Asian Journal of Research and Reviews in Physics

Volume 8, Issue 3, Page 20-28, 2024; Article no.AJR2P.121196
ISSN: 2582-5992

First Principles Study of Structural, Electronic, Mechanical and Density of State Properties of the Half - heusler Alloy NaCrGe

Emmanuel Benjamin Ettah [a++#*]

[a] Cross River University of Technology Calabar Nigeria.

Author's contribution

The sole author designed, analysed, inteprted and prepared the manuscript.

Article Information

DOI: https://doi.org/10.9734/ajr2p/2024/v8i3167

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/121196

Original Research Article

Received: 04/06/2024
Accepted: 06/08/2024
Published: 14/08/2024

ABSTRACT

In this study, the investigated structural parameters revealed that NaCrGe is stable at beta phase. We 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

[++] *Associate Professor;*
[#] *Senior Researcher of Solid States Physics and Electronic;*
**Corresponding author: E-mail emmanuelettah@gmail.com, emmanuelettah@unicross.edu.ng;*

Cite as: *Ettah, Emmanuel Benjamin. 2024. "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 8 (3):20-28. https://doi.org/10.9734/ajr2p/2024/v8i3167.*

positive value of C11 – C44 (+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.

Keywords: Half heusler; half-metallic gap; electronic band structure; mechanical properties; density of state; alloys.

1. INTRODUCTION

"Half-Heusler alloys are ternary intermetallic compounds with the general formula XYZ, where X and Y are typically transition or rare-earth metals, and Z is usually a main group element. They are known for their versatile electronic, magnetic, and thermoelectric properties, making them of interest for various applications, including spintronics, thermoelectric devices, and topological insulators" [1,2].

"Half-metallic ferromagnets represent a relatively new class of materials which have recently attracted a lot of interest due to their possible applications in spin electronics (also known as magnetoelectronics)" [3,4]. "The two spin bands behave entirely differently in these materials. A typical metallic behavior is displayed by one of them (typically the majority-spin band, also called the spin-up band) with a non-zero density of states (DOS) at the Fermi level EF, while the minority (spin-down) band displays a semiconducting behavior with a gap at EF. As a result, these half-metals can be regarded as semiconductor and metal hybrids" [5].

Theoretical investigations using first-principles calculations based on Density Functional Theory (DFT) have proven to be invaluable in understanding and predicting the properties of materials with high accuracy. DFT enables the exploration of electronic structures, mechanical behaviors, and thermodynamic properties without the need for experimental data, providing insights into the fundamental nature of materials and guiding experimental efforts [6,7,8].

Half-Heusler alloys have garnered significant attention due to their intriguing electronic, magnetic, and mechanical properties, which make them suitable for a wide range of applications, from thermoelectrics to spintronics [9,10,11]. The NaCrGe alloy, a member of the half-Heusler family, is of particular interest due to its potential high thermoelectric performance and favorable electronic structure. In this study, we employ first-principles calculations to investigate the structural, electronic, mechanical, and density of state properties of NaCrGe, aiming to elucidate its potential for future technological applications [12,13].

This table gives the rational behind choosing NaCrGe material. The pattern of choosing is presented in Fig. 1 X(blue), Y(red) and Ge(Green). Half-metallic materials have the unique property of exhibiting different conductive behaviors for electrons with different spin orientations. This property is highly desirable for spintronics, a field that aims to manipulate electron spin for information processing and storage. Understanding and identifying new half-metallic materials, like those proposed in your study, could lead to the development of more efficient spintronic devices.

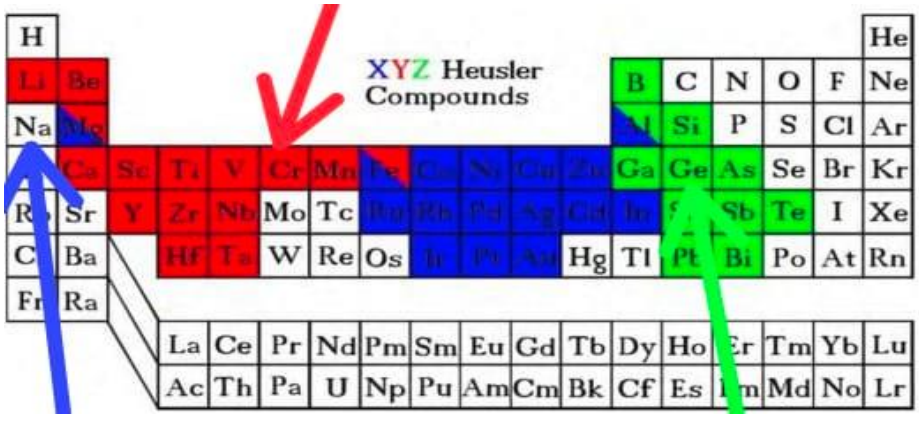

Fig. 1. Periodic Table of Half- Heusler alloy. Source: Sharon, (2023)

