International Astronomy and Astrophysics Research Journal

Volume 6, Issue 1, Page 49-58, 2024; Article no.IAARJ.123147

Density Functional Theory(DFT) Study of Alkali-Metal-Based Half-Heusler Compound NaCrSb

Michael E. Ishaje [a*], Anozie Faustina [a] and Godwin O. Igomah [b]

[a] University of Cross River State, Calabar, Nigeria.
[b] University of Calabar, Calabar, Nigeria.

Authors' contributions

This work was carried out in collaboration among all authors. Author MEI designed the method and conducted the computational simulation using quantum espresso simulation software. Author AF wrote the introductory background, literature, and materials. Author GOI managed the analyses of the study. All authors read and approved the final manuscript.

Article Information

Open Peer Review History:
This journal follows the Advanced Open Peer Review policy. Identity of the Reviewers, Editor(s) and additional Reviewers, peer review comments, different versions of the manuscript, comments of the editors, etc are available here: https://www.sdiarticle5.com/review-history/123147

Original Research Article

Received: 12/07/2024
Accepted: 15/09/2024
Published: 23/09/2024

ABSTRACT

In this study we investigated half-heusler alloy (NaCrSb) using density functional theory as implemented in Quantum espresso software version qe-6.8 for simulation on ubuntu operating system version 22.04LTS. The Perdew-Burke-Ernzerhof (PBE) generalized gradient approximation (GGA) was used for the exchange-correlation potential. The projector augmented-wave (PAW) method was employed to described the core electrons. The Quantum ESPRESSO input file used sets up a self-consistent field (SCF) calculation for a spin-polarized system within a face-centered cubic (fcc) lattice structure. The electrons section focuses on convergence settings for the SCF procedure, specifying the mixing factor (mixing_beta) and the diagonalization algorithm (Davidson).

**Corresponding author: E-mail: ishajemichael@unicross.edu.ng;*

Cite as: *Ishaje, Michael E., Anozie Faustina, and Godwin O. Igomah. 2024. "Density Functional Theory(DFT) Study of Alkali-Metal-Based Half-Heusler Compound NaCrSb". International Astronomy and Astrophysics Research Journal 6 (1):49-58. https://www.journaliaarj.com/index.php/IAARJ/article/view/103.*

The atomic species and atomic positions sections detail the types of atoms present, their masses, and the corresponding pseudopotentials. The material NaCrSb is structurally stable from studied at beta (β)-phase. The half-Heusler alloy has measured band gap of 1.93eV was obtained for NaCrSb, with a range of values. This indicates that NaCrSb is an indirect bandgap semiconductor material. The compound NaCrSb exhibits behavior during spin up and down that is characteristic of both metals and semiconductors, which foretells the half-metallic Heusler alloy. The B/G ratio of 2.53 indicates that the NaCrSb material is ductile. The material's resistance to impact is addressed holistically by the Vicker's hardness. Na-1s and Na-3s; Cr-1s, Cr-2p, Cr-3s; and Sb-1s, Sb- 2s, Sb - 3p has high orbital contribution for the Na,Cr, and Sb-atoms. At fermi energy both the spin up and spin down is at zero point in plot of partial density of state(PDOS) against energy. It became vivid from this that NaCrSb is a half-metallic Heusler alloy. Positive frequencies were detected in the phonon dispersion curves along the $\Gamma - X - \mathrm{K} - \Gamma - \mathrm{L} - \mathrm{W} - X$ high symmetry directions. This suggests that NaCrSb is dynamically stable. The search for new materials with special qualities is what propels progress in materials research and technology.

Keywords: Half-heusler; Half-metallic; electronic band structure; mechanical properties; density of state; phonon; alloy.

1. INTRODUCTIONS

The origin of the name half Heusler" stems from their structural similarity to heusler alloys which have similar crystal structure but are composed of equal proportions of two metallic elements. The thermoelectric applications of half heusler alloy are particularly noteworthy, as they can efficiently convert waste heat into electricity or vice versa. This property is crucial for energy harvesting and power generation technologies.

Additionally, half heusler alloys have shown promise in magnetic refrigeration, spintronics and catalysis. [1] Half-Heusler alloy exhibit promising thermoelectric properties. [2] Half Heusler thermoelectric materials for applications in power generation and refrigeration. Half-Heusler alloy are a class of intemetallic compounds with the chemical formula xyz, where x is typically a transition metal. Y is a metal (e.g. Co, Fe), and Z is metalloid (e.g. Ti, Zr). [3].

