FrYBi (Y = Ca, Sr, Ba) Semiconductors for Visible-Light Harvesting: A multifunctional platform for energy conversion and optoelectronic applications

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This study presents a comprehensive first-principles investigation of the structural, electronic, optical, elastic, and thermoelectric properties of the novel half-Heusler compounds FrYBi (Y = Ca, Sr, Ba). Employing density functional theory (DFT) with both the GGA-PBE and mBJ-GGA approximations, we determine that these compounds crystallise in the cubic Clb structure and exhibit indirect band gaps ranging from 0.97 to 1.35 eV, confirming their semiconducting nature. Detailed optical analyses reveal high absorption coefficients, pronounced reflectivity, and favourable dielectric responses within the visible spectrum, indicating potential for optoelectronic applications. Calculations of the elastic properties demonstrate that all compounds are mechanically stable and exhibit ductile behaviour. Thermoelectric analysis indicates high Seebeck coefficients alongside good electrical conductivity, particularly at low to moderate temperatures, suggesting promising performance for energy conversion applications. These findings position FrYBi alloys as compelling candidates for next-generation thermoelectric and optoelectronic devices.

Keywords: Half Heusler; energy conversion; thermoelectric; Wien2k; semiconductor.

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1. Introduction

Heusler compounds constitute a technologically important family of materials with diverse functionalities ranging from spintronics and thermoelectric to optoelectronics. They was discovered for the first time by Frédérique Heusler [1]. This alloy, with the formula Cu_2MnAl [2–4], had an unknown crystal structure for several years until 1934 when Bradley and Rodgers determined its well-defined organisation at room temperature through X-ray analyses [5, 6]. Subsequently, in 1983, Groot and co-workers identified the compound NiMnSb as the first half-metallic material through electronic structure studies [7].

Heusler alloys are categorised into four groups based on chemical composition [8]:

1. Full Heusler alloys (X_2YZ), where X and Y are transition metals and Z is a group III, IV, or V element. These crystallise in a face-centred cubic structure, exhibiting remarkable magnetic properties [9, 10].

2. Inverse Heusler alloys, characterised by distinct atomic arrangements where Y atoms occupy X sites and Y possesses higher electron counts than X, leading to unconventional magnetic behaviour [11, 12].

3. Quaternary Heusler alloys (exemplified by LiMgPdSb-type compounds) [13, 14].

4. Half-Heusler alloys (XYZ), conceptually divisible into covalent and ionic components. Here, cationic atoms X and Y (transition metals or rare earths) and anionic atom Z (main-group elements like Ge, Sn, or Sb) form compounds such as LiAlSi, ZrNiSn, and LuAuSn [15–18].

Half-Heusler alloys crystallise in a non-centrosymmetric cubic structure (space group $F\bar{4}3m$, No. 216) known as the Cl_b phase [19]. This configuration originates from the tetrahedral arrangement of ZnS-type structures, where atoms occupy octahedral lattice sites. The structure comprises three interpenetrating face-centred cubic sublattices, with atoms X, Y, and Z occupying Wyckoff positions 4a (0, 0, 0), 4b (1/2, 1/2, 1/2), and 4c (1/4, 1/4, 1/4), respectively [20, 21]. While classical half-Heuslers (*e.g.*, NiMnSb, ZrNiSn) exhibit metallic or half-metallic behaviour governed by d-state hybridisation, emerging systems composed of elements such as Li, Na,

K, Ca, Sr, and Ba display qualitatively different electronic behaviour due to their s- and p-electron dominated bonding networks. Recent publications [22–24] have demonstrated that alkali-metal-based Heuslers can exhibit large band gaps, high optical absorption, and promising thermoelectric transport [25, 26].

These materials constitute an extensive family with significant technological potential. A key characteristic is their tunable band gap (0–4 eV), governed by electrostatic interactions among constituent atoms [27, 28].

Recent years have witnessed the emergence of a novel group of Heusler compounds incorporating elements beyond the conventional transition metal framework [29–33], distinguishing them structurally and electronically from traditional Heusler compounds. Comprising alkali and alkaline-earth metals, these materials exhibit distinctive properties arising from their ionic bonding nature and unique valence electron configurations. This behaviour contrasts with the predominantly covalent or metallic bonding observed in conventional transition-metal-based Heusler systems. Owing to their distinctive composition involving alkali and alkaline-earth elements, these compounds show considerable promise for innovative structural, electronic, and thermoelectric applications [34].

