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A FP-LAPW Study of $LuGa_3$ and $ScGa_3$ compounds

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Abstract

In the present paper we study the structural, electronic, elastic, mechanical and thermal properties of isostructural and isoelectronic nonmagnetic RGa_3 (R= Lu and Sc) compounds, which crystallize in $AuCu_3$-type structure using first principles density functional theory based on full potential linearized augmented plane wave (FP-LAPW) method. The calculations are carried out within PBE-GGA, WC-GGA and PBE-sol GGA for the exchange correlation potential. Our calculated ground state properties such as lattice constant (a_0), bulk modulus (B) and its pressure derivative (B') are in good agreement with the available experimental and other theoretical results. We predict the elastic constants for these compounds using GGA approximations. Cauchy pressure and B/G_H ratio are also investigated to explore the ductile and brittle nature of these compounds. The computed electronic band structures and density of states shows the metallic character of these compounds. The elastic properties including Poisson's ratio (σ), Young's modulus (E), shear modulus (G_H) and anisotropy factor (A) are also determined using the Voigt-Reuss-Hill (VRH) averaging scheme. The average sound velocities (v_m), density (ρ) and Debye temperature (θ_D) of these RGa_3 compounds are also estimated from the elastic constants. We first time report the variation of elastic constants, elastic moduli, sound velocities and Debye temperatures of these compounds as a function of pressure. Contour plots of the electron charge densities are also computed to reveal the nature of bonding in these compounds.

Introduction

In the last several years, the superconductivity remains a dynamic area of research in condensed matter physics with a number of discoveries of novel materials and with an increasing demand for novel devices for sophisticated technological applications. Although there are a large number of known conventional and unconventional superconductors (SCs), new findings still emerge even from simple, binary intermetallic systems. Recently Svanidze *et. al*. [1] have shown that single crystals of $ScGa_3$ is a type-I superconductor with *T*c = 2.1 K. The patterns for $ScGa_3$ and $LuGa_3$ were refined with the cubic space group Pm3m, with lattice parameters a = 4.09 °A and a = 4.19°A, respectively. Previous investigations involved only with the synthesis of polycrystalline sample of $ScGa_3$, and characterization of Fermi surface by dHvA measurements on single crystals [2]. The band structure calculations on $ScGa_3$ and $LuGa_3$ reveal that there is a great similarity between the electronic properties of $ScGa_3$ and $LuGa_3$ [3]. The magnetic properties have also been studied experimentally within the temperature range 0-3K [1]. The experimental studies have been performed to investigate structural and electronic properties [1-2] of $ScGa_3$. The elastic, optical and thermodynamical properties of $ScGa_3$ and $LuGa_3$ were studied by FP-LAPW method by using the PBE-GGA and TB-mBJ schemes [4]. Ramesh et.al [5] calculated the electronic structure and transport properties of ScX_3 (X=Ga, In). They also computed the vibrational frequencies to study the nature of instabilities in these compounds. The electronic structure of $ErGa_3$ and its isostructural compounds with Tm, Yb, and Lu have been investigated with a highly accurate band structure scheme in LDA and GGA and warped muffin-tin approximation by Bross [6].

In the present work an attempt is made to study the structural, electronic, elastic, mechanical and thermal properties of RGa_3 (R=Sc and Lu) compounds using three different approaches under generalized gradient approximation (GGA) at ambient pressure as well as at high pressure. The elastic parameters like Poisson ratios, Young’s moduli and anisotropy factors have been evaluated under high pressures for the first time for $LuGa_3$ and $ScGa_3$.The paper is organized as follows: “Computational method” section briefly describes the computational details regarding the methods used in our calculations. It is followed by result and discussion where the results are presented and compared with the available experimental and theoretical data.

Calculation method

The structural, electronic, elastic, mechanical and thermal properties of RGa_3(R= Lu and Sc) compounds are investigated using first principle full potential-linearized augmented plane wave method within density functional theory. We used Perdew and Wang-generalized gradient approximation, which is based on exchange correlation energy [7].The wave vector cut-off for the plane wave expansion of the wave function in the interstitial region was chosen, $R_{MT}*K_{max}= 7$ where R_{MT} is the smallest muffin-tin radius in the unit cell and K_{max} is the maximum of reciprocal lattice vector. A dense mesh of 10×10×10 k points is used and tetrahedral method [8] has been used for the Brillouin Zone integration. The calculations are iterated until the total energies are converged below 10^{-4} Ry. The total energies are calculated as a function of volume and fitted to Birch-Murnagan equation of state [9] to obtain the ground state properties like zero-pressure equilibrium volume. Information on the influences of pressure and temperature on the elastic moduli and related aggregate properties of single crystals plays an essential role in predicting and understanding the interatomic interactions, strength, mechanical stability, phase transition mechanisms and dynamical response of materials. For a cubic crystal, the three elastic moduli C_{11}, C_{12} and C_{44} fully describe its elastic behavior. C_{11} and C_{12} can be determined from the bulk modulus B and shear constant Cs.

