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Research Article

The Electronic Behavior and Mechanical Characteristics of $CuGa_5S_8$

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Abstract: In this theoretical study, it is presented that the electronic behavior and mechanical characteristics of $CuGa_5S_8$ compound having face centered cubic structure with space group $F\bar{4}3m$ and space number 216. All calculations based on density functional theory (DFT) were performed by Generalized Gradient Approximation (GGA). It is understood from the observed electronic band structure of this system that it has semiconducting behavior close to zero-band gap. Also, the high similarity between spin-up and spin-down states indicates that the magnetic nature of this compound may be paramagnetic. Furthermore, the elastic constants were calculated by the stress-strain method, and then, the mechanical stability of this system was determined. Finally, these constants were used to predict some important mechanical properties of the mentioned system.

***Key words**:* Semiconductor, Paramagnet, *ab* initio calculations, Mechanical properties.

$CuGa_5S_8$'in Elektronik Davranışı ve Mekaniksel Karakteri

Öz: Bu teoriksel çalışmada, $F\bar{4}3m$ uzay grubu ve 216 uzay numarası ile yüzey merkezli kübik yapıya sahip olan $CuGa_5S_8$ bileşiğinin elektronik davranışı ve mekaniksel özellikleri sunulmaktadır. Yoğunluk fonksiyonel teorisine dayanan (YFT) tüm hesaplamalar, Genelleştirilmiş Gradient Yaklaşımı (GGY) ile gerçekleştirilmiştir. Bu sistemin gözlemlenen elektronik bant yapısından yaklaşık sıfır-bant aralıklı yarıiletken bir davranışa sahip olduğu anlaşılmıştır. Ayrıca, yukarı-spin ve aşağı-spin durumlarındaki yüksek benzerlik bu bileşiğin manyetik doğasının paramanyetik olabileceğine bir işarettir. Bunun yanısıra, zor-zorlanma yöntemi ile elastik sabitler hesaplanmış ve sonra bu elastik sabitler, söz konusu sistemin bazı önemli mekaniksel özelliklerini tahmin etmek için kullanılmıştır.

***Anahtar kelimeler**:* Yarı-iletken, Paramanyetik, *ab* initio hesaplamaları, Mekaniksel özellikler.

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1. Introduction

$CuInSe_2$ compound which is a semiconductor, belongs to the chalcopyrite family, is a good candidate for solar cell applications [1-2]. Moreover, it was reported that, in this type of materials, when *Ga* or *Al* element was used instead of *In* element, the band gap of the material increased. Thus, the releated systems were more suitable materials for solar cell applications. Among such materials, copper-based selenide ($CuAl_5Se_8$) was increased optical performance and so, it was more useful for photovoltaic applications [3]. Therefore, the intriguing physical properties of these type materials are need to be focused on. Although in literature, there were some reports about selenides and sulfides [4-13], up to now, the electronic nature and mechanical characteristic of $CuGa_5S_8$, which has a spinel-like structure and crystallizes in the face centered cubic with $F\bar{4}3m$ space group and 216 space number, have not yet been studied in detail. So, we focused on electronic behavior and some elasticity properties of the $CuGa_5S_8$ system by use of the *ab* initio simulation methods.

In this computational study, the semiconducting behavior with nearly zero-band gap electronic band structure of novel $CuGa_5S_8$ compound is in paramagnetic phase and its some elasticity properties were reported hypothetically. The observed semiconductor makes this compound significant for many applications in technology. As we know from the literature, there is no detailed experimental or theoretical research about the magnetic and electronic behaviors and elasticity properties of the cubic $CuGa_5S_8$ yet. Therefore, we hope that the present study can help to better understand these types of materials and encourage related experimental works.

