

Heat to energy conversion: Unlocking high thermoelectric performance in NaMgBi-based half-Heusler compounds via Lithium alloying

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Heat to energy conversion: Unlocking high thermoelectric performance in NaMgBi-based half-Heusler compounds via Lithium alloying

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Abstract

A thermoelectric material converts heat to electricity. Alkali-metal magnesium bismuthides are promising thermoelectric materials due to their favourable electronic structures and low lattice thermal conductivity. Using density functional theory, including the effect of spin-orbit coupling and in combination with semiclassical Boltzmann transport, we study the thermoelectric properties of pristine and Lithium (Li)-alloyed NaMgBi of stoichiometries $\text{Na}_{1-x}\text{Li}_x\text{MgBi}$ ($x = 0.25, 0.50, 0.75$). Li atomic substitution preserves structural and mechanical stability, induces lattice softening, and enhances phonon scattering while reducing the lattice thermal conductivity. Also, band structure modifications suppress electron-hole compensation and enhance the Seebeck coefficient without significantly affecting electrical conductivity. Consequently, Li-alloyed NaMgBi attains enhanced figure-of-merit (ZT) relative to the pristine NaMgBi for the temperature range considered. Specifically, we found that $\text{Na}_{0.75}\text{Li}_{0.25}\text{MgBi}$ achieves a maximum $ZT \sim 1.78$ albeit at an elevated temperature. Our study suggests that alkali-metal alloying can effectively optimize both electronic and phonon transport in semi-metallic half-Heusler thermoelectrics, in particular magnesium bismuthides, with attendant increase in the ZT .

Keywords: Density functional theory, NaMgBi, Thermoelectrics, Half-Heusler, Alloy, Boltzmann transport

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1. Introduction

Thermoelectric (TE) materials, which enable the direct and reversible conversion of heat into electricity and vice versa, have attracted considerable attention due to their potential in sustainable energy harvesting, waste-heat recovery, and solid-state cooling applications [1, 2]. The efficiency of a TE material is quantified by the dimensionless figure of merit,

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

where S is the Seebeck coefficient, σ is the electrical conductivity, T is the absolute temperature, and $\kappa = \kappa_e + \kappa_l$ is the total thermal conductivity, composed of the electronic (κ_e) and lattice (κ_l) contributions. High ZT requires an optimal combination of a large Seebeck coefficient, high electrical conductivity, and low thermal conductivity. However, these transport parameters are strongly interdependent: increasing the carrier concentration to enhance σ often reduces S , while reducing κ_l via alloying or nanostructuring can also impact the electronic transport [3, 4]. Consequently, designing materials with high thermoelectric efficiency demands a careful balance between electronic and phononic contributions.

Historically, high-performance TE materials such as Bi_2Te_3 , PbTe , and SnSe have demonstrated ZT values in the range of 1–2, establishing benchmarks for practical applications [5, 6, 7]. Bi_2Te_3 exhibits a ZT of approximately 1 near room temperature and has been widely employed in low-temperature thermoelectric devices. Crystalline PbTe alloys show peak $ZT \sim 1.5$ at elevated temperatures (around 800 K), largely due to their high carrier mobility and favorable electronic band structure. SnSe single crystals display ultralow lattice thermal conductivity and high Seebeck coefficients, resulting in exceptionally high ZT values approaching 2.6 at 923 K [8, 9, 10]. Furthermore, layered chalcogenide and Mg_3Sb_2 -based alloys have emerged as promising TE systems, achieving ZT values close to 2 through careful defect engineering, alloying, and microstructural optimization [11]. The concept of alloying to simultaneously reduce thermal conductivity and maintain or improve electronic transport has also been applied to HH compounds. Previous studies on FeVSb -based and other half-Heusler systems have shown that mass and strain-field fluctuations induced by substitution can significantly enhance phonon scattering, resulting in lower lattice thermal conductivity without compromising electrical performance [12, 13]. Similarly, layered chalcogenides such as SnSe achieve high ZT values primarily due to intrinsically low lattice thermal conductivity and strong anharmonicity [8, 9, 10]. These findings underscore the potential of rational chemical substitution strategies to achieve high-performance thermoelectric materials in systems that are mechanically robust and environmentally benign.

Half-Heusler (HH) compounds with the general formula XYZ have attracted significant attention because of their favourable electronic structures, high mechanical strength, tunable band gaps, and excellent thermal stability [14, 15]. This has motivated extensive studies of this class of materials, both experimentally and theoretically for the aforementioned properties. Half-Heusler compounds also offers a promising platform for thermoelectric optimization due to their sensitivity to chemical substitution. With regards to the latter, we note that previous studies suggest that alkali-metal substitution can be effective in enhancing thermoelectric performance of potential TE materials. For example, incorporation of Na or K into PbTe has been shown to modify band structures and carrier concentrations, leading to improvements in the power factor and ZT [7, 16]. Similarly, Na

and Li substitution in copper chalcogenides reduces lattice thermal conductivity via mass-disorder scattering while enhancing the Seebeck coefficient [17, 18]. These improvements arise from a combination of electronic band tuning, enhanced phonon scattering due to mass fluctuations, and lattice softening, demonstrating the effectiveness of alkali-metal alloying in optimizing both electronic and phononic contributions [19, 20]. Therefore, the concept of alloying to simultaneously reduce thermal conductivity, maintain or improve electronic transport and improve the overall TE performance in materials have been firmly established

Mg-based bismuthide such as NaMgBi possess narrow-gap or semi-metallic electronic structures that are highly sensitive to alloying and chemical substitution [21, 22]. This suggests that their properties which are sensitive to electronic structures perturbation can be tuned by chemical alloying. Motivated by this and previous studies which show the effect of alkali-metal alloying on the TE properties of the widely studied PbTe, Cu-chalcogenides, and FeVSb-based HH materials [7, 17, 18], we investigate possible enhancement of thermoelectric performance of similarly important NaMgBi compound through alkali-metal doping. Our model systems consist in NaMgBi in which the Na site is replaced with the Li atom to form $\text{Na}_{1-x}\text{Li}_x\text{MgBi}$ compound. Here, x represents the concentration of the Li and it varies as $x = 0.25, 0.50$ and 0.75 . We believe that the three concentrations considered are sufficient to give insights into the interplay between the concentration of Li dopant, electronic band structure and electronic transport properties, phonon properties and thermoelectric performance. Our approach can guide investigations into rational design of HH alloys with optimized transport properties thus bridging the gap between theoretical predictions and practical thermoelectric applications.