The elastic moduli required knowledge of the derivative of the energy as a function of the lattice strain. The symmetry of the cubic lattice reduced 21 elastic constants to three independent elastic constants, namely C_{11}, C_{12} andC_{44}. The elastic stability criteria for a cubic crystal at ambient conditions are $C_{11} + 2C_{12}>0$, $C_{44}>0$, $C_{11}- C_{12}>0$ and $C_{12}<B<C_{11}$. In the present work, the elastic constants were calculated using the tetrahedral and rhombohedral distortions on the cubic structure using the method developed by Charpin and integrated it in theWIEN2k package [10]. The systems were fully relaxed after each distortion in order to reach the equilibrium state.C_{44} is proportional to the shear modulus and could be used as a measure of shear resistance. The longitudinal and transverse sound velocities (v_l and v_t) were obtained by using these elastic constants as follows:

$$v_l = \sqrt{\frac{\left[C_{11} + \frac{2}{5}\left(2C_{44} + C_{12} - C_{11}\right)\right]}{\rho}} \qquad (1)$$

$$v_t = \sqrt{\frac{\left[C_{44} - \frac{1}{5}\left(2\mathrm{C}_{44} + C_{12} - C_{11}\right)\right]}{\rho}} \tag{2}$$

Where C_{11}, C_{12} and C_{44} are second-order elastic constants and ρ is mass density per unit volume, and the average sound velocity v_m was approximately calculated from [11, 12]:

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

One of the standard methods to calculate the Debye temperature was from elastic constants, since θ_D may be estimated from v_m by the following equation [11, 13]:

$$\theta_D = \frac{h}{k_B}\left[\frac{3n}{4\pi V_a}\right]^{\frac{1}{3}} v_m \tag{4}$$

where h is Planck’s constant, k_B is Boltzmann’s constant, and V_a is the average atomic volume.

Result and discussion

Ground state properties

In order to calculate the ground state properties, the total energies are calculated in $AuCu_3$ type structure for different volumes around the equilibrium cell volume V_0. The variation of total energy as a function of volume using PBE-GGA for these compounds is shown in Figure. 1 (a-b).The calculated total energies are fitted to the Birch-Murnaghan equation of state [9] to determine the ground state properties like lattice constant (a_0), bulk modulus (B) and its pressure derivative (B') at minimum equilibrium volume V_0 using exchange correlation as PBE-GGA, Wu–Cohen (WC) GGA and PBE-sol GGA. All these GGA functionals have the same correlation functional but they differ in the exchange energy. Both WC GGA and PBE-sol GGA have an enhancement factor $F_x(s)$ that increases more slowly with the reduced density gradient as compared to PBE-GGA. The WC and PBE sol GGAs overestimate the atomization energies much more than PBE-GGA [14-17]. It is seen from Table 1 that our calculated values of lattice parameter a_o with PBE-GGA are found to be in close agreement with the available experimental and other theoretical data than other GGA approximations. The further calculations have been carried out using only PBE-GGA. The variation of volume with pressure is studied for these compounds in $AuCu_3$ structure and is presented in Figure 2 (a-b).

Table-1 Calculated lattice constant (a_o), bulk modulus (B), pressure derivative of bulk modulus (B') and number of density of states $N(E_F)$ for RGa$_3$ compounds.

Solid	**Work**	**Approximation**	**a_o (Å)**	**B (GPa)**	**B'**	**$N(E_F)$ States/eV**
LuGa$_3$	Pre.	PBE-GGA	4.204	68.72	4.37	2.94
		WC-GGA	4.132	78.12	4.19	2.50
		PBE-sol GGA	4.124	79.40	4.36	2.43
	Expt.		4.180[a]	-	-	-
			4.191[b]	-	-	-
			4.169[c]	-	-	-
	Other		4.212[d]	-	-	-
			4.2[e]	68.23[e]	4.23[e]	-
ScGa$_3$	Pre.	PBE-GGA	4.116	72.46	4.85	2.57
		WC-GGA	4.051	83.52	4.79	2.22
		PBE-sol GGA	4.044	84.60	4.80	4.41
	Expt.		4.096[a]	-	-	-
			4.095[f]	-	-	-
			4.092[g]	-	-	-
			4.097[h]	-	-	-
	Other		4.09[i]	87.46[i]		1.44[i]
			4.05[j]	83.8[j]	4.24[j]	-
			4.12[e]	73.1[e]	4.18[e]	-
			4.13[k]	74.2[k]	-	-

[a]Ref.[18];[b]Ref.[19];[c]Ref.[20];[d]Ref.[21];[e]Ref. [4]; [f]Ref.[22];[g]Ref.[23]; [h]Ref.[24];[i]Ref.[1];[j]Ref.[25]; [k]Ref.[26]

Electronic Properties

In order to study the electronic properties of RGa$_3$ compounds, the electronic band structures (BS) are presented in Figure 3(a-b) and density of states (DOS) are shown in Figure 4(a-b).