2. Material and Method

For all first principle calculations [14-15] in this study, the projector augmented wave (PAW) method [16] within the VASP (Vienna Ab initio Simulation Package) [17-18] code was employed. To describe interactions between electrons of atoms in the related composition, Perdew-Burke-Ernzerhof (PBE) [19] type pseudopotentials based on the Generalized Gradient Approach (GGA) were considered. The valence electron configurations of *Cu, Ga,* and *S* atoms in cubic $CuGa_5S_8$ system, are as follows: $3d^{10}4s^1$, $3d^{10}4s^24p^1$, and $3s^23p^4$. The obtained crystallographic parameters after the optimization process, were realized with the help of an automatically generated 10×10×10 Monkhorst-Pack scheme [20] with 110 k-points and also, the kinetic energy cutoff value was selected as 600 eV. For the relaxation process of primitive cell of this composition, the quasi-Newton method was performed and this process was realized until the forces on each atom less than 10^{-9} eV/Å. Furthermore, the convergence criteria was chosen as 10^{-10} eV to solve Kohn-Sham equations iteratively. After obtaining the well optimized structural parameters of the related system, its electronic band structure and some important elasticity characteristics were investigated.

3. Results

Initially, for this composition, the relaxation process was carried out to get appropriate atomic locations in the primitive cell and structural parameters accurately. The optimized crystallographic positions of atoms in this composition are tabulated in Table 1. Also, in Figure 1, X-Ray diffraction pattern (XRD) and the primitive cell of the related system including 14 atoms is illustrated as a three-dimensional crystallographic shape.

Table 1. The crystallographic positions of atoms in the primitive cell of this system.

Atoms	*x*	*y*	*z*	Site	Symmetry
Ga1	0.75000	0.75000	0.75000	4d	-43m
Ga2	0.89591	0.36803	0.36803	48h	..m
Ga3	0.36803	0.36803	0.89591	48h	..m
Ga4	0.36803	0.36803	0.36803	16e	.3m
Ga5	0.36803	0.89591	0.36803	48h	..m
Cu	0.00000	0.00000	0.00000	4a	-43m
S1	0.61647	0.15058	0.61647	48h	..m
S2	0.61647	0.61647	0.61647	16e	.3m
S3	0.61647	0.61647	0.15058	48h	..m
S4	0.15058	0.61647	0.61647	48h	..m
S5	0.60869	0.13044	0.13044	48h	..m
S6	0.13044	0.13044	0.60869	48h	..m
S7	0.13044	0.13044	0.13044	16e	.3m
S8	0.13044	0.60869	0.13044	48h	..m