2. LITERATURE REVIEW

"Intermetallic Heusler alloys are amongst the most attractive half-metallic systems due to their high Curie temperatures and their structural similarity to binary semiconductors. In this review we present an overview of the basic electronic and magnetic properties of both Heusler families: the so-called half-Heusler alloys like NiMnSb and the full-Heusler alloys like Co2 MnGe. Ab initio results suggest that both the electronic and magnetic properties in these compounds are intrinsically related to the appearance of the minority-spin gap. The total spin magnetic moment Mt scales linearly with the number of the valence electrons Zt , such that Mt = Zt − 24 for the full-Heusler and Mt = Zt − 18 for the half-Heusler alloys, thus opening the way to engineer new half-metallic alloys with the desired magnetic properties" [14].

"In this paper, novel perovskite compounds XMgO3 (X = Na, K and Rb) have been investigated intensively in the framework of density functional theory. The results of the magnetic and electronic properties of the perovskite reveal that the three perovskites are ferromagnets and are half-metals which make them ideal for spintronic devices. The magnetic moment of each perovskite is 3 μB . The compounds are also found to be mechanically and thermodynamically stable. From their B/G ratios, it is found that they are ductile and have high specific heat capacities. When subjected to strains below their equilibrium lattice constants, the three compounds lose their magnetic moment". Babalola and Iyorzor [8].

2.1 Mathematical Background

Bulk Moduli(B): Bulk modulus is a measure of the strenght of a substance to withstand changes in volume when under compression on all sides.

$$B = \frac{C_{11}+2C_{12}}{3} \quad (1)$$

Shear Modulus (G): The shear modulus is the structure material response to the shear deformation.

$$G = \frac{C_{11}-C_{12}+3C_{44}}{5} \quad (2)$$

Young's Modulus (E): Young's modulus(E) is a fundamental property of materials that measures their stiffness or resistance to elastic deformation under stress.

$$E = \frac{9GB}{3B+G} \quad (3)$$

Anisotropy factor (A): 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.

$$A = \frac{2C_{44}}{C_{11}-C_{12}} \quad (4)$$

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.

$$C_p = C_{12} - C_{44} \quad (5)$$

Mechanical Stability Criteria (Born Criteria for cubic crystals)

$$C_{11} > 0, C_{44} > 0, C_{11} - C_{12} > 0, C_{11} + 2C_{12} > 0 \quad (6)$$

(Félix, 2014) ; where C_{11} , C_{12}, C_{44} are elastic constant

Equations Source: [15].

3. METHODOLOGY

We performed first-principles calculations using the density functional theory (DFT) 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 describe the core electrons. A plane-wave cutoff energy of 400 eV was set for the basis set expansion, and a k-point mesh of 8x8x8 was used for Brillouin zone integration.

Optimized input file used for simulation:

```
&control¶
Ý calculation ='scf', Ý Ý Ý Ý Ý Ý Ý!.self-consistent calculation¶
Ý prefix='NaCrGe'Ý Ý Ý Ý Ý Ý!.Prefix for output files¶
 Ý pseudo_dir='/home/ishajemichael/PSEUDOPOTENTIALS/', Ý !.Directory containing pseudopotentials¶
 Ý outdir='./', Ý Ý Ý Ý Ý Ý Ý!.Directory for temporary files¶
Ý/¶
Ý &system¶
Ý ibrav=2,Ý Ý Ý Ý Ý Ý Ý!.Index for the bravais lattice¶
Ý celldm(1)=11.857, Ý Ý Ý Ý Ý!.lattice parameter a¶
 Ý nat=3, Ý Ý Ý Ý Ý Ý!.Number of atoms in the unit cell¶
 Ý ntyp=3, Ý Ý Ý Ý Ý Ý Ý!.Number of atom types¶
 Ý occupations='smearing', smearing='mv', degauss=0.02 ÝÝ!.Occupation type, !smearing method¶
Ý ecutwfc= 65, Ý Ý Ý Ý Ý Ý Ý!.Planewave kinetic energy cutoff¶
Ý/¶
Ý &electrons¶
 Ý mixing_beta = 0.7 Ý Ý Ý Ý Ý Ý!.Convergence threshold for scf iterations¶
 Ý diagonalization='david' Ý Ý Ý Ý Ý!.Diagonalization¶
 Ý electron_maxstep = 400Ý Ý Ý Ý Ý!.Electron maximum step¶
Ý/¶
Ý ATOMIC_SPECIES Ý Ý Ý Ý!.Type of atom used, atomic mass, and pseudopotential¶
Ý Na 22.98976928 Na.pbe-spn-kjpaw_psl.0.2.UPF¶
Ý Cr 51.9961 Cr.pbe-spn-kjpaw_psl.0.2.3.UPF¶
Ý Ge 72.64 Ge.pbe-dn-kjpaw_psl.0.3.1.UPF¶
Ý¶
Ý ATOMIC_POSITIONS Ý Ý Ý Ý Ý Ý!.Position of atom with respect to the crystal¶
Ý Na 0.500 0.500 0.500¶
Ý Cr 0.250 0.250 0.250¶
Ý Ge 0.000 0.000 0.000¶
Ý¶
Ý K_POINTS (automatic) Ý Ý Ý!.Points in the reciprocal space used to sample the Brillouin zone¶
Ý 8 8 8 0 0 0¶
```