The Fermi level is fixed at origin. It is clear from band structure that both the studied non-magnetic RGa$_3$ compounds exhibit metallic nature. The band structure calculations on ScGa$_3$ and LuGa$_3$ reveal that there is a great similarity between the electronic properties of ScGa$_3$ and LuGa$_3$ [3].In ScGa$_3$ it is observed that the bands below the Fermi level upto -10.8 eV is mainly due to the '*4s'* state of Ga with very little contribution of '*4p'* state of Ga. On the other hand, the energy bands from - 3 eV to the Fermi level is mainly from Ga-*4p* state with small contributions of Sc-*3d* and Ga-*4s* states. Similarly in LuGa$_3$ the lowest energy bands lying between -10.8 eV arise mainly from the Ga-*4s* states with very little contribution from Ga-*4p* states. The major contribution at the Fermi level is mainly due '*4s'* and '*4p'* state of Ga with contribution of '*d'* state of Lu. The flat band is situated at -4.8eV which is mainly due to the *'4f'* states of Lu. The band above the Fermi level in RGa$_3$ is mainly due to the '*d'* state of Lu and Sc respectively. Hence we can say that at the Fermi level, the main contribution to the total DOS in both the compounds comes from the Ga atoms. The valence and conduction bands overlap considerably, and there is no band gap at the Fermi level for these compounds which confirms the metallic nature of these compounds. On the whole, the band structure calculations on $ScGa_3$ and $LuGa_3$ reveal that there is a great similarity between the electronic properties of $ScGa_3$ and $LuGa_3$ [3]. The density of states (DOS) plot provides an even more comprehensive picture of the elemental contributions to the electronic states of the compounds. The total and partial densities of states for these compounds at ambient pressure are presented in Figure 4 (a-b). At Fermi level, the density of states for these compounds is greater than zero, hence exhibiting metallic behavior. The '*4f* 'states can be easily identified as sharp peaks in the total DOS in the case of $LuGa_3$ compound while in $ScGa_3$ the peak is observed above the Fermi level is mainly due to *'d'* like states of Sc. The total density of states for $LuGa_3$ and $ScGa_3$ at ambient pressure is obtained as 2.94 and 2.57 states/eV, given in Table 1.

Electronic charge density

The charge density distribution is an important property of solid materials and provides good information about the chemical bonding. Figure 5(a-b) shows the contour plots of the distribution of the electron charge densities in the (100) plane for RGa_3 compounds. It is observed that the charge density distribution around Sc and Ga atoms are spherical-like. There is almost no overlapping electron distribution between Sc and Ga atoms, indicating an ionic bonding nature. For covalent and ionic materials, the typical relations between bulk and shear moduli are $G_H = 1.1B$ and $G_H = 0.6B$ [27] respectively. In our case, the G_H/B ratio for $LuGa_3$ is 0.90 indicating the covalent nature and for $ScGa_3$ is 0.56 confirms the ionic nature.

Elastic properties

Elastic properties of a solid give important information on the mechanical and dynamical properties, such as interatomic potentials, equation of state and phonon spectra. The elastic moduli require knowledge of the derivative of the energy as a function of the lattice strain. We have calculated the second order elastic constants (SOECs) of RGa_3 (R = Lu and Sc) compounds in $AuCu_3$ phase at ambient pressure using the method developed by Charpin and as integrated it in the WIEN2k package [10]. The calculated values of elastic constants are given in Table 2 together with the other experimental and theoretical data. It can be noted that our calculated elastic constants satisfy the elastic stability criteria for a cubic crystal at ambient conditions are $C_{11} + 2C_{12}>0$, $C_{44}>0$, $C_{11} - C_{12}>0$ and $C_{12}<B<C_{11}$which clearly indicate the stability of these compounds in $AuCu_3$ structure. It can be noted that our calculated elastic constants satisfy the elastic stability criteria for a cubic crystal at ambient conditions. Our calculated elastic constants for $LuGa_3$ and $ScGa_3$ vary slightly from other theoretical calculations and are in closer agreement with available experimental data. This might be due to the different exchange correlation approximations used. The pressure dependence behavior of the second order elastic constants is also investigated up to 18 GPa (see Figure 6(a-b)) for these compounds. It is clear from Figure. 6(a-b) that for all these compounds, $C_{11}>0$, $C_{12}>0$ and $C_{44}>0$, which implies that these compounds are stable in $AuCu_3$ structure over the pressure range 0 - 18 GPa. We found that all the three elastic constants (C_{11}, C_{12} and C_{44}) increase linearly with the applied pressure and stable against pressure.