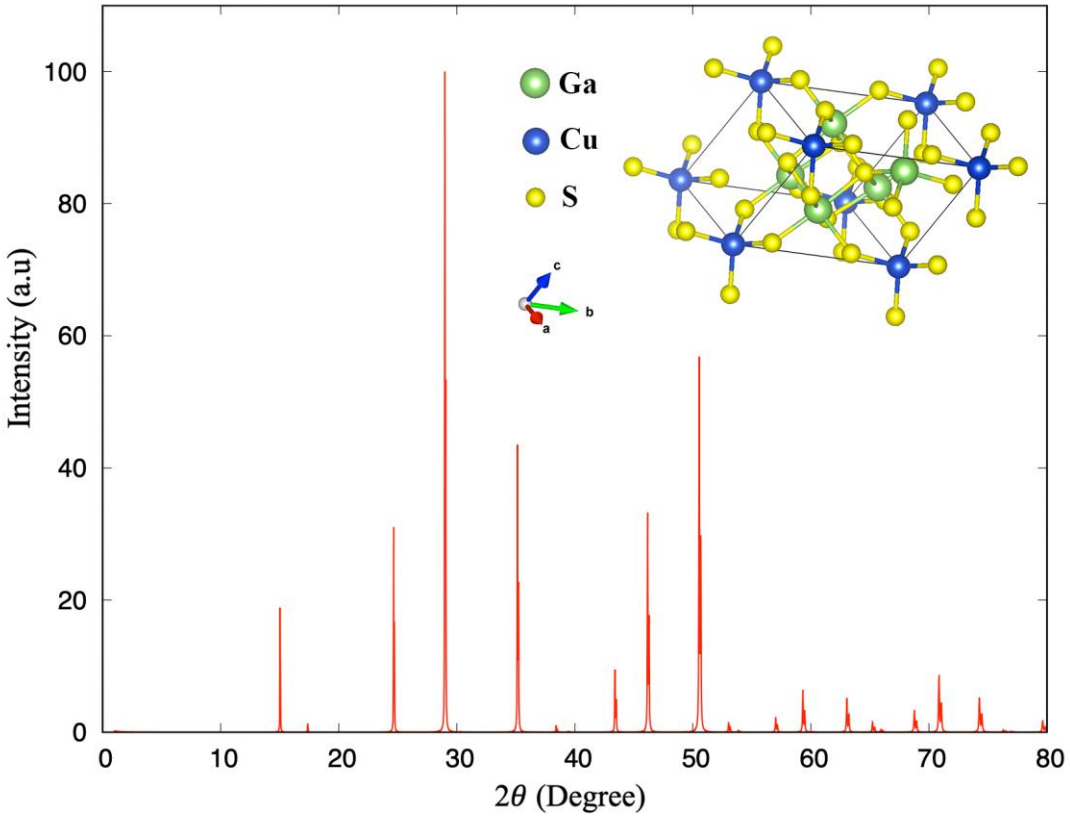

Figure 1. The illustration of three-dimensional primitive cell and X-Ray diffraction pattern (XRD) of $CuGa_5S_8$ system. Where a.u. is arbitrary unit.

The information about the preferred orientation along the crystallographic direction of any solid composition can be obtained from XRD pattern simulation. The obtained value for the maximum 2θ value along the [-2 1 0] direction is 28.99^0. Also, in the mentioned Figure above, some minor peaks were observed as $2\theta = 50.54^0$, $2\theta = 35.14^0$, $2\theta = 46.18^0$, $2\theta = 24.65^0$, and $2\theta = 15.06^0$ to the [-4 -2 -2], [-2 -2 0], [-3 -3 -3], [-2 -1 -1], and [-1 -1 -1] directions, respectively. The thermodynamic stability or structural synthesizability of any solid material which are so important for some industrial and technological applications, can be understood from the calculated formation (ΔE_{for}) and

cohesive energies (ΔE_{coh}). The formation energy (ΔE_{for}) can be calculated by using the internal energy changes [21] as given below in Equation 1:

$$\Delta E_f = E_{CuGa_5S_8} - \left(E_{Cu}^{bulk} + 5E_{Ga}^{bulk} + 8E_S^{bulk}\right) \quad (1)$$

where, $E_{CuGa_5S_8}$ is the total energy of the related composition while E_{Cu}^{bulk} , $E_{Ga}^{bulk}$and E_S^{bulk} are the ground state energies of *Cu*, *Ga* and *S* atoms in crystalized forms. As presented in Equation 2 below, the cohesive energy of any solid crystal which can be calculated from the total energy difference between the bulk form of crystal and the isolated free atoms [22], gives information about the energy required to dissociate a crystal into free constituent atoms.

$$\Delta E_{Coh} = E_{CuGa_5S_8} - (E_{Cu}^{iso} + 5E_{Ga}^{iso} + 8E_S^{iso}) \quad (2)$$

For this system, the calculated negative formation and cohesive energies as given in Table 1, show that the related material has thermodynamical stability and structural synthesizability. Then, the electronic behavior and also some elasticity characteristics of the mentioned system were investigated.

Table 1. The optimized lattice parameter (*a*), bond lengths (*d*), the formation (ΔE_{for}) and cohesive energies (ΔE_{coh}) of $CuGa_5S_8$ composition.

Compound	*a* (Å)	$d_{Cu\text{-}S}$ (Å)	$d_{Ga\text{-}S}$ (Å)	ΔE_{for} (eV)	ΔE_{coh} (eV)
$CuGa_5S_8$	7.218	2.306	2.425	-18.113	-50,919