Importance of density functional theory (DFT) density functional theory is a powerful computational method used to study the electric structure, energetic and properties of materials at the atomic scale. It provides a theoretical framework for predicting the behaviour of materials base on the principles of quantum mechanics, without the need for empirical parameters. DFT calculations have been widely employed to investigate the properties of Half-Heusler Alloys, offering insights into their structural stability, electronic properties, mechanical behaviour, thermodynamic stability and phonon properties.DFT calculations are used to determine the equilibrium crystal structure of Half-Heusler alloys including lattice parameters, atomic positions and structural stability. Studies have investigate the effects of composition, doping and strain on the structural properties of Half-Heusler alloys [4].

DFT enables the calculations of electronic band structures, density of states (DOS) and change densities of Half-Heusler alloys. These properties are crucial for understanding the materials electrical conductivity, band gap and electronic transport behavour, first principles calculations have been used to predict the electronic properties of Half-Heusler alloys and identify potential candidates for thermoelectric application [5]. DFT can determine various mechanical properties of Half-Heusler alloys, such as elastic constants, bulk modulus, shear modulus and young's modulus. These properties are essential for understanding the materials stability, deformation behaviour and response to external forces. [6]

DFT calculations can predict the thermodynamic stability, formation enthalpy and phase diagrams of Half-Heusler alloys under different temperature and pressure conditions. These thermodynamic properties provides insights into the materials' stability range and phase transitions, guiding experimental synthesis effects [7].

DFT-based phonon properties calculations can be determine dispersion relations, phonon densities of states and thermal properties (e.g. specific heat capacity thermal conductivity) of Half-Heusler alloys phonon properties are crucial

for understanding the materials' thermal transport behaviour and phonon-mediated thermal conductivity [8].

In addition to their electronic and magnetic properties, Half-Heusler alloys also demonstrate excellent mechanical stability and computability making them suitable various structural applications their robustness and resistance to corrosion further enhance their appeal for engineering application in harsh environments. Overall, the rich and tunable properties of Half-Heusler alloys continue to fuel research interest and exploration in materials science and engineering, with ongoing advancements in synthesis, characterization techniques and computational modeling, these alloys hold great promise for addressing challenges in energy conversion, electronics and beyond, paving the for innovative technologies with enhanced performance and efficiency. The project is aimed at studying that structural, electronic, mechanical, density of state, and phonon properties of Half-Heusler alloy NaCrSb using density functional theory [9].

2. LITERATURE REVIEW

Our DFT calculation reveal the crystal structure, electronic band structure, phonon dispersion curves and thermodynamic stability of CoTiSb. Additionally, we analyze its mechanical properties, including elastic constants and shear modulu our findings provide valuable insights into the material's suitability for applications such as thermodynamics, spritronics, and catalysis. Overall, CoTiSb is a fascinating material with a wide range of potential applications. Its properties can be further optimized and tailored through careful material design, synthesis and characterization, paving the way for its use in advanced technologies [9].

Half-Heusler alloys, exemplified by the alloy NiMnSb, have garnered significant interest in the scientific community for their potential applications across various technological domains due to their distinct amalgamation of properties. This investigation utilizes density functional theory (DFT) calculations to delve into the intricies of structural, electronics, mechanical, thermodynamic and phonon attributes of NiMnSb. Employing DFT methodologies, we elucidate the crystalline framework, electronic band manifestation, phonon dispersion behaviours and thermodynamic robustness of the alloy. Additionally, mechanical traits such as elastic moduli and shear modulus are scrutinized, offering insights into the alloy's mechanical integrity. The outcomes of this study furnish valuable perspectives on the aptness of NiMnSb for diverse applications, encompassing fields such as thermodynamics, spintronics and catalysis. [10].

In this study it was revealed that NaCrGe is stable at beta phase. He obtained that the material is a narrow bandgap semiconductor half-Heusler alloys with measured gap of 1.050 eV. The structure NaCrGe conduction band minimum (CBM) position at gamma(Γ) and the valence band maximum (VBM) located at X-point of the Brillouin zone. This indicates that the alloy NaCrGe has indirect bandgap semiconductors. The material NaCrGe is considered hybrids between metals and semiconductors. Hence, NaCrGe is Half-metallic heusler alloy. The calculated mechanical properties indicate that NaCrGe possesses good mechanical stability, making it suitable for structural applications. B/G ratio for NaCrGe is 2.40. This implies that NaCrGe is "ductile" in nature at ambient condition. Also NaCrGe is confirmed "ductile" in nature at positive value of $C_{11} – C_{44}$ (+48.07). PDOS shows that Na-4p, Cr-4p and Ge- 2p has the highest orbital contribution for Na, Cr and Ge atoms respectively. At fermi energy both spin up and spin down is at zero point in the plot of projected density of state (PDOS) against energy. This revealed that NaCrGe is a half metallic heusler alloy. [11]