Before proceeding, we should state the following regarding the structural form of half-Heusler XYZ compounds, including the NaMgBi. We note that the face-centered cubic structure with the space group $F\bar{4}3m$ has been widely adopted for this material, ostensibly due to the preponderance of this structural type in the class of material [21, 23-27]. Furthermore, this structural type for the XYZ HH compounds has been characterized extensively for their novel electronic and electro-optical properties. Therefore, in order to deepen our current understanding of the structure-property relationship in this material, we have equally considered the much-studied cubic structure for the investigation of its thermoelectric properties. The present study therefore serves as a further exploration of this class of compound using a consistent structural motif, i.e., cubic structure as has been extensively studied in previous reports as cited above. However, we should emphasize that recent experimental study has shown that NaMgBi in particular can exist in tetragonal $P4/nmm$ structure under equilibrium conditions [28] but has not been considered presently due to the aforementioned reasons. To achieve our study objective as highlighted above, we have employed a comprehensive computational framework which encompasses density-functional theory (DFT)[29] calculations, including the effect of spin-orbital coupling (SOC) to account for the presence of heavy element Bi in the material system, elastic property evaluation, semiclassical transport theory, and semi-empirical thermal conductivity modeling. Our approach provides a robust and consistent approach (with respect to previous studies of similar material structure) for predicting and understanding the thermoelectric behavior of NaMgBi-based material compound. The rest of the paper is structured as follows: In section 2, we describe the full details of DFT computational parameters and the empirical formalism underpinning the thermoelectric properties of a material. The atomic models considered are also described in this section. Section 3 presents a comprehensive results and analysis of the data while important results are summarized in section

2. Computational Methodology and Atomic Models

All first-principles calculations in this work were performed using the *Quantum-ESPRESSO* (QE) package [30] which implements density functional theory (DFT) within a plane-wave and pseudopotential formalism. The interaction between valence electrons and ionic cores was treated using norm-conserving pseudopotentials obtained from the official QE pseudopotential library. The valence electronic configurations considered were Li ($2s^1$), Na ($3s^1$), Mg ($3s^2$) and Bi ($6s^2 6p^3$). Exchange–correlation effects were described within the generalized gradient approximation (GGA) using the Perdew–Burke–Ernzerhof (PBE) functional [31]. The electronic wave functions were expanded in a plane-wave basis set with a kinetic energy cutoff of 150 Ry, ensuring full convergence of total energy and stress. Brillouin zone integrations were carried out using a Monkhorst–Pack $15 \times 15 \times 15$ k -point mesh. Structural relaxations were performed until the total energy and atomic forces converged to within 10^{-6} Ry and 10^{-3} Ry/Bohr, respectively. Spin–orbit coupling (SOC) effects were explicitly included in all electronic structure calculations to properly account for relativistic effects, particularly important for heavy elements such as bismuth [32]. The elastic properties were evaluated using the Thermo_PW module [33] within the QE package. From the calculated elastic constants, the mechanical stability of each compound was assessed, and macroscopic elastic moduli including the bulk modulus (B), shear modulus (G), and Young’s modulus (E) were derived using the Voigt–Reuss–Hill averaging scheme [34].

Thermoelectric transport properties were calculated using the BoltzTraP2 code [35], which solves the semi-classical Boltzmann transport equations within the constant relaxation time approximation (CRTA) [36]. Dense non-self-consistent k -point meshes were employed to accurately interpolate the electronic band structure and evaluate the energy derivatives required for transport coefficients. The Seebeck coefficient (S), electrical conductivity (σ), electronic thermal conductivity (κ_e), and power factor (PF) were computed over a temperature range of 100–1000 K. A constant relaxation time of 10 fs was adopted consistently for comparative evaluation of all investigated compositions. Although deformation-potential based relaxation-time calculations may provide a more rigorous quantitative description of carrier scattering processes [37, 38, 39], the CRTA approach remains the widely employed approach for comparative screening and trend analysis in thermoelectric materials research [40]. Within the Slack model, i.e., a semi-empirical model for estimating the lattice thermal conductivity (κ_L , in W/mK) [41]:

$$\kappa_L = A \frac{\theta_D^3 D V^{\frac{1}{3}} m_{av}}{\gamma^2 n^{\frac{2}{3}} T} \quad (1),$$

where A is a material-dependent constant, θ_D is the Debye temperature in K, V is the volume per atom or formula unit in ($\text{\AA}^3$), γ is the Grüneisen parameter (dimensionless, measuring anharmonicity), n is the number of atoms in the primitive unit cell, T is the absolute temperature in K, and m_{av} is the average atomic mass in (amu). The Debye temperature was obtained from the elastic constants and sound velocities according to [42]:

$$\theta_D = \frac{h}{\kappa_B} \left[\frac{3n}{4\pi V_m} \right]^{\frac{1}{3}} \quad (2),$$

where h is Planck’s constant, κ_B is Boltzmann’s constant, V is the atomic volume, and V_m is the average sound velocity derived from the longitudinal (v_l) and transverse (v_t) sound velocities:

$$V_m = \left[\frac{1}{3} \left(\frac{2}{v_t^3} + \frac{1}{v_l^3} \right) \right]^{\frac{-1}{3}} \quad (3),$$

The sound velocities were obtained from the elastic constants using

$$v_l = \sqrt{\frac{3B+4G}{3\rho}} ; \quad v_t = \sqrt{\frac{G}{\rho}} \quad (4),$$

where ρ is the mass density of the material. The Grüneisen parameter γ , which quantifies lattice anharmonicity, was estimated from the Poisson ratio ν using the empirical relation

$$\gamma = \frac{3(1+\nu)}{2(2-3\nu)} \quad (5).$$

The Slack model is primarily intended for capturing comparative trends rather than fully quantitative anharmonic phonon transport behavior. More rigorous treatments based on third-order interatomic force constants and anharmonic phonon scattering as implemented in Phono3py package [43]. Within the CRTA, the electrical conductivity and electronic thermal conductivity are given by [42]:

$$\sigma = \sigma_0 \tau \quad \text{and} \quad \kappa_e = L \sigma T \quad (6) ,$$

where σ_0 is the conductivity pre-factor obtained from the electronic band structure, τ is the carrier relaxation time, L is the Lorenz number, and T is the absolute temperature. The transport coefficients are evaluated through the transport distribution function $\Sigma(\varepsilon)$, defined as [42]

$$\Sigma(\varepsilon) = \frac{1}{N_k} \sum_{n,k} v_{nk}^2 \tau_{nk} \delta(\varepsilon - \varepsilon_{nk}) \quad (7),$$

where v_{nk} is the group velocity of band n at wavevector k , τ_{nk} is the relaxation time, and ε_{nk} is the band energy. The Seebeck coefficient S is then obtained from the first and zeroth moments of the transport distribution function as [44]

$$S = \frac{1}{eT} \frac{K_1}{K_0} \quad (8) ,$$

where

$$K_1 = \int \Sigma(\varepsilon) (\varepsilon - \mu)^i \left(-\frac{\partial f}{\partial \varepsilon} \right) d\varepsilon \quad (9) ,$$

with e being the elementary charge, μ the chemical potential, f the Fermi–Dirac distribution function, and T the absolute temperature.