3.1. The Electronic Character of $CuGa_5S_8$

In this subsection, it was needed to calculate the electronic band structure to decide how the electronic nature of the mentioned cubic system. The electronic band structure and the total density of states (TDOS) were calculated within the classical PBE-GGA approach and graphed along the high symmetry directions for both majority and minority spin channels, as presented in Figure 2. It can be observed from the related figure that, the electronic behavior of this cubic system is close to a zero-band-gap semiconductor. Also, to understand better the dominancy of orbitals on electronic nature of this system, the orbital projected partial density of states for the atoms in the primitive cell were plotted, as presented in Figure 3. It can be obviously seen from the related figure that, especially near the Fermi energy level in the valence band, the *p*-states of sulphide (*S*) atoms and the filled *3d*- orbitals of the copper (*Cu*) atoms have dominancy on the electronic band character of this material. There are noticeable hybridizations between *d*- states of copper (*Cu*) atoms and *3p*- states of sulphide (*S*) atoms in the valence band which is below the Fermi level. In the conduction band above Fermi level, there are similar hybridizations between *4s* states of gallium (*Ga*) atoms and *3p* states of sulphide (*S*) atoms (between around 0.9 eV and 2.8 eV). It can be understood that *p*- and *d*- orbitals of gallium (*Ga*) atoms, *s*- and *p*- orbitals of copper (*Cu*) atoms and *s*- orbitals of sulphide (*S*) atoms have not major role in the electronic character of $CuGa_5S_8$. The semiconductor characteristic near the zero-band gap of the

related system can be defined by the hybridizations between *d*- orbitals of copper (*Cu*) atoms and *p*- orbitals of sulphide (*S*) atoms.

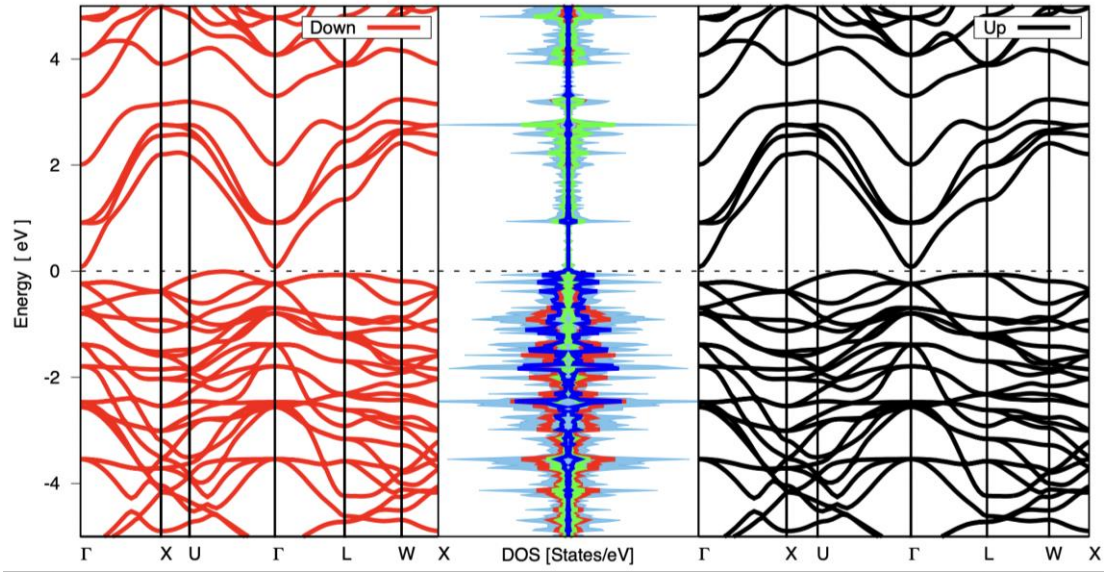

Figure 2. The electronic band structure and the TDOS of $CuGa_5S_8$ system.