Table -2. Calculated second order elastic constants, Young’s modulus (E), shear modulus (G_H), Anisotropic factor (A), Poisson’s ratio (σ) Cauchy’s pressure (C_{12}-C_{44}) for RGa_3 compounds

Solids	**Work**	**C_{11} (GPa)**	**C_{12} (GPa)**	**C_{44} (GPa)**	**E (GPa)**	**G_H (GPa)**	**A**	**B/G_H**	**σ**	**C_{12}-C_{44} (GPa)**
$LuGa_3$	Pre.	149.20	33.08	65.23	144.89	62.26	1.12	1.15	0.16	-32.15
	Oth.	99.97[e]	54.82[e]	28.68[e]	71.80[e]	26.05[e]	1.27[e]	0.37[e]	0.37[e]	-
$ScGa_3$	Pre.	131.70	44.26	39.76	104.33	41.29	0.90	1.77	0.26	4.50
	Oth.	116.97[e]	53.16[e]	16.39[e]	60.02[e]	21.47[e]	0.51[e]	0.28[e]	0.39[e]	-
		153.2[j]	49.6[j]	37.5[j]	--	42.7[j]	-	-	0.28[j]	12.1[j]
		151.4[k]	35.6[k]	41.3[k]	117[k]	47.3[k]	0.71[k]	-	0.24[k]	-

[e]Ref.[4];[j]Ref.[25]; [k]Ref.[26];

Mechanical properties

The main mechanical parameters, i.e. Young’s modulus (*E*), shear modulus (G_H), Poisson’s ratio (σ) and anisotropic ratio (*A*), which are important for industrial applications are calculated and presented in Table 2 with the theoretical ones. These important parameters are used to characterize the mechanical behavior of a material.

The shear modulus G_H describes the material’s response to shearing strain using the Voigt-Reuss-Hill (VRH) method [28-30]; the effective modulus for the polycrystals could be approximated by the arithmetic mean of the two well known bounds for monocrystals.

The bulk and shear modulus, defined as-

$$B = \frac{1}{3}\left(C_{11} + 2C_{12}\right) \qquad (5)$$

$$G_H = \frac{G_V + G_R}{2}$$

where

$$G_V = \frac{C_{11} - C_{12} + 3C_{44}}{5}$$ is the Voigt shear modulus (6)

And

$$G_R = \frac{5C_{44}(C_{11} - C_{12})}{4C_{44} + 3\left(C_{11} - C_{12}\right)}$$ is the Reuss shear modulus (7)

The anisotropy factor (A) is an indicator of the degree of anisotropy in the solid structures. For a completely isotropic material, the A factor takes the values of 1, when the value of A is smaller or greater than unity it is a measure of the degree of elastic anisotropy.

$$A = \frac{2C_{44}}{C_{11} - C_{12}} \tag{8}$$

The calculated elastic anisotropic factor for RGa_3 (R = Lu and Sc) compounds is greater than 1, which indicates that these compounds are not elastically isotropic. The bulk modulus is a measure of resistance to volume change by applied pressure [31].

The ratio of bulk modulus to shear modulus B/G_H can be used to calculate the ductile/brittle character of a material [32]. If B/G_H ratio is greater than 1.75, then the material will be considered as a ductile otherwise it will be of brittle nature. Pettifor and Chen *et al*. [33, 34] have demonstrated the brittle versus ductile transition in intermetallic compounds from the first principles calculations. They demonstrated that the higher the value of B/G_H, the more ductile the material would be. The B/G_H ratio of RGa_3 is given in Table 2 which shows that $LuGa_3$ is brittle in nature whereas $ScGa_3$ is ductile in nature.

The Cauchy pressure is another interesting elastic parameter used to describe the angular characteristic of atomic bonding in a compound [33]. The positive value of Cauchy pressure is responsible for an ionic bonding, while a material with negative Cauchy pressure requires angular or directional character in bonding (covalent bonding). The calculated values of the Cauchy's pressure are given in Table 2 which shows that $ScGa_3$ compound with positive value of Cauchy pressure exhibit ionic bonding and ductile in nature, while $LuGa_3$ compound with negative value of Cauchy pressure posses more directional covalent bonding and brittle in nature.

The Young's modulus is defined as the ratio of the tensile stress to the corresponding tensile strain, and is an important quantity for technological and engineering applications. It provides a measure of the stiffness of a solid, and the material is stiffer for the larger value of Young's modulus. And the stiffer solids have covalent bonds [35].