The formation energy (E_f) of the pristine and doped compounds was evaluated to assess thermodynamic stability using:

$$E_f = E_{tot} - \sum_i n_i \mu_i \quad (11) ,$$

where E_{tot} is the total energy of the compound, n_i and μ_i represent the number and chemical potential of the constituent elements, respectively. The chemical potentials of Na, Li, Mg and Bi, were taken from their most stable elemental phases. For doped systems such as $\text{Na}_{0.75}\text{Li}_{0.25}\text{MgBi}$, $\text{Na}_{0.50}\text{Li}_{0.50}\text{MgBi}$ and

$\text{Na}_{0.25}\text{Li}_{0.75}\text{MgBi}$, the formation energies were evaluated relative to the corresponding pristine and elemental reference states.

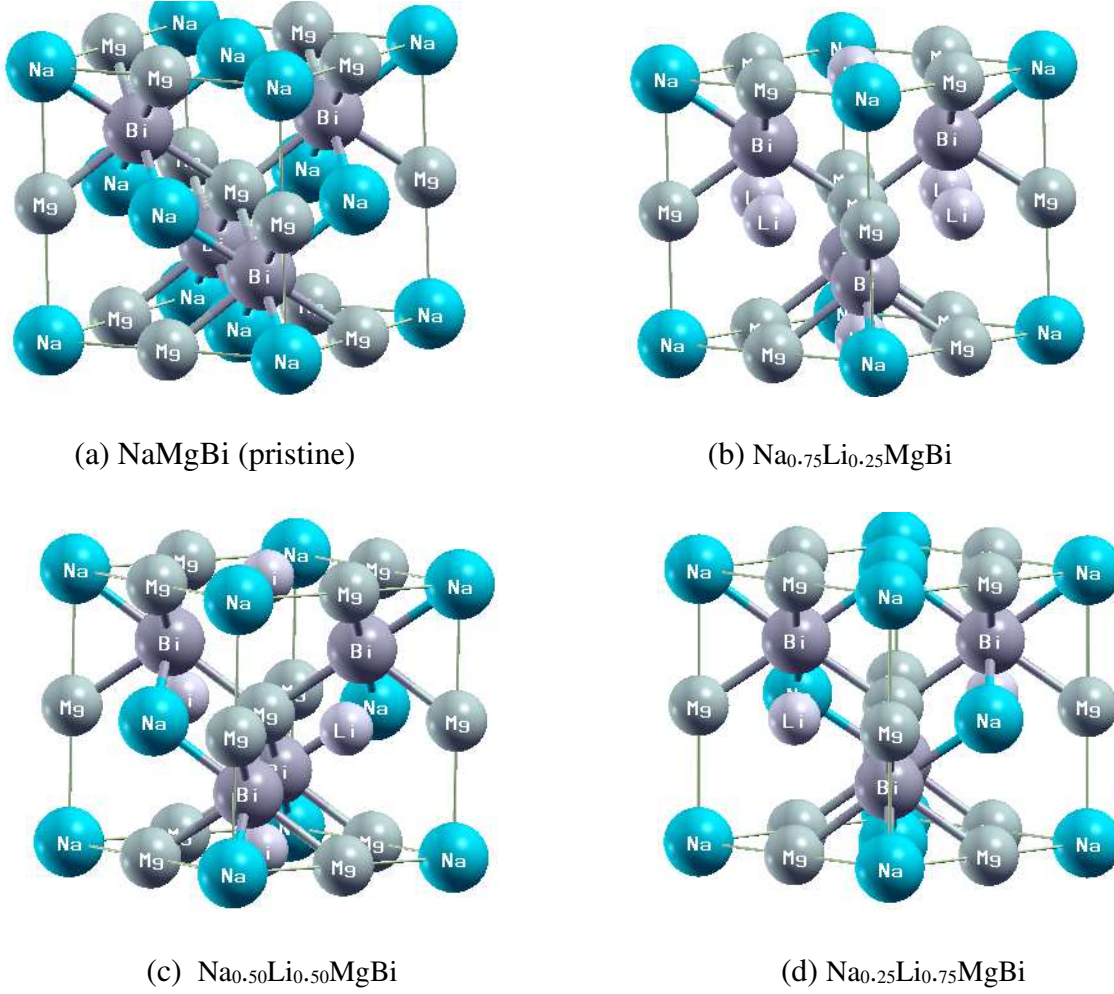


Figure 1: Optimized crystal structures of $\text{Na}_{1-x}\text{Li}_x\text{MgBi}$ compounds: (a) NaMgBi ($x = 0$) (b) $\text{Na}_{0.75}\text{Li}_{0.25}\text{MgBi}$ ($x = 0.25$) (c) $\text{Na}_{0.50}\text{Li}_{0.50}\text{MgBi}$ ($x = 0.50$) and (d) $\text{Na}_{0.25}\text{Li}_{0.75}\text{MgBi}$ ($x = 0.75$)

The optimized crystal structures of NaMgBi and its Li-alloyed derivatives, $\text{Na}_{1-x}\text{Li}_x\text{MgBi}$ ($x = 0.25, 0.50, 0.75$), were obtained by fully relaxing both atomic positions and lattice parameters until the residual forces and total energy converged within the selected thresholds.

3. Results and Discussion

In this section, we present the analysis of the structural, mechanical, electronic, and thermoelectric properties of NaMgBi and $\text{Na}_{1-x}\text{Li}_x\text{MgBi}$ ($x = 0.25, 0.50, 0.75$) alloys. The results are discussed in the context of both the underlying atomic and electronic structure and their impact on thermoelectric performance. Emphasis is placed on understanding how Li alloying influences lattice stability, electronic band dispersion, carrier transport, and phonon scattering, thereby governing the overall figure of merit (ZT). Comparisons with previously reported theoretical and experimental studies are

made to highlight the significance of the observed trends and the potential of these half-Heusler compounds for high-efficiency thermoelectric applications.