This Quantum ESPRESSO input file 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 (Giannozzi, 2017) [16-18].

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 [16,17,19,20].

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 germanium(Ge) 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 [21].

4. RESULTS AND DISCUSSION

4.1 Structural Properties

Fig. 2. Shows that crystal structure of NaCrGe compoud for beta(β) – phase. The structure is a face centre cubic system with it atomic position. While Table 1 contained calculated structural parameter of NaCrGe material. The lattice constant (a_o) for non magnetic calculation is 11.5174a.u. bulk modulus(B) is 60.1Gpa, pressures derivative $B^{/}$ is 4.77 and minimum energy Eg is -672.79eV. Fig. 2 is a plot of energy against lattice parameter which shows that the compound NaCrGe is stable at beta phase . The results was presented in thesamepatterned as seen in Guo et al., [22], and Laref and Laref, [23].

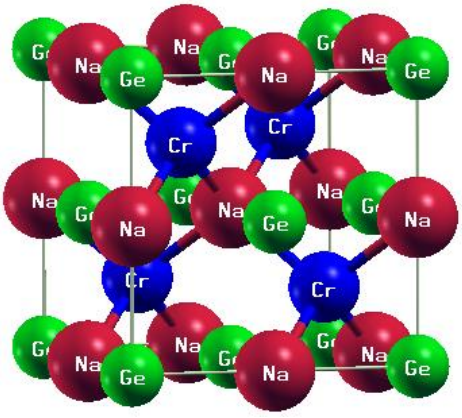

Fig. 2. Crystal structure of β - phase of NaCrGe ma terial

Table 1. Structural Parameters for NaCrGe compound

Compound	a_0 (a.u)	B(Gpa)	$B^{/}$	E_g(eV)
NaCrGe	11.5174	60.1	4.77	672.79

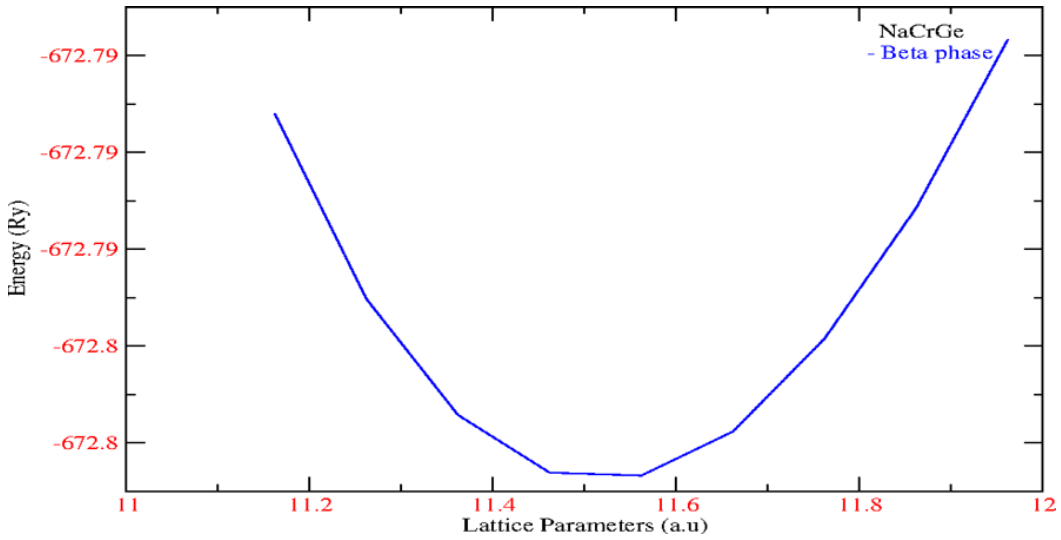

Fig. 3. Enery(Ry) versus Lattice parameter (a.u) for NaCrGe compound

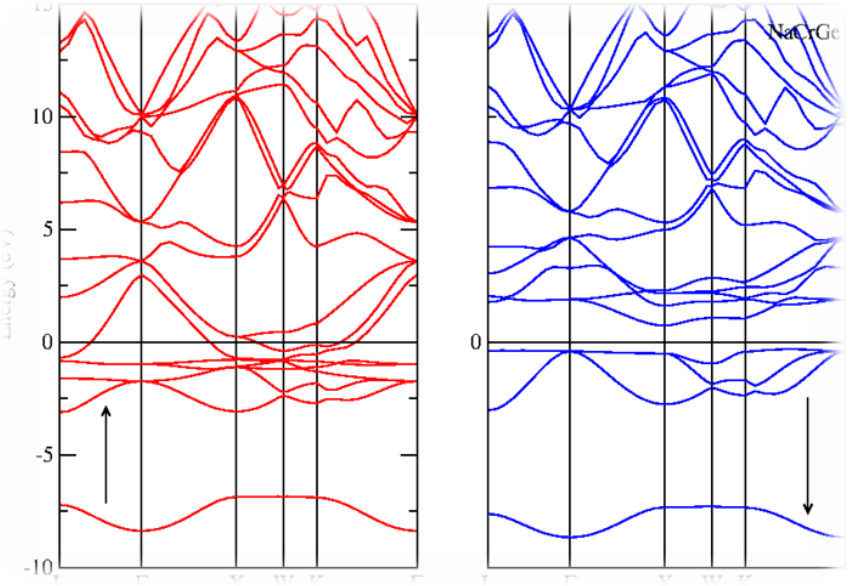

Fig. 4. Calculated Electronic Band Structure for NaCrGe

4.2 Electronic Band Structure

The electronic band gap structural properties of NaCrGe alloys has been calculated using the optimized latticed constants in high symmetry directions of the first Brillouin zone M – Γ – R – W – k – Γ as presented in Fig. 4.