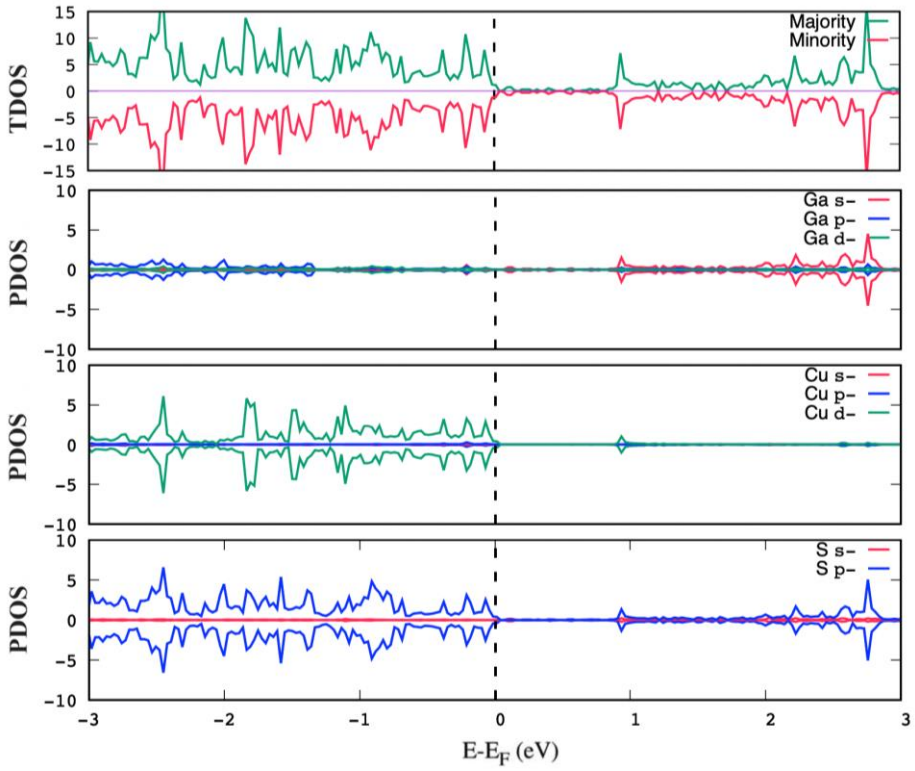

Figure 3. The total (TDOS) and the partial density of states (PDOS) of $CuGa_5S_8$ system.

Also, due to the fact that the total magnetic moment which is obtained as a result of the calculations, is equal to zero and the similarity in the minority and majority channels of the observed electronic band structure, the magnetic character of the material in this study is likely to be paramagnetic.

2. The Mechanical Characteristics of $CuGa_5S_8$

The elastic constants of a solid crystal are used to determine its elastic properties and mechanical stability having so important for technology and industry. In this regard, a material is usually preferred if it has mechanical stability in such applications. In this subsection, to predict some elastic properties such as ductility, hardness, atomic bonding type in the crystal, etc., and also mechanical stability, the elastic constants of this composition were calculated from the stress-strain approach [23]. It is well known from the literature that, a crystal having cubic symmetry has three independent elastic constants as C_{11}, C_{12} and C_{44} [24] and for this composition, the computed elastic constants are presented in Table 2.

Table 2. The elastic constants (C_{ij}) and Cauchy pressure ($C_p = C_{12} - C_{44}$) of cubic $CuGa_5S_8$ system.

Material	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	C_p (GPa)
$CuGa_5S_8$	99.45	71.77	55.74	16.03

In order to decide on the mechanical stability of a crystal, it should be checked whether it meets the conditions known as Born-Huang criteria [24] and for cubic crystals, these criteria are shown in Equation 3.

$$C_{11} - C_{12} > 0, \quad C_{11} + 2C_{12} > 0, \quad C_{11} > 0 \quad \text{and} \quad C_{44} > 0 \tag{3}$$

According to given criteria above, it can be said that this material having face centered cubic structure (FCC) has mechanical stability. Moreover, to have an idea about brittleness of this system, the Cauchy pressure [25] can be calculated as $C_p = C_{12} - C_{44}$. The related material can be stated as ductile since this pressure is positive value. Since ductile type materials can absorb more energy rather than brittles and plastically deform without fracturing easily, $CuGa_5S_8$ composition may have importance for some technological applications.

In order to estimate and making discussion on some mechanical properties, the elastic constants were employed which are computed under stress-strain method based on ab initio calculations. The estimated some elasticity properties of the mentioned compound are presented in Table 3. The upper, the lower and the average values of the bulk (B) and shear (G) modulus, were calculated by employing Voigt [26], Reuss [27] and Hill [28] approximations, as given in Equations 4-7, respectively.