3.1. Structural Properties and Stability

All compositions retain the cubic half-Heusler structure with space group F-43m, confirming that Li substitution preserves the overall crystal symmetry of the pristine compound. The relaxed pristine and Li-doped NaMgBi are shown in Figure 1. Also, Table 1 presents the optimized lattice parameters and formation energies of NaMgBi and $\text{Na}_{1-x}\text{Li}_x\text{MgBi}$ alloys. The calculated lattice parameters of the investigated cubic model structures are consistent with previously reported theoretical studies on cubic half-Heusler type NaMgBi system [21]. The negative formation energies suggest relative energetic favourability of the investigated configurations. We note however that the calculated formation energies for Li-doped systems are relatively small and, in some cases, slightly positive, indicating possible metastable character within the adopted structural framework. Such metastable phases may remain experimentally accessible under non-equilibrium synthesis conditions [44, 45, 46]. It should be stated also that formation energy alone does not provide a complete assessment of thermodynamic stability with respect to competing phases. A more rigorous evaluation involving AIMD simulations, phonon or/and convex-hull analysis would further clarify the synthesizability of the investigated compounds [37-39]. This remains an important subject for our future study of this and similar materials.

Table 1: Calculated lattice parameter a , unit cell volume, and formation energy of $\text{Na}_{0.50}\text{Li}_{0.50}\text{MgBi}$ and $\text{Na}_{1-x}\text{Li}_x\text{MgBi}$ alloys compared with available literature data.

Compound	a (This work)	A (Literature)	Volume ($\text{\AA}^3$)	E_{form} (eV/atom)
NaMgBi	6.99	7.06 [14]	341.5	-0.732
$\text{Na}_{0.75}\text{Li}_{0.25}\text{MgBi}$	7.08	—	354.9	-0.006
$\text{Na}_{0.50}\text{Li}_{0.50}\text{MgBi}$	7.00	—	343.0	0.006
$\text{Na}_{0.25}\text{Li}_{0.75}\text{MgBi}$	6.91	—	329.9	-0.009

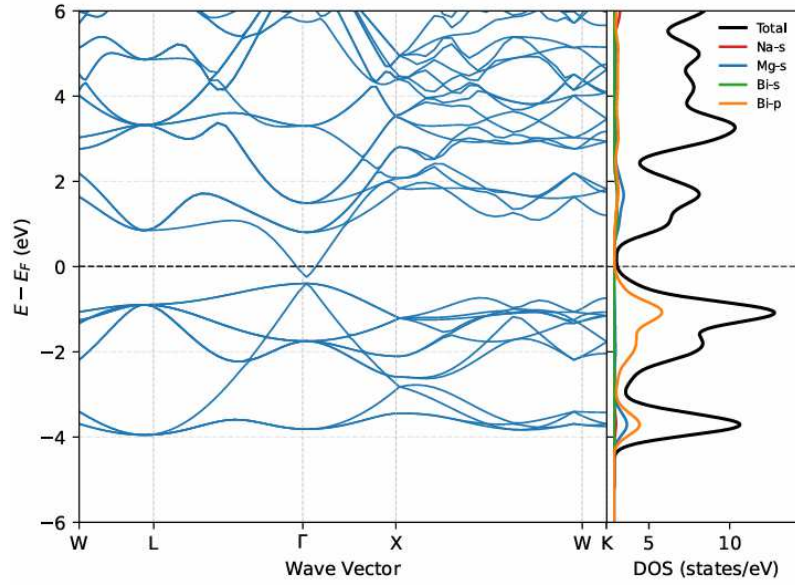
The mechanical stability of the $\text{Na}_{1-x}\text{Li}_x\text{MgBi}$ compounds was examined through their elastic properties. For a cubic structure, Born stability criteria are: $C_{11} > 0$, $C_{44} > 0$, $C_{11} - C_{12} > 0$, and $C_{11} + 2C_{12} > 0$. Using the calculated values of elastic constants for all the stoichiometries as stated Table 2, we confirm that the stability criteria are indeed satisfied. Furthermore, calculated bulk, shear, and Young's moduli indicate that the investigated compounds possess adequate resistance to both volume and shear deformations. Poisson's ratios suggest that these materials exhibit predominantly ductile mechanical behavior, which is desirable for thermoelectric devices subjected to thermal cycling and fabrication processes [21].

Table 2: Calculated elastic constants (C_{ij}), bulk modulus (B), shear modulus (G), Young's modulus (E) in GPa, Poisson's ratio (ν), and Debye temperature (Θ_D) for NaMgBi and $\text{Na}_{1-x}\text{Li}_x\text{MgBi}$ compounds.

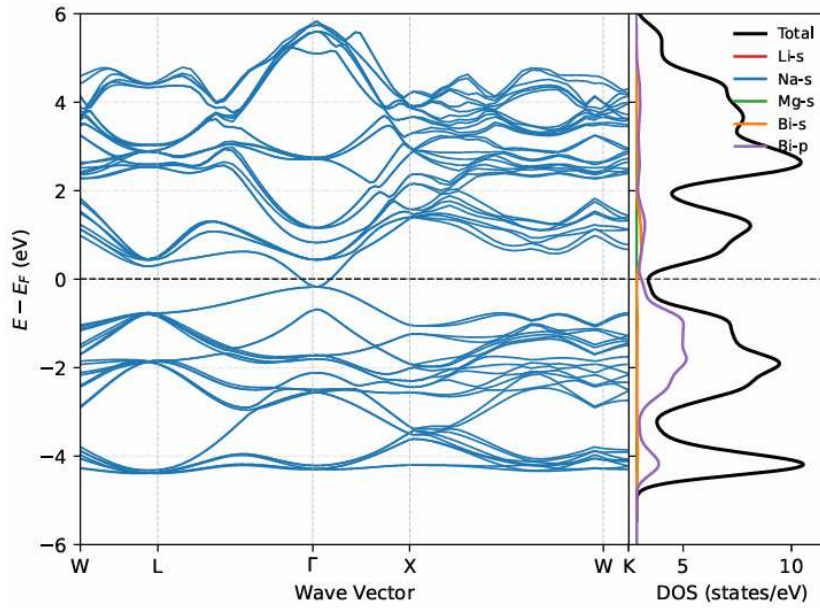
Compound	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	B (GPa)	G (GPa)	E (GPa)	ν	Θ_D (K)
NaMgBi	48.4	15.3	22.6	26.4	19.9	47.8	0.20	217.4
$\text{Na}_{0.75}\text{Li}_{0.25}\text{MgBi}$	46.1	12.5	22.8	23.7	20.2	47.2	0.17	219.5
$\text{Na}_{0.50}\text{Li}_{0.50}\text{MgBi}$	33.1	0.9	14.9	11.6	15.2	31.8	0.04	193.2
$\text{Na}_{0.25}\text{Li}_{0.75}\text{MgBi}$	48.9	13.9	25.9	25.6	22.1	51.5	0.16	229.8