Their semiconducting behaviour is primarily governed by the number of valence electrons, which can be deliberately modified to achieve a broad range of band gap values. This tunability enhances their suitability for thermoelectric and photovoltaic technologies [35–37]. Recent *ab initio* studies on energy storage materials, such as $LiRuPO_4$, demonstrate the critical role of DFT in predicting electronic properties for tailored band gaps, further validating our computational approach. Forty-two years ago, Groot *et al*. identified in their analysis of NiMnSb an energy gap at the Fermi level for minority spin states, while majority spin states exhibited metallic character. This spin-asymmetric electronic structure led to the formulation of the term "half-metal" [38, 39]. Subsequent investigations have identified numerous half-Heusler compounds as half-metals, and contemporary research suggests this emerging group may also display semi-metallic or semiconducting behaviour with tunable electronic properties [40, 41].

Although several studies have examined Li-, Na-, and Mg-based half-Heuslers, no prior work has reported structural, electronic, optical, or thermoelectric properties of FrYBi compounds. Their potential as visible-light semiconductors and ductile thermoelectric also remains unexplored. The present work fills this gap by: (i) Establishing the structural and thermodynamic stability of FrYBi (Y = Ca, Sr, Ba), (ii) Investigating their electronic band structures and optical transitions, (iii) Providing detailed analyses of mechanical stability and bonding-driven anisotropy, (iv) Evaluating thermoelectric parameters, including Seebeck coefficient, electronic conductivity, and the figure of merit. The choice of FrYBi is supported by recent findings showing alkaline-earth substitutions can strongly modulate thermoelectric performance [42, 43]. These considerations position the FrYBi series as promising candidates for multifunctional energy applications. Their tunable semiconducting nature positions them as promising candidates for transparent conductive materials and optoelectronic systems. Cost-effective photovoltaic studies in regions like Saudi Arabia [44] underscore the urgent need for scalable materials with optimal visible-light absorption, as demonstrated by FrYBi compounds.

2. Computational details

Half-Heusler alloys with stoichiometric composition XYZ (1:1:1 ratio) crystallise in a face-centred cubic (fcc) structure, belonging to space group F-43m (No. 216). The atomic Wyckoff positions are 4a (0, 0, 0), 4b (1/2, 1/2, 1/2), and 4c (1/4, 1/4, 1/4). Three distinct atomic arrangements are possible for half-Heusler compounds based on these positions, as detailed in Table I. This work investigates the structural, optoelectronic, elastic, and thermoelectric properties of the FrYBi series (Y = Ca, Sr, Ba).

All calculations were performed using the WIEN2k code, which implements density functional theory (DFT) via the full-potential linearised augmented plane wave (FP-LAPW) method. The exchange-correlation functional was treated with the generalised gradient approximation (GGA-PBE) of Perdew, Burke, and Ernzerhof, supplemented by the modified Becke-Johnson potential (mBJ-GGA) for band structure accuracy.

Within this framework:

- Basis functions, electronic densities, and potentials are expanded in spherical harmonics inside atomic spheres and as Fourier series in interstitial regions.
- The convergence parameter $R_{MT} \cdot K_{\max}$ was set to 8, where R_{MT} is the smallest muffin-tin radius and $K_{\max}$ is the maximum reciprocal lattice vector magnitude.
- Additional parameters include $G_{\max} = 14$ a.u^{-1} and an energy threshold of -7.0 Ry separating core and valence states.
- Brillouin zone integration employed a $14 \times 14 \times 14$ k-mesh (3000 k-points in the irreducible wedge).
- Self-consistent cycles terminated when total energy convergence fell below 10^{-5} Ry.

The robust predictive capability of DFT for Heusler alloys is well-established. Prior studies have demonstrated strong agreement between DFT predictions and experimental structural and electronic properties [45,46]. These works validate the reliability of the computational methods employed here.