$$B_V = B_R = \frac{C_{11} + 2C_{12}}{3} \tag{4}$$

$$G_V = \frac{C_{11} - C_{12} + 3C_{44}}{5} \tag{5}$$

$$G_R = \frac{5(C_{11} - C_{12})C_{44}}{4C_{44} + 3C_{11} - 3C_{12}} \tag{6}$$

$$B_H = \frac{B_V + B_R}{2} \quad ; \quad G_H = \frac{G_V + G_R}{2} \tag{7}$$

Also, to characterize the stiffness of our material in detail, the Young's modulus [29] which is among the vital parameters about hardness, was calculated from Equation 8.

$$E = \frac{9BG}{3B + G} \tag{8}$$

This material can be considered as a hard material in the view of the bulk (*B*) and Young's modulus (*E*) values tabulated in Table 3. Also, the brittleness of the related system was predicted from Pugh's ratio (*B/G*) [30]. It is known that when the mentioned ratio is greater than 1.75 critical value, the compound can be regarded as ductile material. According to this, this system can be considered as ductile. Furthermore, the Poisson's ratio (σ) [29], which can be calculated with the help of Equation 9, can be used to predict the compressibility of any material. Accordingly, this material has nearly compressibility character since the Poisson's ratio (σ) is less than 0.5 value as given in Table 3. Also, the mentioned ratio can give an idea about the atomic bonding type in a solid crystal. If the related ratio is around 0.25, the material can be considered to have ionic type bonding, and if it is close to 0.1, the material can be considered to have covalent type bonding [31-32]. In this view, this composition can be considered as nearly an ionic character.

$$\sigma = \frac{3B - 2G}{6B + 2G} \tag{9}$$

Table 3. The estimated bulk (*B*), Young's (*E*) and shear (*G*) modulus, Pugh's (*B/G*) and Poisson's (*σ*) ratios of cubic $CuGa_5S_8$ system.

Material	*B(GPa)*	G_V*(GPa)*	G_R*(GPa)*	G_H*(GPa)*	*E(GPa)*	*B/G*	*σ*	*A*
$CuGa_5S_8$	81.00	38.94	25.15	32.00	84.80	2.531	0.325	4.036

One of the properties of a material to be known is whether it is mechanically isotropic. Therefore, to understand anisotropic behavior of this system, the anisotropy shear factor (*A*) [33] which is another vital parameter, was calculated as given below in Equation 10. As shown in Table 3 above, the calculated anisotropy shear factor value indicates a strongly anisotropic characteristic of this system.

$$A = \frac{2C_{44}}{C_{11} - C_{12}} \tag{10}$$

In addition, two-dimensional Young's modulus (*E*), linear compressibility (β), shear modulus (*G*) and Poisson's ratio (σ) were plotted for the related cubic system, as can be seen in Figure 4, in order to better explain the isotropicity. According to these figures, it can be said that this material has anisotropic nature except linear compressibility (β).