The measured band gap is 1.050eV was obtained for NaCrGe. Hence, the material is a narrow bandgap semiconductor half-Heusler alloys. Azzouz, (2019) studied that to be considered for photovoltaic and photochemistry, semiconductors must have an optimal band gap more than 1.4 and less than 3.0 eV. We observed that the structure NaCrGe conduction band minimum (CBM) 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. In these materials the two spin bands show a completely different behaviour. While one of them (usually the majority-spin band, henceforth also referred to as spin-up band in red color) shows a typical metallic behaviour at the Fermi level E_F line. Meanwhile, the minority (spin-down, blue color) band exhibits a semiconducting behaviour with a gap at E_F line. The material NaCrGe is considered hybrids between metals and semiconductors. Hence, NaCrGe is Half-metallic heusler alloy.

4.3 Mechanical Properties

The calculated mechanical properties indicate that NaCrGe possesses good mechanical stability, making it suitable for structural applications. The empirical relationship between bulk and shear moduli B/G is proposed by [24] could be used to describe the mechanical strength of materials. He suggested that if the B/G ratio is less than 1.75, the material is “britle” in nature otherwise its “ductile”. Relaying on this assumptions, we found that B/G ratio for NaCrGe is 2.40. This implies that NaCrGe is “ductile” in nature at ambient condition. It also aggreed with the fact that if $C_{11} – C_{44}$ is negative the material is brittle, when positive the material is ductile. $C_{11} – C_{44}$ (64.26 − 16.19) is +48.07. Hence NaCrGe is “ductile” in nature at positive value of $C_{11} – C_{44}$.