3. Results and discussions

3.1. Structural properties and formation Energy

We first compute the structural characteristics and formation energies for FrYBi (Y = Ca, Sr, Ba). These compounds crystallise in the Cl_b structure (space group F-43m, No. 216). To determine the stable phase, we optimise the total energy as a function of unit cell volume and fitted the resulting curves using the Murnaghan equation of state (EOS) [47], with results presented in Fig. 1.

$$E(V) = E_0 + \frac{B_0}{B_0'(B_0'-1)}\left[V\left(\frac{V_0}{V}\right)^{B_0'} - V_0\right] + \frac{B_0}{B_0'}(V - V_0), \quad (1)$$

where B_0 denotes the bulk modulus, B_0' its first derivative, E_0 the equilibrium energy, and V_0 the equilibrium volume. The volume-pressure relationship is given by:

$$V = V_0\left[1 + \frac{B_0'P}{B_0}\right]^{-1/B_0'}. \quad (2)$$

The bulk modulus is defined as:

$$B = V\frac{\partial^2 E}{\partial V^2}. \quad (3)$$

To further justify the selection of the Type-1 atomic configuration as the most stable structure, we carried out a complete structural optimisation for all three possible half-Heusler arrangements (Type-1, Type-2, and Type-3) as presented in Table II. For each compound in the FrYBi series (Y = Ca, Sr, Ba), the Type-1 configuration systematically exhibited the lowest total energy and most negative formation energy, confirming its thermodynamic preference. This energetic behaviour is consistent with the chemical environment established by the Type-1 arrangement, where the highly electropositive Fr atom occupies the 4a site, the alkaline-earth element (Ca/Sr/Ba) resides at 4b, and the more electronegative Bi atom is positioned at 4c. Such an arrangement promotes stronger Y-Bi bonding and minimises electrostatic repulsion, yielding a more compact and energetically favourable structure.

Calculated equilibrium parameters including volume, lattice parameter, bulk modulus, its pressure derivative, equilibrium energy, and formation energy, are summarised in Table II. The results confirm that FrYBi compounds exhibit greatest stability in the Type 1 configuration, with lattice parameters of 8.4918 Å (FrCaBi), 8.6752 Å (FrSrBi), and 8.8360 Å (FrBaBi). Table II further reveals negative formation energies for the most stable FrYBi configurations. This signifies exothermic compound formation from constituent elements, indicating thermodynamic stability relative to isolated atoms. Such energetically favourable formation implies spontaneous synthesis under appropriate conditions and structural robustness, highlighting their potential for thermally stable applications.

3.2. Electronic properties

We computed the electronic band structures of FrYBi (Y = Ca, Sr, Ba) along high-symmetry paths in the first Brillouin zone using both GGA-PBE and mBJ-GGA approximations. The results are presented in Fig. 2. These figures indicate an indirect band gap between the valence band maximum and conduction band minimum along the X–Γ direction, with mBJ-GGA values of 0.98 eV (FrCaBi), 0.97 eV (FrSrBi), and 1.35 eV (FrBaBi).

The density of states (DOS) provides essential insight into material properties by identifying orbital contributions to charge and thermal transport, along with electron energy distributions. Our DOS calculations employed the mBJ-GGA approximation. Figure 3 displays the total (TDOS) and partial (PDOS) density of states for FrYBi compounds within the energy range [1, 3.5] eV. Within the valence band, the dominant contribution originates from Bi p-orbitals, with minor contributions from Fr p-orbitals and Y d-orbitals. In the conduction band, Y d-orbitals (Y = Ca, Sr, Ba) provide the principal contribution, while other orbital contributions remain negligible.

3.3. Optical properties

The dielectric function comprises real (ε_1) and imaginary (ε_2) components, expressed as:

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega). \quad (4)$$

Figure 4a) illustrates variations in the real part of the dielectric function $\varepsilon_1(\omega)$ for FrYBi (Y = Ca, Sr, Ba). The response exhibits three distinct regions:

- At zero frequency, $\varepsilon_1(0)$ values are 7.06 (FrCaBi), 6.71 (FrSrBi), and 6.59 (FrBaBi).
- In the visible spectrum, $\varepsilon_1(\omega)$ ascends to maxima of 11.895 (FrCaBi), 12.145 (FrSrBi), and 11.602 (FrBaBi), followed by sharp attenuation with increasing energy.
- Within the UV spectrum, $\varepsilon_1(\omega)$ displays oscillatory behaviour, attaining negative values at specific energies (Table III), signifying electromagnetic wave reflection. Beyond $\sim$ 7.5 eV, $\varepsilon_1(\omega)$ becomes positive and increases gradually with energy.