3.2. Electronic properties and thermoelectric characteristics

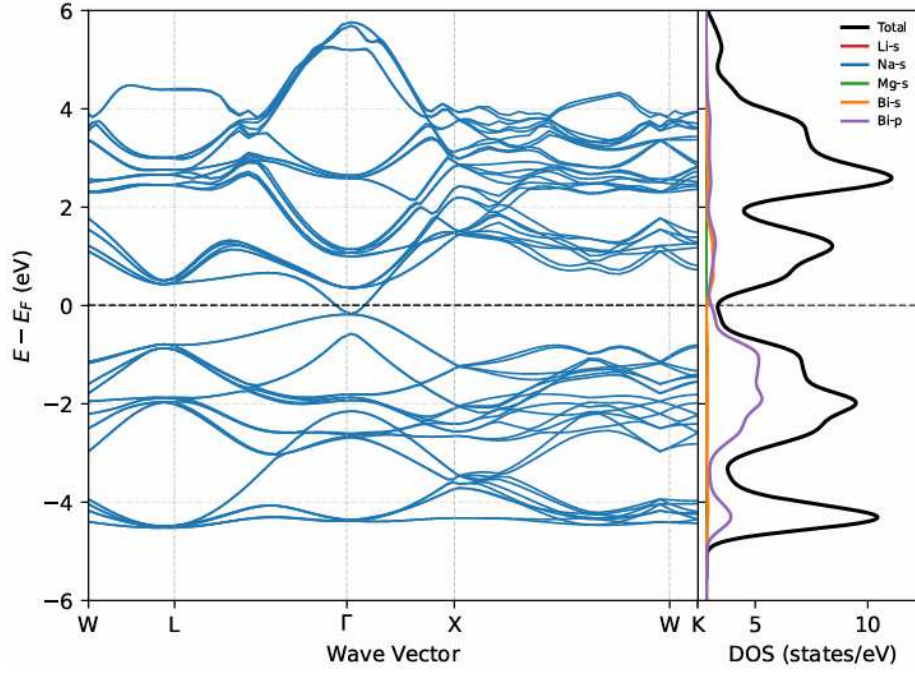
The electronic band structures and the density of states (DOS) as obtained for NaMgBi and $\text{Na}_{1-x}\text{Li}_x\text{MgBi}$ ($x = 0.25, 0.50, 0.75$) stoichiometries are shown in Fig. 2(a-d). The effect of spin-orbit coupling (SOC) has been included. All the investigated compositions exhibit a semi-metallic or near-zero-gap electronic band character, with pristine NaMgBi displaying a very small gap of approximately 0.01 eV. Increasing Li content drives the system toward a fully gapless electronic structure.



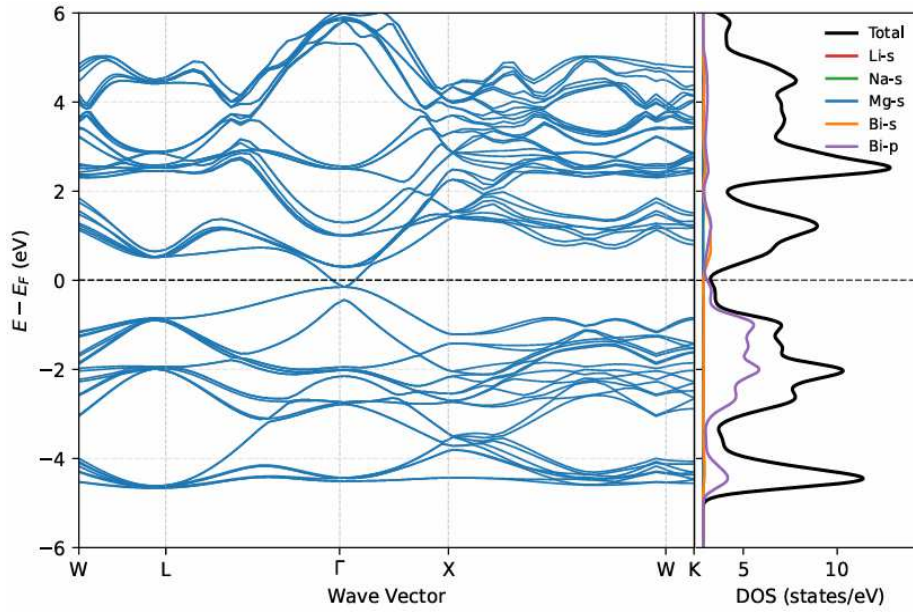
(a)



(b)



(c)



(d)

Figure 2: Electronic band structures (left) and the density of states (DOS, right) of (a) NaMgBi ($x = 0$) (b) $\text{Na}_{0.75}\text{Li}_{0.25}\text{MgBi}$ ($x = 0.25$) (c) $\text{Na}_{0.50}\text{Li}_{0.50}\text{MgBi}$ ($x = 0.50$) and (d) $\text{Na}_{0.25}\text{Li}_{0.75}\text{MgBi}$ ($x = 0.75$) calculated with spin-orbit coupling. The figures illustrate the evolution of the semi-metallic character and band dispersion near the Fermi level with increasing Li content, highlighting the influence of Li alloying on the electronic structure.

This behaviour is characteristic of Bi-based half-Heusler compounds [22], where strong relativistic effects lead to band inversion and narrow-gap or semi-metallic states near the Fermi level. In NaMgBi, the valence- and conduction-band edges occur near high-symmetry points of the Brillouin zone [22, 47], however, Li substitution modifies their relative positions and curvature, resulting in enhanced band overlap and increased dispersion near the Fermi level. These changes modify the relative contributions of electron-like and hole-like carriers near the Fermi level and introduce increased asymmetry in the electronic transport distribution, which is beneficial for FeNbSb-based alloys performance [3]. This behavior contributes to enhanced thermopower through increased density-of-states effective mass and favorable carrier-energy filtering effects.