The structural, electronic, mechanical, and thermodynamic properties of N_2CaNa full Heusler alloys using density functional theory (DFT). Results for the structural analysis establish structural stability with a minimum formation energy of 29.9 eV. The compound is brittle and mechanically stable, having checked out with the Pugh criteria. The B/G ratio of bulk modulus B to shear modulus G for N2CaNa is 4.766, hence the material is ductile. N2CaNa alloy is ductile in nature. The Debye model correctly predicts the low-temperature dependence of heat capacity, which is proportional to Debye's T 3 law. Just like the Einstein model, it also recovers the Dulong–Petit law at high temperatures, suggesting the thermodynamic stability of the compounds at moderate temperatures. The results demonstrate potential N2CaNa for applications in spintronics, structural engineering, and other fields requiring materials with tailored properties. [12].

3. METHODOLOGY

In this study, we are delving into the structural, electronic, mechanical, thermodynamic and phonon properties of half heusler alloy (NaCrSb) using a computational technique of Density Functional Theory (DFT). This method is widely used in materials science to study how atoms arrange themselves in material and how they interact with each other. Quantum espresso software version qe-6.8 for simulation on ubuntu operating system version 22.04LTS. The Perdew-Burke-Ernzerhof (PBE) generalized gradient approximation (GGA) was used for the exchange-correlation potential. The projector augmented-wave (PAW) method was employed to describe the core electrons.

The Quantum ESPRESSO input file used sets up a self-consistent field (SCF) calculation for a spin-polarized system within a face-centered cubic (fcc) lattice structure. The control section specifies the type of calculation, file prefixes, and directories for pseudopotentials and temporary files. The system section defines key parameters such as the Bravais lattice index (ibrav=2), lattice parameter (celldm(1)), and the number of atoms (nat) and types (ntyp) in the unit cell. Additionally, it handles electronic state occupations using Marzari-Vanderbilt smearing and sets initial magnetizations for each atomic type, with a specified plane-wave kinetic energy cutoff (ecutwfc) to ensure the accuracy of the wavefunctions.[11,13,14,15]

The electrons section focuses on convergence settings for the SCF procedure, specifying the mixing factor (mixing_beta) and the diagonalization algorithm (Davidson). It also sets the maximum number of iterations (electron_maxstep) to ensure the calculation converges properly. These parameters are crucial for achieving a reliable and efficient solution to the electronic structure problem, especially for complex systems involving multiple atom types and spin polarization. [11,13,14,16,17].

The atomic species and atomic positions sections detail the types of atoms present, their masses, and the corresponding pseudopotentials. This includes sodium (Na), chromiun (Cr) , and Antimony(Sb) each with specific pseudopotential files. The k-points section defines the mesh for sampling the Brillouin zone, using an 8x8x8 grid with no shift, which is essential for accurately capturing the electronic properties of the material. This comprehensive setup ensures a thorough and precise simulation of the material's electronic and magnetic properties [11,18].

4. RESULTS AND DISCUSION

4.1 Structural Properties

In order to find the ground state geometry, geometry optimization for the purpose of determining structural attributes entails volume optimization, cell shape determination, and atomic position optimization. Making DFT calculations for every possible values of a=b and c and figuring out which one yields the lowest total energy is one method of figuring out a cell's shape. Using an DFT optimization process within QE is an alternate (and faster) method that looks for the set of lattice parameters, unit cell angles, and internal positions that result in a zero stress tensor (which automatically equates to a minimal total energy). The regular full-Heusler and half-Heusler compounds crystallize in the centrosym-metric and noncentrosymmetric cubic C1b structure, respectively, with the F $\bar{4}$3m (no. 216) space group in the centrosym-metric cubic L21 structure with the F $\bar{m}$3m (no. 225) space group, respectively. [19]. The phase is β(4b 4a 4c) phase. Fig. 1 is extracted using Xcrysden tools from the obtimizeds input files. The crystal structure of the β-phase phase of NaCrSb compound in Fig. 1 shows structural positions of atoms in their respective phases.

We performed Series of self-consistent calculations to optimised the structure of NaCrSb. The informational collections produced from the self-consistent energy computations were fitted to the third and fourth-order Birch-Murnaghan condition of state [20] and the optimized Lattice Constant(α_o), Bulk Modulus(B), pressure derivative(B') and minimum energy (E_{min}) were obtained. The bulk modulus estimates how safe a material is to impressibility and its pressure derivative estimates its reaction to slight expansion in pressure.