Figure 4b) illustrates the energy-dependent behaviour of the imaginary dielectric function $\varepsilon_2(\omega)$ for FrYBi (Y = Ca, Sr, Ba). Initially, $\varepsilon_2(\omega)$ remains negligible across low energies, confirming the absence of optical absorption below the band gap. A sharp increase onset occurs at energies corresponding to each compound's band gap, signifying interband electronic transitions. The response rises steeply to visible-spectrum maxima of 12.676 (FrCaBi), 13.957 (FrSrBi), and

11.582 (FrBaBi), followed by pronounced oscillatory attenuation toward minima in the ultraviolet (UV) region. This behaviour reflects characteristic dispersion in semiconductors under high-energy photon absorption.

Figure 4c) presents photon-energy-dependent absorption coefficients $\alpha(\omega)$ for FrYBi. The absorption onset aligns precisely with each compound's band gap energy, indicating interband transition thresholds. Beyond this threshold, $\alpha(\omega)$ increases rapidly, peaking in the visible region at 5849.65 cm^{-1} (FrSrBi), 5193.72 cm^{-1} (FrCaBi), and 4890.61 cm^{-1} (FrBaBi). Subsequent oscillatory decreases occur as photon energies extend into the UV region, revealing complex high-energy transition dynamics.

Optical conductivity characterises electronic responses to electromagnetic radiation, providing critical insights into band structure and charge carrier dynamics. This parameter intrinsically links to optical constants including the dielectric function, absorption coefficient, and refractive index. The real component $\sigma_1(\omega)$ is expressed as [48]:

$$\sigma(\omega) = \alpha(\omega)n(\omega)\frac{\omega}{2\pi}. \tag{5}$$

Figure 4d) illustrates the photon-energy-dependent optical conductivity $\sigma(\omega)$ of FrYBi (Y = Ca, Sr, Ba). This trend corresponds closely to the absorption coefficient behaviour: $\sigma(\omega)$ remains negligible at low energies, rising sharply at each compound's band gap energy. It increases rapidly to visible-region maxima of 5.26×10^{15} s^{-1} (FrSrBi), 4.67×10^{15} s^{-1} (FrCaBi), and 4.39×10^{15} s^{-1} (FrBaBi). Beyond these peaks, $\sigma(\omega)$ decreases gradually with oscillatory behaviour as photon energies extend into the ultraviolet (UV) range, characteristic of high-energy interband transitions.

Reflectivity characterises light-matter interactions by probing electronic structure, providing critical insights into band gaps, electronic transitions, and electromagnetic radiation reflection. This parameter is particularly relevant for reflective coatings, photovoltaics, and optical sensors. Reflectivity $R(\omega)$ is defined as [49]:

$$R(\omega) = \frac{(n-1)^2 + K^2}{(n+1)^2 + K^2}, \tag{6}$$

where n is the refractive index and K the extinction coefficient.

Figure 5a) presents photon-energy-dependent reflectivity for FrYBi (Y = Ca, Sr, Ba). Initial reflectivity values at low energy are 20.55% (FrCaBi), 19.31% (FrSrBi), and 19.62% (FrBaBi). Reflectivity increases sharply with photon energy, peaking in the visible spectrum at 42.85% (FrCaBi), 44.59% (FrSrBi), and 40.00% (FrBaBi). Beyond these maxima, reflectivity decreases oscillatory into the ultraviolet (UV) range. Notably, FrBaBi exhibits a secondary peak of 43.74% at ~ 5.35 eV. Prominent features between 2–7 eV signify strong photon-electron interactions and potential interband transitions.

The energy loss function characterises a material's capacity to dissipate energy from fast-moving electrons, offering critical insights into plasmonic behaviour and dielectric responses. This function is directly related to the complex dielectric function and is defined as:

$$L(\omega) = \frac{\varepsilon_2(\omega)}{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)}, \tag{7}$$

where $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ denote the real and imaginary components of the dielectric function, respectively.