Although the calculated band structures indicate semi-metallic or near-gapless electronic behavior, the transport properties are governed not only by the position of the Fermi level but also by the asymmetry of carrier velocities and density of states near the Fermi energy [36]. Consequently, hole-like transport contributions remain dominant, leading to positive Seebeck coefficients across the investigated temperature range [48]. Projected density of states (PDOS) analysis indicates that electronic states near the Fermi level are dominated by Bi-*p* orbitals, with minor contributions from Mg-*s* states, while Na and Li states are largely absent. This confirms that alkali-metal substitution acts primarily as a band structure modulator rather than a direct carrier dopant [18]. Li incorporation induces a redistribution of Bi-*p* states and a moderate flattening of bands near the valence-band maximum. This leads to an increase in the density-of-states effective mass and enhanced the Seebeck coefficient (*S*), in particular for Na_{0.25}Li_{0.75}MgBi. Also, at a moderate Li concentration such as $x = 0.25$, i.e., Na_{0.75}Li_{0.25}MgBi, sufficient band dispersion is retained to support high carrier mobility. It should be noted that high *S* and high electrical conductivity (σ) result in a high figure of merit (*ZT*). In essence, the electronic band analysis shows that Li alloying of NaMgBi may serve as an effective control over band dispersion and carrier asymmetry near the Fermi level thus establishing alkali-metal substitution as a viable electronic optimization strategy for Bi-based half-Heusler thermoelectric materials, as we have shown. Other reported approaches for enhancing thermoelectric properties include bandgap modification via heavy doping as has been demonstrated for conventional semiconducting half-Heusler thermoelectrics such as TiNiSn, ZrNiSn, and HfCoSb. [49, 50, 51]

3.3. Thermoelectric properties

Here, the thermoelectric properties of pristine NaMgBi and Na_{1-x}Li_xMgBi ($x = 0.25, 0.50, 0.75$) alloys are systematically investigated. The key transport parameters examined include the Seebeck coefficient (*S*), electrical conductivity (σ), electronic thermal conductivity (κ_e), lattice thermal conductivity (κ_L), power factor (*PF*), and the dimensionless figure of merit (*ZT*). A comparative analysis of these quantities for the pristine and alloyed systems enables a clear assessment of the impact of Li substitution on thermoelectric performance and its underlying electronic origin. Figures 3(a–f) illustrates the temperature evolution of these key thermoelectric parameters. Collectively, these trends provide a coherent picture of how alkali-metal alloying simultaneously modifies electronic structure and phonon transport, thereby governing the overall thermoelectric efficiency of NaMgBi-based half-Heusler alloys.

3.3.1. Seebeck Coefficient, *S*

The temperature dependence of the Seebeck coefficient for NaMgBi and Na_{1-x}Li_xMgBi alloys is presented in Fig. 3(a). All compositions exhibit positive Seebeck coefficients throughout the investigated temperature range, indicating dominant *p*-type charge carrier transport. The Seebeck

coefficient initially increases with temperature and subsequently exhibits a gradual reduction at higher temperatures, consistent with the onset of thermally activated bipolar transport effects commonly observed in narrow-gap and semi-metallic thermoelectric systems [48, 52]. Although bipolar transport effects become increasingly noticeable at elevated temperatures, relatively high Seebeck coefficients are maintained due to favorable band asymmetry and the modified electronic structure induced by Li alloying [36]