4.2 Electronic Band Structure

As shown in Fig. 2, the optimized latticed constants in high symmetry directions of the first Brillouin zone L – Γ – X – W – k – Γ have been used to compute the electronic band gap structural properties of the KCrAs alloy.

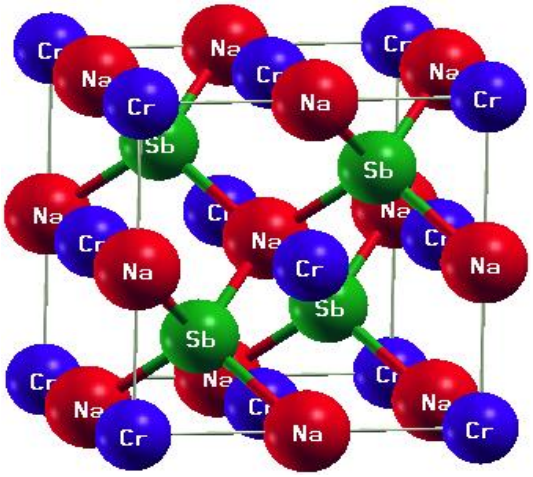

Fig. 1. The crystal structure of (a) α -phase (b) β -phase (c) γ -phase of NaCrSb compound

Table. 1. Structural Parameters for NaCrSb for β -phase phases considered

Compounds	Configurations	E(Ry)	a(Å)	B(Gpa)	B′
NaCrSb	β - Phase(4b 4a 4c)	455.75	12.81	37.2	4.58

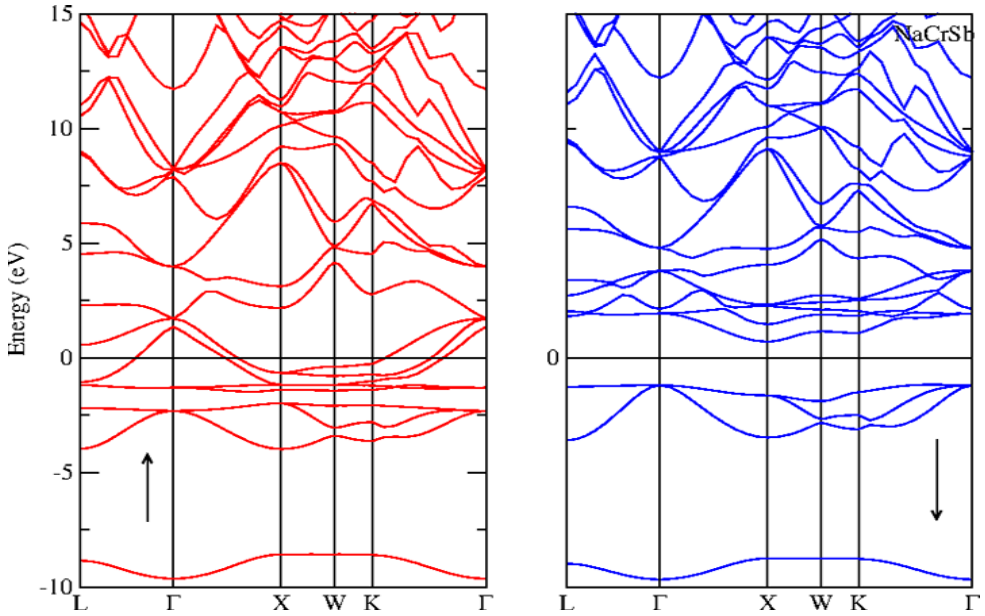

Fig. 2. Calculated electronic band structure of NaCrSb

For NaCrSb, a low bandgap semiconductor half-Heusler alloy at spin down, the measured band gap was 1.93eV, with a range of values. The structure NaCrSb, with its valence band maximum (VBM) situated at the Γ-point of the Brillouin zone and its conduction band minimum (CBM) at the X-point, has been identified in Fig. 2. This suggests that NaCrSb is a material with an indirect bandgap semiconductor. The two spin bands in this material, NaCrSb, showed entirely different behaviors. At the Fermi level (E_F) line, one of the typically the majority-spin band, also called the spin-up band in red displays characteristic metallic behavior. Meanwhile, the minority band which is blue in hue and spin-down shows semiconductor behavior with a gap at the EF line. The material NaCrSb demonstrates both semiconductor and metal behavior at different spin up and down orientations. Therefore, half-metallic heusler alloy is predicted by NaCrSb. These results correspond with [21].