Figure 5b) illustrates the photon-energy-dependent energy-loss function for FrYBi (Y = Ca, Sr, Ba). In the low-energy regime ($0 - 2$ eV), energy loss remains negligible for all compounds, indicating minimal electron interactions and high transparency. Between $2 - 8$ eV, energy loss increases oscillatory with rising photon energy, corresponding to enhanced electronic excitations and plasmonic behaviour. Each compound reaches a distinct peak within this range, after which the function decreases gradually with further energy increase. This behaviour suggests strong interband transitions and highlights the dynamic electronic response in the mid-energy region.

The complex refractive index characterises light-matter interactions and relates directly to the dielectric function. It comprises two components: the real part (refractive index, n) and the imaginary part (extinction coefficient, k). This relationship is expressed as [50, 51]:

$$N(\omega) = n(\omega) + ik(\omega). \tag{8}$$

The complex refractive index components are derived from the dielectric function as follows. The frequency-dependent refractive index is given by

$$n(\omega) = \frac{1}{\sqrt{2}}\left[\left(\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)\right)^{1/2} + \varepsilon_1(\omega)\right]^{1/2}, \tag{9}$$

The static refractive index ($\omega = 0$) relates directly to the static dielectric constant:

$$n(0) = \sqrt{\varepsilon_1(0)}. \tag{10}$$

The imaginary part of the complex refractive index is given by:

$$k(\omega) = \frac{1}{\sqrt{2}}\left[\left(\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)\right)^{1/2} - \varepsilon_1(\omega)\right]^{1/2}. \tag{11}$$

Figure 5c) depicts the photon-energy dependence of the refractive index for half-Heusler compounds FrYBi (Y = Ca, Sr, Ba). The static refractive index values are 2.658 (FrCaBi), 2.567 (FrSrBi), and 2.590 (FrBaBi). With increasing photon energy, $n(\omega)$ rises to visible-spectrum maxima at:

- 3.61 (FrCaBi, 472 nm, blue region).
- 3.65 (FrSrBi, 440 nm, violet region).
- 3.58 (FrBaBi, 515 nm, green region).

Beyond these peaks, $n(\omega)$ gradually decreases with higher energy, exhibiting weak oscillatory behaviour in the ultraviolet (UV) regime. This trend reflects the material's dispersive optical response and interband electronic transitions. Figure 5d) illustrates the photon-energy dependence of the extinction coefficient $k(\omega)$ for FrYBi (Y = Ca, Sr, Ba). This parameter quantifies electromagnetic wave attenuation through absorption and scattering. $k(\omega)$ increases with photon energy, peaking in the visible spectrum before gradually decreasing with mild oscillations into the ultraviolet (UV) range.

Comparative analysis with Figs. 4b) and 4c) reveals close alignment between the peak positions of $k(\omega)$, optical conductivity, and the imaginary dielectric function. This consistency underscores their intrinsic relationship, governed by interband electronic transitions and dielectric responses. Such correlation validates the calculated optical properties and their coherence with fundamental optical theory.

The FrYBi compounds exhibit distinctive optical characteristics characterised by significant peaks in reflectivity, absorption coefficient, and dielectric functions across $0-10$ eV. Prominent features within the visible spectrum ($1-3.2$ eV) indicate small energy gaps and effective visible-light absorption. All three compounds demonstrate analogous optical behaviour with intensity variations, rendering them promising candidates for solar cells, photodetectors, and visible-light optical devices. Comparative studies on efficiency enhancement, such as Usman *et al.* work on engineered coatings [54], highlight the importance of material-surface interactions in maximizing light absorption for photovoltaic systems.

The optical response of FrYBi is strongly influenced by atomic size, electronegativity, and bonding characteristics. The following insights clarify the physical origins:

- FrCaBi shows the highest dielectric constant due to stronger ionic–covalent bonding.
- FrSrBi exhibits the highest absorption coefficient, likely driven by optimal orbital overlap between Sr-d and Bi-p states.
- FrBaBi shows slightly reduced absorption because Ba's larger radius weakens interband transition probability.

These differences reflect systematic variations in charge-transfer strength and electronic hybridisation.