Young's Modulus (E) is given by

$$E = \frac{9BG_H}{3B + G_H} \tag{9}$$

Poisson's ratio is the measure of the compressibility, i.e. it is the ratio of lateral and longitudinal strain in uniaxial tensile stress. The Poisson's ratio is small (σ=0.1) for covalent materials, and it has a typical value of σ=0.25 for ionic materials [36].

$$\sigma = \frac{3B - 2G_H}{2(3B + G_H)} \tag{10}$$

In the present case the σ values are 0.16, 0.26 for $LuGa_3$ and $ScGa_3$ respectively. We have also observed the dependency of elastic moduli with the pressure in the range of 0-18GPa for these RGa_3 compounds and presented in Figure 7(a-b). It is found that all the three elastic moduli (bulk modulus B, Young modulus E and shear modulus G_H) increase linearly with the applied pressure.

Thermal properties

The Debye temperature is an important fundamental parameter closely related to many physical properties such as elastic constants, specific heat and melting temperature. At low temperature Debye temperature calculated from elastic constants. There are various methods to obtain the values of Debye temperature. A usual method for estimating the θ_D value can be obtained from the values of the elastic constants and the wave velocities such as average wave velocity, transverse and longitudinal elastic wave velocities. The predicted sound velocities, Debye temperature and density are given in Table 3.We have studied first time the variation of sound velocities with pressure and presented in Figure 9 (a-b).

Table - 3. Calculated density (ρ), Longitudinal (v_l), transverse (v_t), average elastic wave velocities (v_m), Debye's temperature (θ_D) for RGa_3 compound

Solids	**p*10^3 (kg/m^3)**	**v_l (m/s)**	**v_t (m/s)**	**v_m (m/s)**	**θ_D (K)**
$LuGa_3$	8.584	4248	2695	2964	264
$ScGa_3$	6.029	4617	2618	2911	264

We have studied the variation of θ_D with pressure and presented in Figure 8. It is observed from the figure that θ_D of these RGa_3 compounds increased as pressure increased which shows quite normal behavior for all these compounds. For lack of experimental results, we could not compare them. Hence, our results can be considered as a prediction for these properties of RGa_3 compounds and it will be testify future experimental work.

Conclusion

First principle study has been performed on RGa_3 compounds (R= Lu and Sc) using full potential linearized augmented plane wave approach within three different forms of generalized gradient approximation. The calculated lattice parameters and bulk modulus are, reasonably, consistent with the literature values. The present elastic constants satisfy the traditional mechanical stability conditions and are agrees reasonably with the available theoretical results. The computed electronic band structures show metallic character. By Pugh's criterion we found that $LuGa_3$ is brittle and $ScGa_3$ is ductile in nature. The polycrystalline bulk modulus B, shear modulus G_H, Young's modulus E, and Poisson's ratio σ were deduced by using Voigt–Reuss–Hill (VRH) approximations The contour plots of the electron charge densities confirm the covalent nature of bonding in $LuGa_3$ compound and ionic bonding in $ScGa_3$ compound. We have also studied the variation of elastic constants and elastic moduli of these compounds with pressure over the range 0-18 GPa. The calculated mechanical properties of RGa_3 compound are in good agreement with the available other theoretical results, presented in the Table 3. We also report the thermal properties of these compounds for the first time, which will be tested in the future experimentally and theoretically.

Acknowledgements

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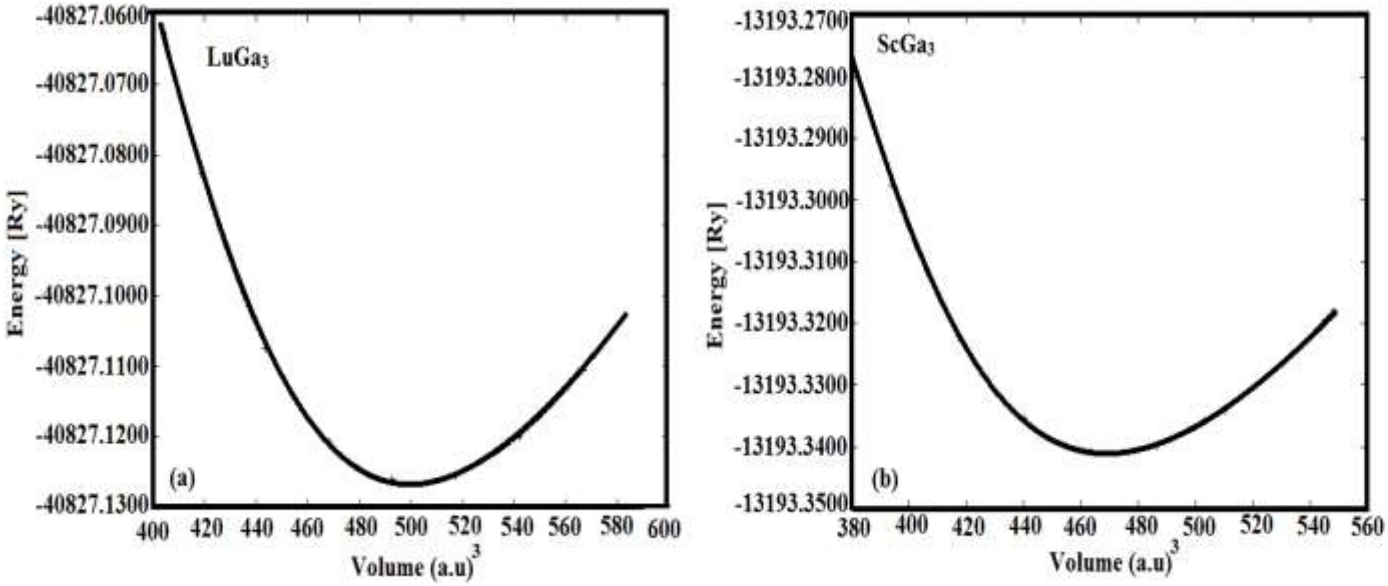