4.3 Elastic and Mechanical Properties

We analysed the elastic properties of the materials in a bid to establish the mechanical stability of the compounds investigated. the Born stability criteria [22].

Mechanical Stability Criteria (Born Criteria for cubic crystals)

$C_{11} > 0, C_{44} > 0, C_{11} - C_{12} > 0, C_{11} + 2C_{12} > 0$(4.1)

where C_{11} , C_{12}, C_{44} are elastic constant

Anisotropy factor (A)

$$A = \frac{2C_{44}}{C_{11}-C_{12}} \quad (4.2)$$

The term anisotropy refers to the fact that the properties of a magnetic material are dependent on the directions in which they are measured. Anisotropy makes an important contribution to hysteresis in magnetic materials and is therefore of considerable practical importance. The anisotropy has a number of possible origins.

Cauchy's pressure (C^p)

Cauchy pressure determined as the difference between two elastic constants. This parameter gives an idea of the type of chemical bond between atoms and, also determines the plasticity of metals and alloys.

$$C_p = C_{12} - C_{44} \quad (4.3)$$

Vick's Hardness (Hv): Vickers hardness, a measure of the hardness of a material, calculated from the size of an impression produced under load by a pyramid-shaped diamond indenter

$$H_v = 0.92\left(\frac{B}{G}\right)^{1.3137} * G^{0.708} \quad (4.4)$$

Equations Source: [23].

The Elastic Constants (C_{11}, C_{12}, and C_{44}), Bulk modulus (B), shear modulus (G), B/G ratio, Cauthy's pressure (Cp), young modulus (E), Poisson ratio (u), Zener Anisotropy factor (A), and Vick's Hardness (Hv) of the Half-Heusler Alloy NaCrSb were calculated using equations (4.1) through (4.4) based on the results shown in Table 2. The potential bonding of the atoms in the compound is suggested by the Poisson ratio and the Cauchy pressure. In their research, [24] reported that the Poisson ratio's crucial value was 0.26. We obtained 0.32 as the Poisson ratio for NaCrSb. A sizeable negative C^p supports directional covalent bonding, while a positive value suggests non directional metallic bonding. Results of C^p for the compound NaCrSb is positive and substantial, supporting a non directional metallic bonding among the atoms. In isotropic materials, the properties of the material are independent of the direction, while the material properties are direction-dependent in anisotropic materials. When a material is measured from different directions, any deviation from unity automatically renders the material anisotropic. The values of the anisotropy/isotropy test for the material is 0.29. The result shows NaCrSb is anisotropic. [25] determined that the reference value between brittleness and ductility in a material is 1.75 at the critical value from the ratio of bulk modulus to shear modulus (B/G) of a material. The material is brittle or ductile when the B/G value is below or above the reference value. In fabrication processes, a material's brittleness or ductility may have an impact on the manner of failure. With a B/G ratio value of 2.53, Table 2's results demonstrate the ductile nature of the NaCrSb material. The material's resistance to indentation is addressed holistically by the Vicker's hardness. It describes how a material's ductility can influence the mechanism of failure throughout the fabrication process. The ductility of the NaCrSb material is supported by Table 2's data. The elastic parameters for a cubic crystal structure. C_{11} and C_{44} described the degree of material's stiffness against principal strains and the stiffness of a crystal structure, which determines the resistance against shear deformation. It is a harder and a stiff material and will resist plastic deformation.

4.4 Density of State

Fig. 3(a) shows that Na-1s and Na-3s has the high orbital contribution for the Na-atoms. While in Fig. 3(b) and (c) Cr-1s, Cr-2p, Cr-3s and Sb-1s, Sb- 2s, and Sb - 3p has high orbital present for Cr-atoms as well. At fermi energy both the spin up and spin down is at zero point in plot of partial density of state(PDOS) against energy. The PDOS plot agreed with the prediction that the material is narrow band. It became clear from this that NaCrGe is a half-metallic Heusler alloy.

4.5 Phonon Dispersion Curve Properties

The phonon spectra were calculated to determine the vibrational characteristics of the NaCrSb molecular structure. Thermo_pw is a code that computes the physical properties of materials using Quantum ESPRESSO routines as the underlying engine.

