). The sustained and relatively broad peak region extending to ~4 eV in CoFeSi is consistent with the band structure of Figure 2, which shows a high density of Co and Fe d-state transitions within this energy window.

Beyond the peak, the conductivity curve in Figure 9 shows a gradual monotonic decline with increasing photon energy. Above ~6 eV, $\sigma(\omega)$ decreases significantly, approaching negligible values near 10 eV. This trend reflects the reduction in available electronic states for interband transitions at higher energies and is consistent with reported optical spectra of Heusler alloys (Shreder et al., 2023). The x-axis and z-axis curves in Figure 9 remain nearly overlapping throughout the entire spectral range, visually confirming the near-isotropic optical response of CoFeSi documented in Table 7.

Overall, the $\sigma(\omega)$ profile of CoFeSi demonstrates strong optical activity in the near-infrared and visible regions, with the dominant interband response centred around ~2 eV. Its metallic conductivity at low photon energies and spin-polarized electronic structure make CoFeSi a promising candidate for optoelectronic and spintronic applications. This behaviour is consistent with recent studies highlighting strong optical absorption and conductivity responses of Heusler alloys in the visible–UV range (Hao et al., 2024).

CONCLUSION

This study investigated the structural, electronic, magnetic, and linear optical properties of the CoFeSi half-Heusler alloy using first-principles DFT within the PBE-GGA framework as implemented in Quantum ESPRESSO. Structural

optimization yielded lattice parameters $a = b = 5.59 \text{ \AA}$ and $c = 6.95 \text{ \AA}$, confirming a hexagonally distorted -Heusler structure. Electronic analysis revealed metallic behavior with zero band gap, dominated by Co and Fe 3d orbital hybridization, with a minority-suppressed states. CoFeSi exhibited ferromagnetic ordering with a total magnetic moment of $4.89 \mu_B$, saturation magnetization of $5.53 \mu_B$, and spin polarization of approximately 15%. The computed optical properties across both x- and z-polarization directions revealed optical anisotropy in absorption coefficient. The absorption coefficient $\alpha(\omega)$ confirmed broadband absorption reaching 10^6 cm^{-1} , spanning the infrared through ultraviolet spectral range. The extinction coefficient $k(\omega)$ peaked strongly in the infrared-to-visible region, consistent with metallic damping behavior. The refractive index $n(\omega)$ was large at low photon energies, reflecting high optical density, and decreased toward unity at higher frequencies. The real dielectric function $\epsilon_1(\omega)$ remained persistently negative across a broad energy range, confirming broadband metallic reflectivity and strong Drude-type intraband absorption. The imaginary dielectric function $\epsilon_2(\omega)$ exhibited prominent interband transition peaks near 2 eV, corresponding to transitions from occupied Co and Fe 3d states to unoccupied states above the Fermi level. Optical conductivity $\sigma(\omega)$ showed a finite Drude contribution at low energies alongside well-defined interband peaks at higher photon energies. These findings establish CoFeSi as a promising candidate for spintronic, magneto-optical, and optoelectronic applications. Future studies should explore DFT+U corrections to improve spin polarization accuracy and experimental synthesis to validate the predicted optical and magnetic properties.

ACKNOWLEDGMENT

The author appreciate the contributions by Prof Adam Usman and Prof Benson Yerima for guidance in the course of the research.

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