Figure 1. (a)–(b) Variation of total energy with volume of RGa_3 compounds in $AuCu_3$ structure

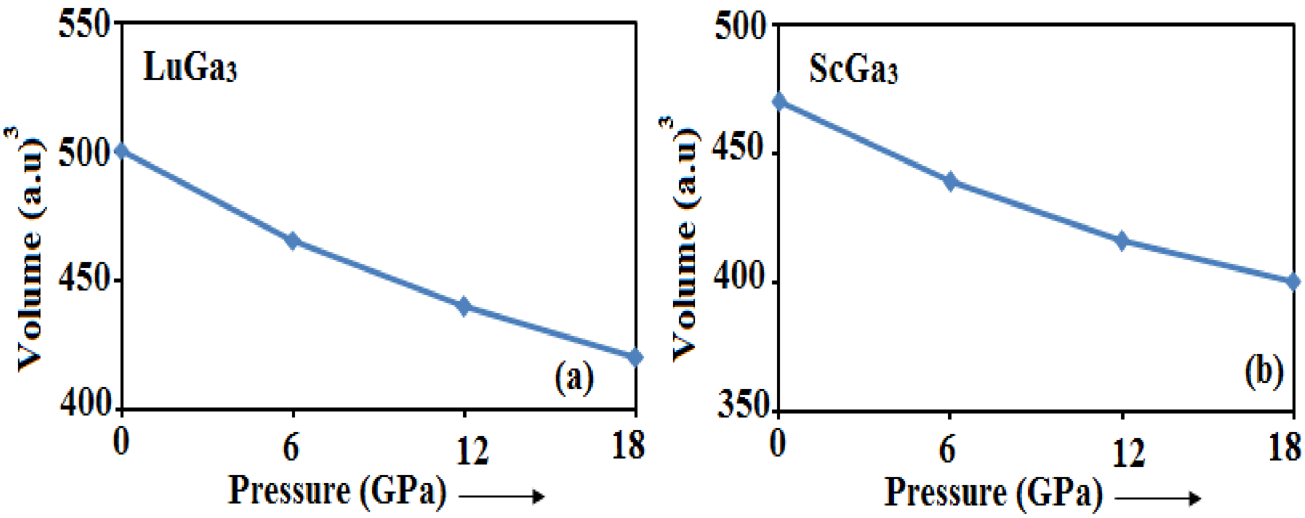


Figure 2. (a)–(b) Variation of volume with pressure of RGa_3 compounds in $AuCu_3$ structure