Table 2. Calculated Elastic Constants (C_{11}, C_{12} and C_{44}) Bulk modulus(B), shear modulus (G), B/G Ratio, Cauthy's pressure (C^p), young modulus (E), Poisson ratio(u), Zener Anisotropy factor(A) and Vick's Hardness (H_v) of Half-Heusler Alloy NaCrSb

Compounds	C_{11} (Gpa)	C_{12} (Gpa)	C_{44} (Gpa)	B (Gpa)	G (Gpa)	B/G (Gpa)	C^p (Gpa)	E (Gpa)	u	A	H_v
NaCrSb	60.41	31.18	17.27	40.92	16.2	2.53	13.91	42.95	0.32	1.18	22.37

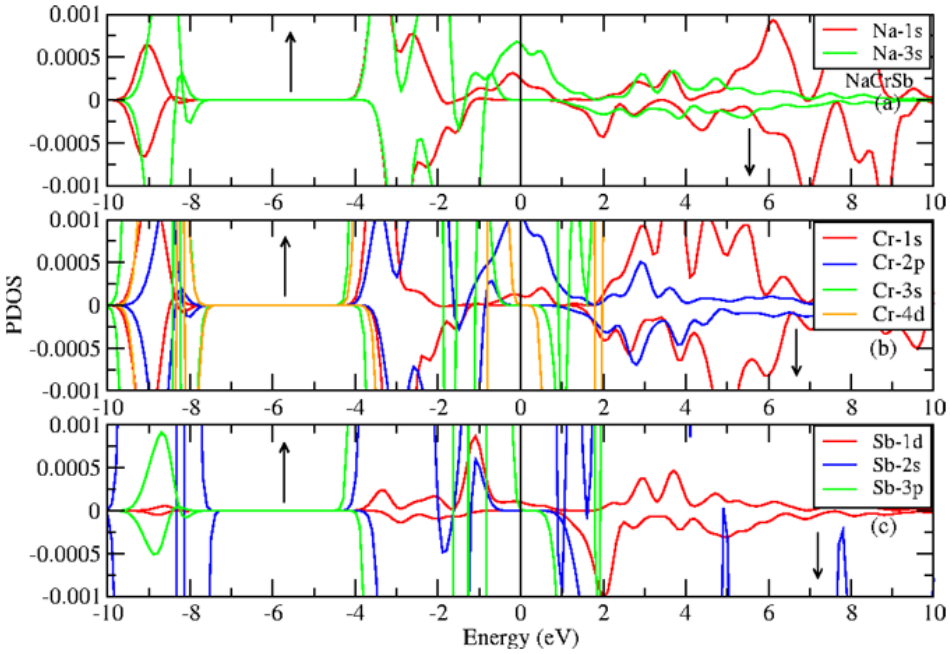

Fig. 3. Plot of PDOS against energy for NaCrSb. Atom projected DOS calculated for the *(a). Na -1s, Na- 3s, (b). Cr-1s, Cr-2p, Cr-3s and Cr- 4d and (c). Sb-1s, Sb- 2s, and Sb - 3p.*

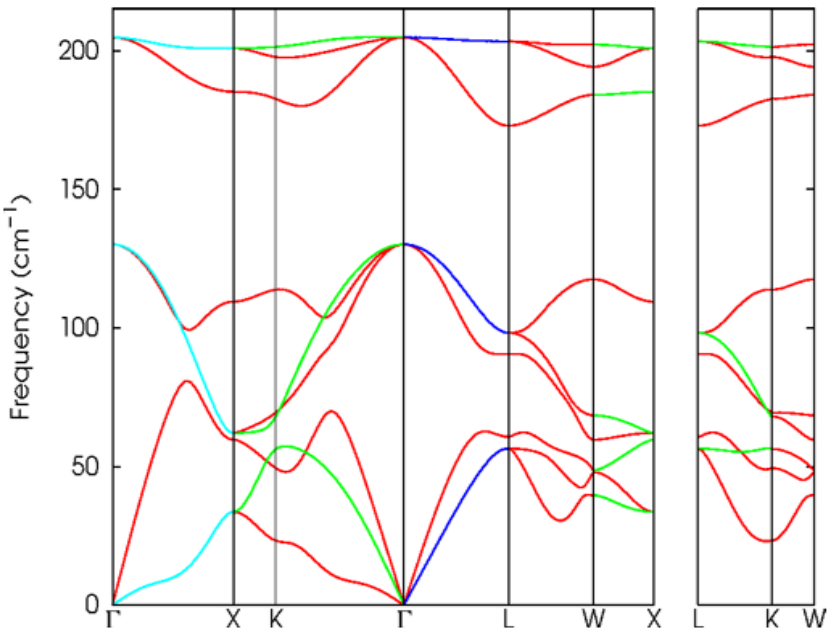

Fig. 4. Calculated phonon frequency versus wave vector coordinate for NaCrSb

Fig. 4 shows the phonon dispersion curves along the $\Gamma - X -$ K $- \Gamma -$ L $-$ W $- X$ high symmetry directions. The compound NaCrSb revealed positive frequencies, which indicates NaCrSb is dynamically stable.