3.4. Mechanical properties

Analysis of elastic and mechanical properties enables the assessment of material suitability for applications. To evaluate mechanical stability, the three independent elastic constants—C_{11}, C_{12}, and C_{44}—must be determined. These constants are essential for calculating key parameters, including the bulk modulus, Young's modulus (E), shear modulus (G), and Poisson's ratio (ν), thereby facilitating comprehensive material characterisation. For cubic crystals, such as the half-Heusler compounds under study, the elastic constants must satisfy specific mechanical stability criteria to ensure structural integrity under external stress [55]:

$$C_{11}-C_{12}>0, \quad C_{11}>0, \quad C_{44}>0,$$
$$C_{11}+2C_{12}>0 \quad \text{and} \quad C_{12}<B<C_{11}. \tag{12}$$

The bulk modulus B (compressibility factor) is calculated from elastic constants using [56]:

$$B=\frac{C_{11}+2C_{12}}{3}. \tag{13}$$

Crystal anisotropy, a vital characteristic for assessing structural faults (*e.g.*, microcracks) during crystal growth, is defined for cubic systems as [57, 58]:

$$A=\frac{2C_{44}}{C_{11}-C_{12}}. \tag{14}$$

The shear modulus G, characterising the shear stress-strain relationship in elastic materials, is given by [59]:

$$G=\frac{C_{11}-C_{12}+3C_{44}}{5}. \tag{15}$$

Young's modulus E, quantifying material stiffness, is expressed as:

$$E=\frac{9BG}{3B+G}. \tag{16}$$

Poisson's ratio ν, indicating the expansion of a material in directions perpendicular to the direction of compression, is defined as:

$$\nu=\frac{3B-2G}{2(3B+G)}. \tag{17}$$

Table IV summarises the elastic properties of half-Heusler compounds FrYBi (Y = Ca, Ba, Sr). All compounds exhibit relatively low bulk and shear moduli, indicating soft and ductile characteristics. The B/G ratio ($1.69-1.90$) exceeds Pugh's critical value of 1.75 [60], confirming mechanical ductility. Poisson's ratio ($\nu=0.253-0.277$) falls within the metallic range [61], indicating elastic deformability and fracture resistance. The anisotropy factor reveals FrBaBi as most anisotropic ($A=1.11$) and FrSrBi as least anisotropic ($A=0.864$), suggesting enhanced isotropic behaviour and structural stability for the latter.

Compared to similar half-Heusler compounds (ScNiSb, LaPtSb, LiMgBi) with analogous elastic properties [62], FrYBi compounds are promising for thermoelectric/mechanical applications requiring low stiffness and ductility. The mechanical data indicate ductile, soft, and moderately anisotropic behaviour, structurally comparable to established ductile systems like YMnSb and LiMgBi [63]. Elastic constants satisfy cubic Born criteria. However, the DFT-calculated elastic constants typically carry uncertainties of $\sim 5-10\%$ due to numerical convergence. This margin was considered when assessing mechanical stability. Anisotropy increases from Sr $\rightarrow$ Ca $\rightarrow$ Ba due to changes in Y–Bi bond stiffness. Ba, having the largest ionic radius, produces weaker directional bonding, resulting in more anisotropic shear response.

3.5. Thermoelectric properties

Addressing the growing demand for sustainable energy necessitates exploring thermoelectric alternatives [64, 65]. These materials enable direct conversion of thermal energy into electricity [66, 67], with Heusler alloys emerging as promising candidates due to their diverse properties. Material efficacy is quantified by the dimensionless figure of merit ZT [68, 69]:

$$ZT = \frac{S^2 \sigma T}{\kappa}, \tag{18}$$

where S denotes the Seebeck coefficient, σ the electrical conductivity, κ the thermal conductivity, and T the absolute temperature.

Thermoelectric characteristics were computed using the BoltzTraP code within WIEN2k, with a relaxation time of 8×10^{-14} s manually specified for FrYBi (Y = Ca, Sr, Ba) compounds [70, 71]. The Seebeck coefficient (S), which quantifies thermoelectric voltage generation under temperature gradients, is presented in Figs. 6a), 7a), and 8a). All compounds exhibit positive S values, confirming p-type semiconducting behaviour and thermoelectric applicability. At 100 K, the Seebeck coefficient reaches 164.57 μV/K (mBJ-GGA) and 156.36 μV/K (GGA) for FrCaBi; 181 μV/K (mBJ-GGA) and 172.71 μV/K (GGA) for FrSrBi; and 199.12 μV/K (mBJ-GGA) and 169.02 μV/K (GGA) for FrBaBi. Peak values occur at 200 K across all compounds, with mBJ-GGA consistently yielding higher magnitudes. Beyond this temperature, S decreases monotonically, though all systems maintain high coefficients at low temperatures.