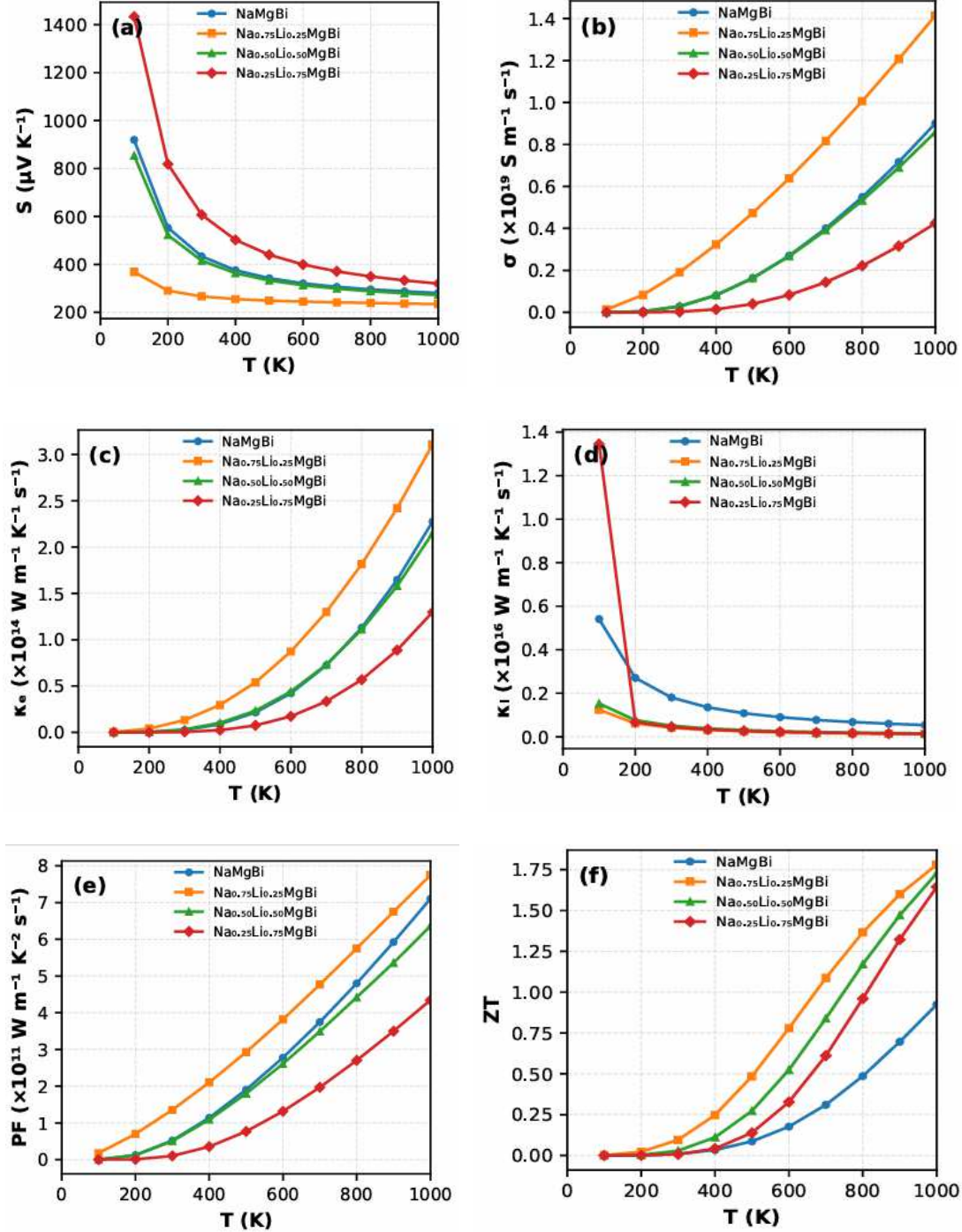


Figure 3: Temperature-dependent thermoelectric transport properties of $\text{Na}_{1-x}\text{Li}_x\text{MgBi}$ ($x = 0$ (blue line); 0.25 (yellow line); 0.50 (green line), 0.75 (red line)) alloys: (a) Seebeck coefficient (S), (b) electrical conductivity (σ), (c) electronic thermal conductivity (κ_e), (d) lattice thermal conductivity (κ_l), (e) power factor (PF), and (f) dimensionless figure of merit (ZT).

3.3.2. *Electrical conductivity, σ*

The temperature dependence of the electrical conductivity is shown in Fig. 3(b). Electrical conductivity generally increases with temperature for all investigated compositions, indicating thermally activated carrier transport behavior characteristic of semi-metallic and narrow-gap systems. As summarized in Table 3, the maximum electrical conductivity obtained for $\text{Na}_{0.75}\text{Li}_{0.25}\text{MgBi}$ is approximately $1.4 \times 10^{19} \text{ S}/(\text{m}\cdot\text{s})$. This enhanced conductivity arises from an optimal balance between carrier concentration and mobility achieved through moderate Li substitution. At this composition, the semi-metallic band structure provides a high carrier density, while alloy disorder remains sufficiently weak to preserve carrier mobility. With increasing Li content beyond $x = 0.25$, the electrical conductivity decreases, as observed for $\text{Na}_{0.50}\text{Li}_{0.50}\text{MgBi}$ and $\text{Na}_{0.25}\text{Li}_{0.75}\text{MgBi}$. This reduction can be attributed to increased alloy disorder and mass fluctuation scattering, which more strongly impede carrier transport despite the continued presence of a high density of states near the Fermi level. In contrast, pristine NaMgBi exhibits lower electrical conductivity than the optimally substituted alloy due to a less favorable balance between band dispersion and carrier scattering [53].

Compared with conventional semiconducting half-Heusler thermoelectric materials such as ZrNiSn and HfCoSb , which typically require heavy doping to achieve comparable conductivity levels, the NaMgBi -based alloys intrinsically possess favourable electrical transport properties owing to their semi-metallic electronic structures. This intrinsic conductivity, combined with tunability through alkali-metal substitution, highlights the effectiveness of Li alloying as a strategy for optimizing charge transport in Bi-based half-Heusler thermoelectrics [49, 50, 51].

3.3.3. *Thermal Conductivity*

The evolution of the total thermal conductivity (κ) for NaMgBi and $\text{Na}_{1-x}\text{Li}_x\text{MgBi}$ alloys is summarized in Fig. 3 (c, d) and quantitatively compared in Table 3. A clear and systematic reduction in κ is observed with increasing Li content, highlighting the role of Li alloying in suppressing heat transport [54]. Specifically, κ decreases from $7.7 \times 10^{14} \text{ Wm}^{-1} \text{ K}^{-1}$ for pristine NaMgBi to $2.6 \times 10^{14} \text{ Wm}^{-1} \text{ K}^{-1}$ for $\text{Na}_{0.25}\text{Li}_{0.75}\text{MgBi}$, corresponding to a reduction of nearly 66%. The reduction in thermal conductivity is associated with enhanced phonon scattering arising from alloy disorder and lattice softening induced by Li substitution [56]. The large mass contrast between Na and Li disrupts phonon propagation, shortens phonon mean free paths, and enhances anharmonic phonon-phonon interactions. In addition, the reduced elastic moduli and Debye temperatures (Table 2) indicate lattice softening, which further suppresses lattice thermal conductivity through increased phonon anharmonicity.

Among the compositions investigated, $\text{Na}_{0.25}\text{Li}_{0.75}\text{MgBi}$ exhibits the lowest κ , reflecting the strongest alloy disorder and phonon scattering effects. While increased Li content leads to a modest reduction in electrical conductivity (Table 3), the substantial suppression of thermal conductivity more than compensates for this effect, resulting in an overall enhancement of the thermoelectric figure of merit. Compared to conventional half-Heusler thermoelectrics, which typically exhibit lattice thermal conductivities exceeding $8\text{--}10 \text{ Wm}^{-1} \text{ K}^{-1}$ and require extensive nanostructuring, the present alloys achieve intrinsically low thermal conductivity through chemical alloying alone [42]. These results demonstrate that Li alloying is an efficient phonon-engineering strategy in NaMgBi -based half-Heusler systems, enabling significant thermal conductivity reduction while maintaining favorable electronic transport properties. Finally, it is important to note that the present analysis is

based on the semi-empirical Slack model and therefore primarily captures relative alloying trends in lattice thermal conductivity. Explicit anharmonic phonon calculations would be valuable for a much detailed and quantitative validation.

Table 3: Calculated thermoelectric transport parameters of NaMgBi and $\text{Na}_{1-x}\text{Li}_x\text{MgBi}$ alloys at 1000 K. The table lists the Seebeck coefficient (S), electrical conductivity (σ), total thermal conductivity (κ), and the resulting figure of merit (ZT). The results show that Li substitution enhances thermoelectric performance, with $\text{Na}_{0.75}\text{Li}_{0.25}\text{MgBi}$ exhibiting the highest ZT .