The phonon dispersion curves along the Brillouin zone $\Gamma - X -$ K $- \Gamma -$ L $-$ W $-$ path were generated using Phonopy code [26] within the quasi-harmonic approximation [27] and are displayed in Fig. 4. The dispersion in Fig. 4 can be classified into the upper (optical) and lower (acoustic) modes. The acoustic modes lie in between L – K – W , while the optical mode extends from 3.90 to 6.14 THz as also shown in L – K – W. Both the optical and acoustic branches are separated. The former shows three acoustic modes, while the latter, which contains both the longitudinal optical (LO) and transverse optical (TO) modes, shows three branches for each of them. Our calculated phonon frequencies gaps ranges from 130 (cm^{-1}) and 280(cm^{-1}) at Γ respectively.

5. CONCLUSION

The research provides valuable insights into the structural, electronic, mechanical, density of state and phonon properties of half-heusler alloy (NaCrSb) using density functional theory. The lowest ground state energy was found in the β-phase, suggesting that the material NaGrSb is tructurally stable at this phase. The materials are semiconductor half-Heusler alloys with small bandgaps, and the measured band gap of 1.93eV was obtained for NaCrSb, with a range of values. This indicates that NaCrSb is an indirect bandgap semiconductor material. The substance NaCrSb exhibits behavior during spin up and down that is characteristic of both metals and semiconductors, which foretells the half-metallic Heusler alloy. The B/G ratio of 2.53 indicates that the NaCrSb material is ductile. The material's resistance to impact is addressed holistically by the Vicker's hardness. It discusses how a material's ductility can influence the mechanism of fracture throughout the fabrication process. Positive frequencies were detected in the phonon dispersion curves along the $\Gamma - X -$ K $- \Gamma -$ L $-$ W $- X$ high symmetry directions. This suggests that NaCrSb is dynamically stable. The acoustic modes lie in between L – K – W , while the optical mode extends from 3.90 to 6.14 THz as also shown in L – K – W. Both the optical and acoustic branches are separated. The former shows three acoustic modes, while the latter, which contains both the longitudinal optical (LO) and transverse optical (TO) modes, shows three branches for each of them. The search for new materials with special qualities is what propels progress in materials research and technology. We suggest that NaCrSb is a promising sort of material with practical applications in spintronics.

DISCLAIMER (ARTIFICIAL INTELLIGENCE)

Author(s) hereby declare that NO generative AI technologies such as Large Language Models (ChatGPT, COPILOT, etc) and text-to-image generators have been used during writing or editing of this manuscript.

ACKNOWLEDGEMENTS

To start, we would like to express my deep and sincere gratitude to my research team members, Prof. Babalola, M. I, and Prof. Iyorzor. B. E for an opportunity to do research under their supervision and also for an invaluable guidance throughout this work. Their dynamism, sincerity and motivation inspires us. We will not fail to commend the efforts of the Director of Research and Development UNICROSS Dr. Lukpata and his staff for the space alot to us in his laboratory to run the simulations using their hybrid computer. May the almighty God rewards you in double fold. Thanks we appreciate.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

REFERENCES

1. Smith J, Johnson A. Exploring the thermoelectric properties of half-heusler alloys. Journal of Material Science. 2023;45(3):789–802.
2. Ettah EB, Kseniia Minakova ME. Ishaje and valentyna sirenko. On the interplay of thermodynamic and structural properties of LiZn-based half-Heusler alloys. Fizyka Nyzkykh Temperatur/Low Temperature Physics. 2023;49(11):1389–1393.
3. Coey JM, Venkatesan M. Half-metallicity of heusler alloys. Journal of Physics: Condensed matter. 2010;22(2): 023201.
4. Zhang Chuan, Fan Zhang, Haoyan Diao, Michael C. Gao, Zhi Tang, Jonathan D. Poplawsky, Peter K. Liaw. Understanding

phase stability of Al-Co-Cr-Fe-Ni high entropy alloys. Materials & Design. 2016; 109(5):425-433.