Electrical conductivity per relaxation time (σ/τ), a critical parameter for thermoelectric efficiency, is shown in Figs. 6b), 7b), and 8b). Both approximations, GGA-PBE and mBJ-GGA, yield closely comparable results. At 100 K under mBJ-GGA, σ/τ ranges from 2.24 (FrBaBi) to 5 (FrCaBi), with FrSrBi intermediate. This parameter increases steadily with temperature, peaking at 1400 K with values spanning 25 (FrBaBi) to 28 (FrCaBi). The compounds demonstrate favourable thermoelectric characteristics, combining sustained high-temperature electrical conductivity with low thermal conductivity at elevated temperatures.

Figures 6 to 8c) and 8d) depict the thermal conductivity per unit temperature (κ/τ) and dimensionless figure of merit (ZT) for FrYBi (Y = Ca, Sr, Ba) calculated using GGA-PBE and mBJ-GGA methods. The κ/τ ratio increases with temperature for all compounds, indicating enhanced phonon and electronic heat transport contributions at elevated temperatures. Throughout the studied range, mBJ-GGA predicts consistently lower κ/τ values than GGA-PBE, suggesting reduced phonon-mediated thermal transfer that benefits thermoelectric efficiency.

The ZT values increase with temperature, reaching maxima in the high-temperature regime: approximately 0.75 for FrCaBi, 0.72 for FrSrBi, and 0.70 for FrBaBi under mBJ-GGA (compared to 0.66, 0.64, and 0.61 for GGA-PBE). These enhanced mBJ-GGA ZT values result from synergistic improvements in the Seebeck coefficient, electrical conductivity, and reduced thermal conductivity. This confirms that electronic structure refinement via the mBJ potential significantly boosts thermoelectric performance.

FrYBi compounds thus show promise for high-temperature waste heat recovery and spintronic applications. Further optimisation through alloying or nano-structuring could reduce lattice thermal conductivity while maintaining electrical transport properties, thereby enhancing ZT.

The maximum ZT values correspond to temperatures where the power factor $S^2\sigma$ is greatest. Although explicit doping calculations were not performed, the broad Seebeck coefficient plateau suggests that moderate p-type carrier enhancement would further optimise performance.

- Larger band gaps in Ba-based compounds reduce intrinsic carrier concentration, lowering σ but increasing S.
- Ca-based compounds balance σ and S better, giving the highest power factor.

These trends indicate possible optimisation paths via chemical doping.

4. Solar cell applications

The optoelectronic and electronic properties of FrYBi (Y = Ca, Sr, Ba) half-Heusler compounds position them as promising candidates for enhancing solar cell efficiency. Their tunable indirect band gaps ($0.97 - 1.35$ eV, mBJ-GGA) align optimally with the solar spectrum's peak photon flux ($1.0-1.5$ eV), enabling efficient visible-light harvesting. The advantages for photovoltaic applications can be resumed as follow:

- FrYBi compounds exhibit strong absorption in the visible range ($4890 - 5849$ cm^{-1}), surpassing conventional silicon ($\alpha \sim 10^3$ cm^{-1}) and rivaling perovskite absorbers like $MAPbI_3$ [Fig. 4c)]. This ensures effective photon-to-electron conversion.

The band gap tunability (via Y-site substitution: Ca $\rightarrow$ Sr $\rightarrow$ Ba) allows customization for tandem solar cells, where FrCaBi (0.98 eV) could serve as a bottom layer and FrBaBi (1.35 eV) as a top layer, maximizing spectral utilisation. This approach aligns with established tandem solar cell design principles, where band gap optimization is critical for achieving high power conversion efficiencies [72]. The integration of such materials with advanced solar tracking systems, as demonstrated by Hasan [73], could further optimize energy harvesting efficiency in real-world deployments.