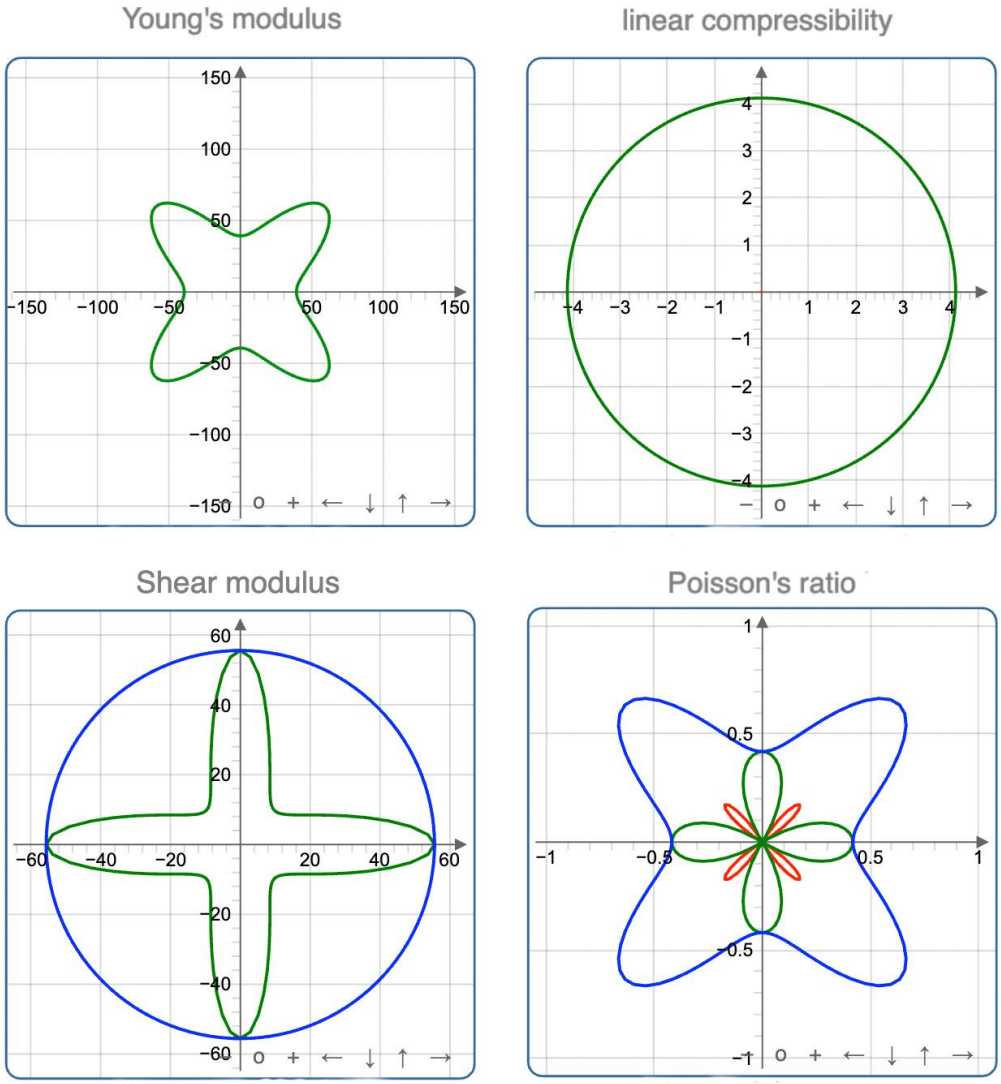

Figure 4. Two-dimensional Young's modulus (E), linear compressibility (β), shear modulus (G) and Poisson's ratio (σ) of cubic $CuGa_5S_8$ compound.

Moreover, among the mechanical properties, sound velocities (the transverse (v_t), longitudinal (v_l) and average (v_m) wave velocities) in the crystal, which can be calculated by using Navier's equation [34], and Debye temperature (Θ_D) are so important parameters to understand thermo-elastic behavior of a material. The predicted parameters for this compound are tabulated in Table 4. As seen in the related Table, the sound conductivity of this system is relatively high while its thermal conductivity is very low.

Table 4. The estimated sound velocities (v_l, v_t and v_m) and Debye temperature (θ_D) for $CuGa_5S_8$.

Material	$v_l\ (m/s)$	$v_t\ (m/s)$	$v_m\ (m/s)$	$\theta_D\ (K)$
$CuGa_5S_8$	5442	2768	3102	32.00

4. Conclusion

In the presented hypothetical study, the nearly zero-band-gap semiconducting character within the paramagnetic phase and some mechanical properties of $CuGa_5S_8$ which has face centered cubic structure, were examined extensively. The calculated relatively great formation and cohesive energies indicate the structural and thermodynamic stability of the related system. The focused system in this study has nearly zero-band-gap semiconductor character due to having similar spin-down and spin-up states in which

the observed electronic band structure under GGA approximation and also, it has paramagnetic nature due to having zero total magnetic moment. These physical characteristics make the mentioned material so important for possible technological applications. Moreover, as a result of the calculations to examine some mechanical properties, it has been concluded that this compound has mechanical stability since the calculated elastic constants satisfy Born-Huang criteria and also, it has a large ductility.

Author Statement

Aytaç Erkişi: Investigation, Original Draft Writing.
Yusuf Özcan: Investigation, Validation, Review and Editing.

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Conflict of Interest

As the authors of this study, we declare that we do not have any conflict of interest statement.

Ethics Committee Approval and Informed Consent

As the authors of this study, we declare that we do not have any ethics committee approval and/or informed consent statement.

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