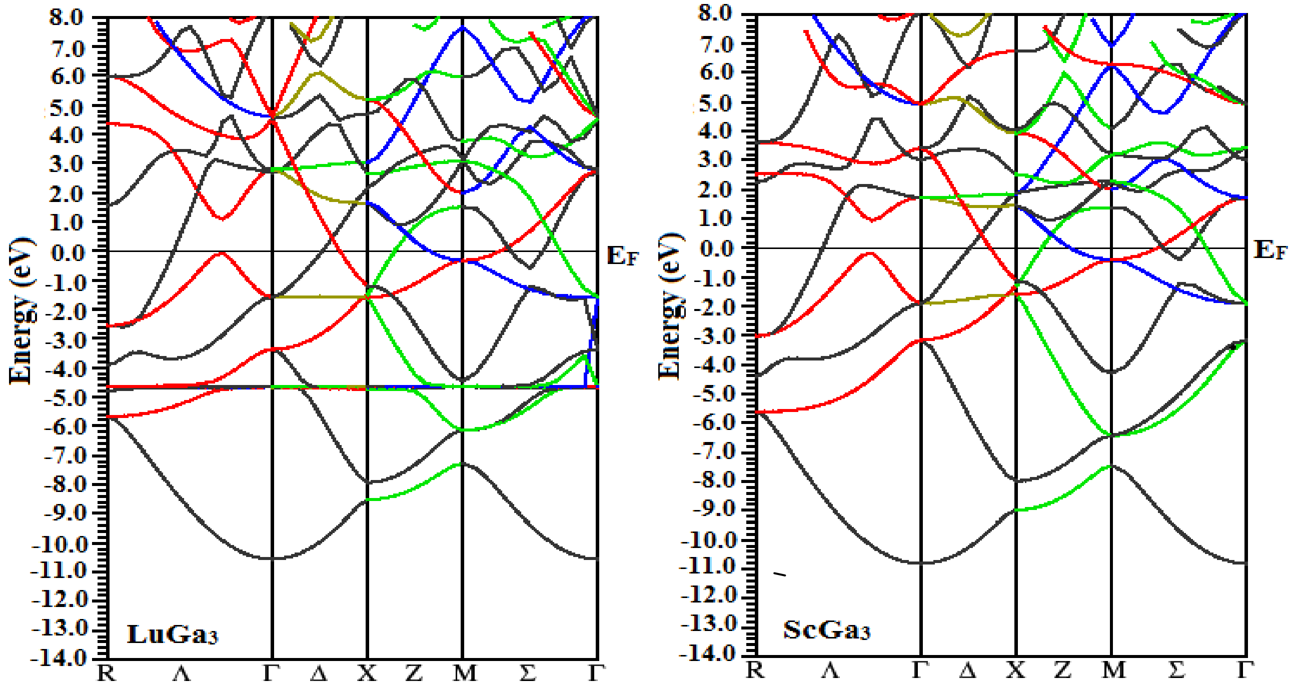
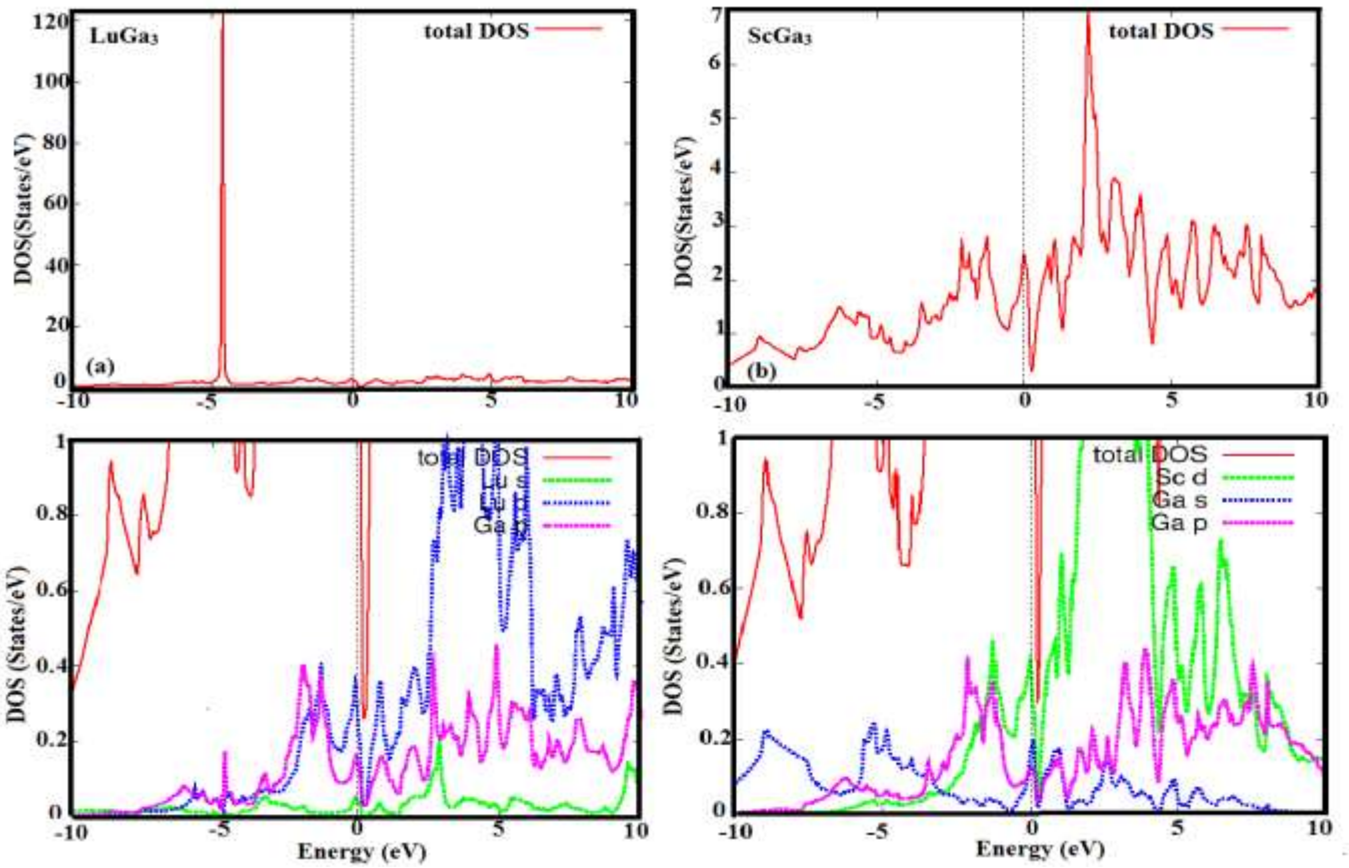