- The dominant Bi-p (valence band) and Y-d (conduction band) orbital contributions (Fig. 3) facilitate delocalized charge carriers, reducing recombination losses.

- High static dielectric constants ($\varepsilon_1(0) = [6.59 - 7.06]$) screen Coulomb interactions, further suppressing charge recombination (Table III).

Values from Table III show that the static dielectric constants $\varepsilon_1(0)$ for the three compounds are: FrCaBi: 7.06, FrSrBi: 6.71, and FrBaBi: 6.59. These high $\varepsilon_1(0)$ values ($6.59 - 7.06$) indicate that these materials effectively screen Coulomb interactions, reducing charge carrier recombination, which is beneficial for optoelectronic applications like solar cells. The trend suggests that FrCaBi provides the strongest screening, followed by FrSrBi and FrBaBi.

4.1. Device integration and Stability

The compounds' ductile nature ($B/G > 1.75$) as reported in Table IV enables flexible solar cell designs resistant to mechanical stress, unlike brittle Si or perovskites. Also, the low thermal conductivity (κ/τ, Figs. 6–8) minimizes heat-induced degradation, critical for concentrated photovoltaics. Table V shows the comparative advantages between the novel half-Heusler compounds FrYBi, c-Si and Perovskites.

4.2. Design recommendations

The following tasks are recommended for such application:

- Integrate FrYBi as an absorber layer in thin-film heterojunctions (*e.g.*, ITO/FrYBi/CdS) or as a spectral-splitting layer in tandem cells.
- Doping: P-Type behavior (positive Seebeck coefficients, Sec. 3.5.) suggests compatibility with n-type oxides (*e.g.*, TiO_2) for p-n junctions.

These properties, combined with scalable synthesis routes (suggested by negative formation energies, Table **??**), make FrYBi alloys compelling for next-generation photovoltaics. Future work should explore experimental validation and interface engineering to optimize power conversion efficiency.

5. Conclusion

This comprehensive DFT study elucidates the fundamental properties of the previously unexplored half-Heusler compounds FrYBi (Y = Ca, Sr, Ba). Structural optimisation confirms their stability in the cubic $F\bar{4}3m$ phase (Type 1), with lattice parameters expanding systematically from FrCaBi to FrBaBi. The negative formation energies further affirm thermodynamic stability, supporting their experimental feasibility.

Electronic structure calculations using mBJ-GGA reveal indirect band gaps (0.97–1.35 eV), primarily governed by Bi-p orbitals in the valence band and Y-d states in the conduction band. Optical properties exhibit strong light-matter interactions in the visible range. Evidenced by high absorption coefficients (4890–5849 cm^{-1}), reflectivity peaks (40–45%), and tunable dielectric responses. These traits align with potential applications in photovoltaic cells and transparent conductive coatings.

Mechanical analyses indicate ductile behaviour (Pugh's ratio $B/G > 1.75$, Poisson's ratio $\nu \approx 0.27$) and moderate anisotropy, comparable to established half-Heusler systems like LiMgBi. The compounds' softness suggests resilience under deformation, favourable for flexible electronics. Thermoelectrically, high Seebeck coefficients (up to 199 $\mu V{\cdot}K^{-1}$ for FrBaBi) and increasing electrical conductivity with temperature highlight their efficiency in heat-to-electricity conversion. While thermal conductivity remains low at moderate temperatures, further optimisation could enhance the figure of merit (ZT).

In summary, FrYBi alloys emerge as multifunctional materials with tailored band gaps, robust optical activity, mechanical ductility, and thermoelectric responsiveness. Future work should explore doping strategies to optimise ZT and experimental synthesis to validate these predictions. Their versatility positions them at the forefront of next-generation optoelectronic and sustainable energy technologies.

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Credit author statement

O. Hammadache executed writing - original draft, conceptualization, methodology, investigation, software, validation, formal analysis, data curation, visualization and editing. M. Houari accomplished supervision, resources, review and editing. S. Mesbah performed formal analysis, data curation, validation, visualization, review and editing. K. Khelifa-Kerfa contributed with formal analysis, software, data curation, resources, review and editing. M. Benghanem contributed with investigation, validation, formal analysis, data curation, review and editing. T. Lantri and B. Belarbi contributed equally with methodology, validation, formal analysis, data curation, visualization, review and editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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