5. Wang X, Pei Y, Lalonde AD. Half-Heusler alloys as thermoelectric materials. Advanced energy material. 2018;8(35): 1800016.
6. Li X, Xu D, Chen L. First-principles study of elastic, electronic and thermodynamic properties of half-heusler alloys Co2TiZ (Z=Al, Ga, In). journal of Magnetism and Magnetic Materials. 2016;414:11-17.
7. Zhang H, Singh S, Singh A. First-principles study of the thermodynamic properties phase stability of half-heusler alloys under various temperature and pressure conditions. Journal of alloys and compounds. 2019;805:50-58.
8. Togo A, Tanaka I. First-principles phonon calculations in materials metals. The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science. 2015;823-843.
9. Falser C, Fecher GH, Balke B. Spintronics: A challenge for materials science and solid-state chemistry. Angewandte chemie international edition. 2007;46(37):668–699.
10. Kandpal, Hem C Gerhard H Fecher, Claudia Felser. Calculated electronic and magnetic properties of the half-metallic, transition metal based Heusler compounds. Journal of Physics D: Applied Physics. 2006;40(6). DOI:10.1088/0022-3727/40/6/S01
11. Ettah, Emmanuel Benjamin. First principles study of structural, electronic, mechanical and density of state properties of the Half - Heusler Alloy NaCrGe. Asian Journal of Research and Reviews in Physics. 2024;8 (3):20-28. Available: https://doi.org/10.9734/ajr2p/2024/v8i3167.
12. Ettah EB, Ishaje ME, Minakova K A, Sirenko V A, Bondar IS. Machine-learning assistant DFT study of half-metallic full-Heusler alloy N2CaNa: structural, electronic, Mechanical, and thermodynamics properties.Fizyka Nyzkykh Temperatur/Low Temperature Physics. 2024;50(10): 928–937
13. Giannozzi P. et al., Quantum ESPRESSO toward the exascale. J. Chem. Phys. 2020;152:154105
14. Giannozzi P. et al., Quantum ESPRESSO: A molular and open-source sotfware project for quantum simulationd of materials. J. Phys.:Condens. Matter. 2009;21:395502
15. Ležaić M, Galanakis I, Bihlmayer G, Blügel S. Structural and magnetic properties of the (001) and (111) surfaces of the half-metal NiMnSb, J. Phys.: Condens. Matter. 2005;17:3121.
16. Katubi KM, Shakil M, Pervaiz H, et al,. Comprehensive computational study of phase stability, half metallicity, elastic and thermal properties of Fe based quaternary heusler alloys for spintronics applications. Indian J Phys. 2023;97(9):1–15. DOI:10.1007/s12648-023-02606-1
17. Pask JE, Yang LH, Fong CY, Pickett WE, Dag S. Six low-strain zinc-blende half metals: An ab initio investigation, Phys. Rev. B. 2003;67:224420.
18. Mouhat F, Coudert FX. Necessary and sufficient elastic stability conditions in various crystal systems. Phys RevB. 2014;90 (22):224104. DOI:10.1103/PhysRevB.90.224104
19. Graf T, Felser C, Parkin SS. Simple rules for the under- standing of Heusler compounds, Prog. Solid State. 2011;39:1.
20. Murnaghan FD. The compressibility of media under extreme pressures. Proc. Natl. Acad. Sci. U.S.A. 1944;30:244-247.
21. Hoang Thuy, Rhim SH. Hong SC. Robust Half-Metallicities of Alkali-Metal-Based Half-Heusler Compounds; 2021. Available:https://ssrn.com/abstract=3990820 or, Available:http://dx.doi.org/10.2139/ssrn.3990820
22. Born M, Huang K. Dynamical theory of crystal lattices. Clarendon press. 1954;
23. Osafile OE, Umukoro JO. Structural, Electronic, Mechanical and Thermodynamic Properties Of Half-Metallic Rh2fez (Z = Ga, In) Full Heusler Compounds From First Principles. Scientia Africana. 2020;19(3):167-180. Available:https://dx.doi.org/10.4314/sa.v19i3.12 ISSN 1118 – 1931.
24. Frantsevich IN, Voronov FF, Bakuta SA. Elastic constants and elastic moduli of metals and nonmetals (In Russian). Kiev, Izdatel'stvo Naukova Dumka. 1982;288.
25. Pugh SF. Relations between the elastic moduli and the plastic properties of polycrystalline pure Scripta materialia. 2009;108:1–5.
26. Atsushi Togo, Isao Tanaka . T“DynaPhoPy: A code for extracting phonon quasiparticles from molecular dynamics simulations” Abel

Carreras, Comput. Phys. Commun. 2017;221: 221-1-14.

27. Wallace DC. Thermodynamics of Crystals; Dover Publications: Mineola, NY, USA; 1998.

Peer-review history:
The peer review history for this paper can be accessed here:
https://www.sdiarticle5.com/review-history/123147