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(Y), Poisson ratio(u), and Zener Anisotropy factor(A) of Half-Heusler Alloy NaCrGe

Compounds	C_{11}	C_{12}	C_{44}	B (Gpa)	G (Gpa)	B/G (Gpa)	C_p (Gpa)	Y (Gpa)	u	A
NaCrGe	64.26	28.56	16.19	40.45	16.85	2.40	12.37	44.03	0.32	12.37

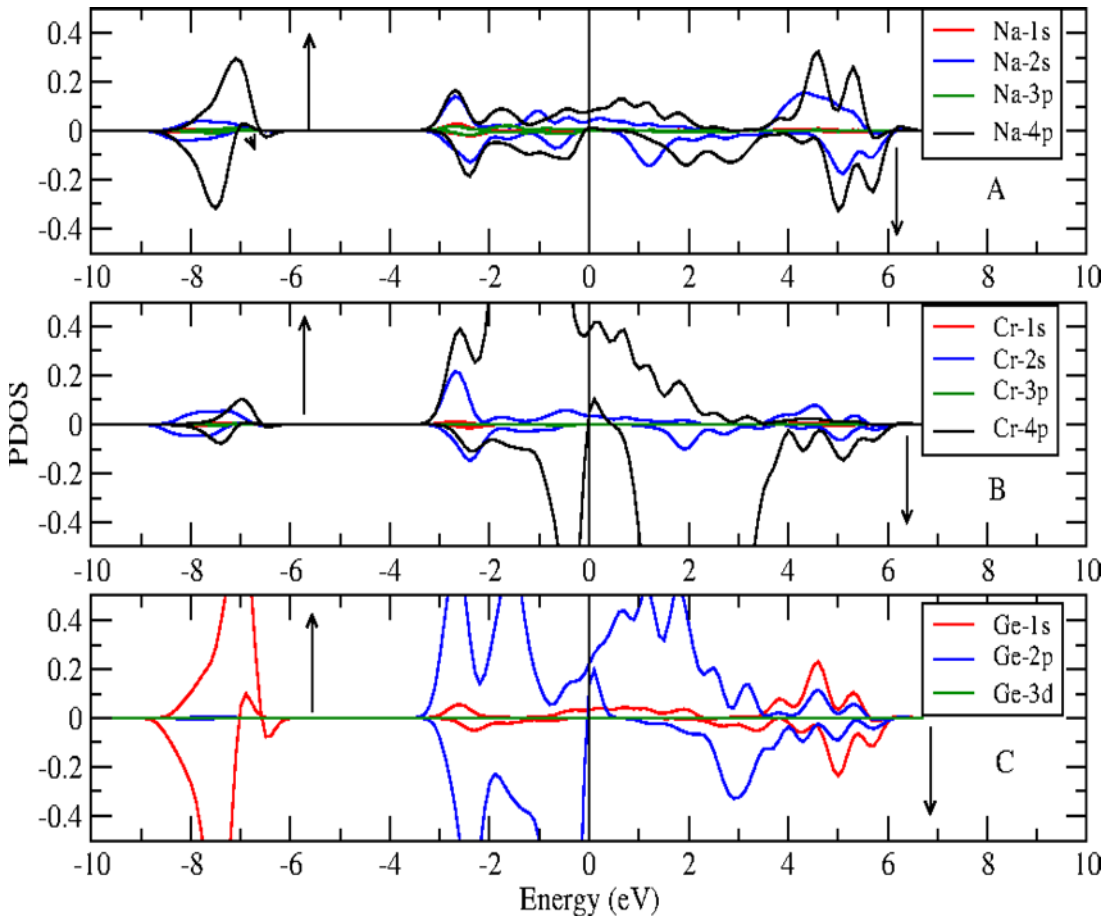

Fig. 5. Plot of PDOS against energy for NaCrGe. Atom projected DOS calculated for the (a). Na -1s, Na- 2s, Na- 3p, and Na- 4p (b). Cr-1s, Cr-2s, Cr-3p and Cr- 4p and (c). Ge-1s, Ge- 2p, and Ge- 3d

4.4 Density of State

Fig. 5a shows that Na-4p has the hightest orbital contribution for the Na-atoms. While in Fig. 4b Cr-4p has the hightest orbital present for Cr-atoms. Also Fig.5c. Ge-2p has more orbital donation for the Ge-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. This revealed that NaCrGe is a half metallic heusler alloy [25,26].

5. CONCLUSION

The research provides valuable insights into this intriguing material NaCrGe. The comprehensive understanding of its electronic band structure and potential applications contributes to the ongoing exploration of advanced materials and opens up exciting opportunities for the development of innovative electronic devices. The investigated strutural parameters revealed that NaCrGe is stable at beta phase.We obtained that the material is a narrow bandgap semiconductor half-Heusler alloys with measured gap of 1.050eV. The structure NaCrGe conduction band minimum (CBM) 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 possessed both metallic and semiconductor features. 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 repectively. At fermi energy both the 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. The exploration of novel materials with unique properties is a driving force behind advancements in materials science and technology. Half-metallic materials represent a class of compounds with unconventional electronic properties that hold promise for future applications.

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 manuscripts.

COMPETING INTERESTS

Author haS declared that no competing interests exist.

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