Compound	S ($\mu\text{V/K}$)	σ (S/ms)	κ (W/mKs)	ZT
NaMgBi	281	9.0×10^{18}	7.7×10^{14}	0.92
$\text{Na}_{0.75}\text{Li}_{0.25}\text{MgBi}$	234	1.4×10^{19}	4.3×10^{14}	1.78
$\text{Na}_{0.50}\text{Li}_{0.50}\text{MgBi}$	272	8.6×10^{18}	3.7×10^{14}	1.72
$\text{Na}_{0.25}\text{Li}_{0.75}\text{MgBi}$	320	4.2×10^{18}	2.6×10^{14}	1.64

3.3.4. Power Factor

The power factor ($PF = S^2\sigma$), shown in Fig. 3(e), exhibits a pronounced enhancement upon Li substitution, highlighting the effectiveness of alkali-metal alloying in optimizing electronic transport [18]. As summarized in Table 3, $\text{Na}_{0.75}\text{Li}_{0.25}\text{MgBi}$ achieves the highest power factor among the investigated compositions. Although its Seebeck coefficient ($234 \mu\text{V/K}$) is slightly lower than those of pristine NaMgBi and Li-rich alloys, this reduction is more than offset by a substantial increase in electrical conductivity ($1.4 \times 10^{19} \text{ S/ms}$), indicating an optimal balance between carrier concentration and mobility [42]. In contrast, higher Li contents (e.g., $\text{Na}_{0.25}\text{Li}_{0.75}\text{MgBi}$) yield enhanced thermopower but suffer from reduced electrical conductivity due to increased alloy disorder scattering, which limits the achievable power factor. The enhanced PF at intermediate Li concentrations is attributed to favorable electronic band structure modifications near the Fermi level, enabling improved carrier transport without severe degradation of thermopower. Notably, the resulting power factor values are comparable to those reported for optimized half-Heusler and PbTe-based thermoelectric materials [4], underscoring the competitiveness of NaMgBi-based alloys and demonstrating that simple alkali-metal alloying can effectively yield high power factors in semi-metallic half-Heusler systems.

3.3.5. Figure of Merit

The cumulative optimization of electronic and thermal transport properties is reflected in the dimensionless thermoelectric figure of merit ZT , presented in Fig. 3 and summarized in Table 3. Relative to pristine NaMgBi ($ZT = 0.92$), all Li-substituted alloys exhibit a pronounced enhancement in thermoelectric performance, demonstrating the effectiveness of alkali-metal alloying in simultaneously tuning charge and heat transport [18]. It is noteworthy to mention that the ZT value obtained for the pristine NaMgBi, of ≈ 0.92 at 1000 K is slightly less than 1.15 reported in [22] for a monolayer (ML) of the same compound at a temperature of 500 K. This underscores the dimensional effect in determining the ZT values of the same compound, i.e., bulk versus monolayer. Compound $\text{Na}_{0.75}\text{Li}_{0.25}\text{MgBi}$ is predicted to exhibit the highest thermoelectric figure of merit, reaching $ZT \approx 1.78$ at 1000 K within the adopted computational framework. This superior performance originates from an optimal interplay between a high-power factor and significantly suppressed thermal conductivity. As shown in Table 3, this composition maintains a high electrical conductivity ($1.4 \times 10^{19} \text{ S/ms}$) while preserving a sizable Seebeck coefficient ($234 \mu\text{V/K}$), resulting in the largest power factor across the series. Concurrently, its thermal conductivity is reduced by

nearly 45% compared with pristine NaMgBi, reflecting enhanced phonon scattering induced by mass fluctuation and lattice disorder [12, 13].

Although Li-rich compositions such as Na_{0.25}Li_{0.75}MgBi exhibit even lower thermal conductivity, their reduced electrical conductivity limits further improvement in ZT , highlighting the necessity of balancing electronic and phononic contributions [34]. The predicted ZT values obtained in the present work are comparable to several reported half-Heusler and Mg₃Sb₂-based thermoelectric systems [11, 12, 45, 46, 47]. For example, FeNbSb-based half-Heusler alloys have achieved ZT values in the range of 1.4–1.6 through band engineering and multicomponent alloying strategies, while optimized Mg₃Sb₂-based compounds have approached $ZT \approx 2$ through defect and microstructural engineering [11]. The competitive performance predicted for Li-alloyed NaMgBi therefore highlights the potential relevance of alkali-metal alloying in tuning thermoelectric transport properties.

4. Conclusions

In this work, we have conducted a comprehensive first-principles investigation of the structural, mechanical, electronic, and thermoelectric properties of NaMgBi and Na_{1-x}Li_xMgBi ($x = 0.25, 0.50, 0.75$) half-Heusler alloys. The investigated cubic model configurations satisfy the elastic stability criteria and exhibit energetically favorable formation characteristics within the adopted computational framework. All the compositions were found to be mechanically stable, while Li substitution of Na induces lattice softening and enhanced mass-disorder scattering with attendant significant reduction of the lattice thermal conductivity. Electronic structure analysis revealed that alkali-metal alloying modifies the band dispersion near the Fermi level, suppresses electron–hole compensation, and increases the Seebeck coefficient while preserving adequate electrical conductivity. Li alloying further modifies carrier asymmetry near the Fermi level, enhances phonon scattering through alloy disorder, and contributes to improved thermoelectric transport behavior. These combined effects result in a pronounced enhancement of thermoelectric performance, with Na_{0.75}Li_{0.25}MgBi achieving a maximum figure of merit $ZT \approx 1.78$ at about 1000 K. The present study demonstrates that Li alloying offers an effective and scalable route for simultaneously optimizing electronic and phonon transport in semi-metallic half-Heusler compounds, highlighting the potential of NaMgBi-based alloys as high-efficiency and environmentally friendly thermoelectric materials. Finally, we wish to stress that the present study primarily aims to provide a comparative first-principles assessment of Li-alloying effects in cubic half-Heusler-type NaMgBi systems. While the approaches employed provide important qualitative insights into the interplay between electronic transport and phonon scattering, more rigorous investigations involving deformation potential-based carrier relaxation times, anharmonic phonon transport calculations, convex-hull stability analysis, and finite-temperature dynamical stability simulations would further strengthen the quantitative predictions and remain important directions for future work [37–39].

CRediT authorship contribution statement

Solomon T. Tonga: Writing – original draft, Software, Methodology, Formal analysis, Conceptualization. **J. B. Yerima:** Writing – review & editing, Supervision. **A. D. Ahmed:** Writing – review & editing. **L. Mongalo:** Writing– review & editing, Software. **Abdulrafiu T. Raji:** Writing – review & editing, Software, Methodology, Formal analysis, Conceptualization.

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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Data availability

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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