Figure 3(a)-(b). Band structure in $AuCu_3$ phase for RGa_3 compounds at ambient pressure.



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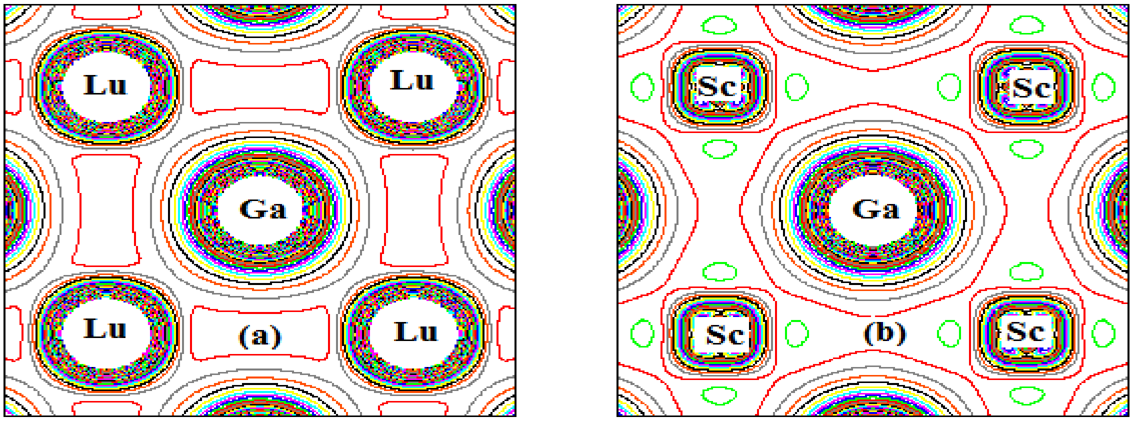

Figure 5: (a) - (b): Electronic charge density plots of RGa_3 at ambient conditions

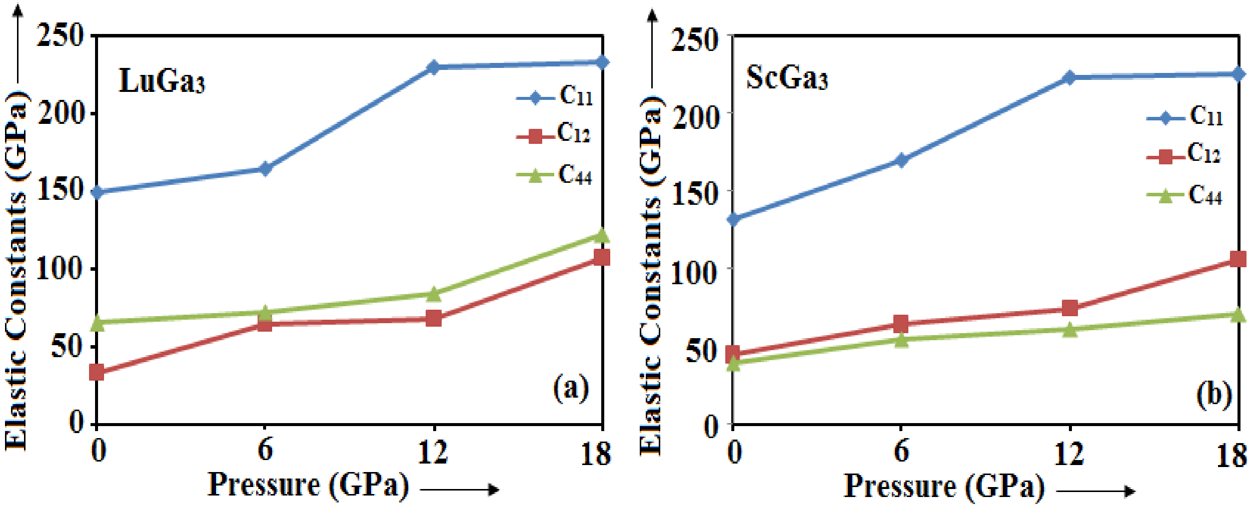

Figure 6: (a) – (b) Variation of elastic constants with pressure of RGa_3 compounds in $AuCu_3$ structure

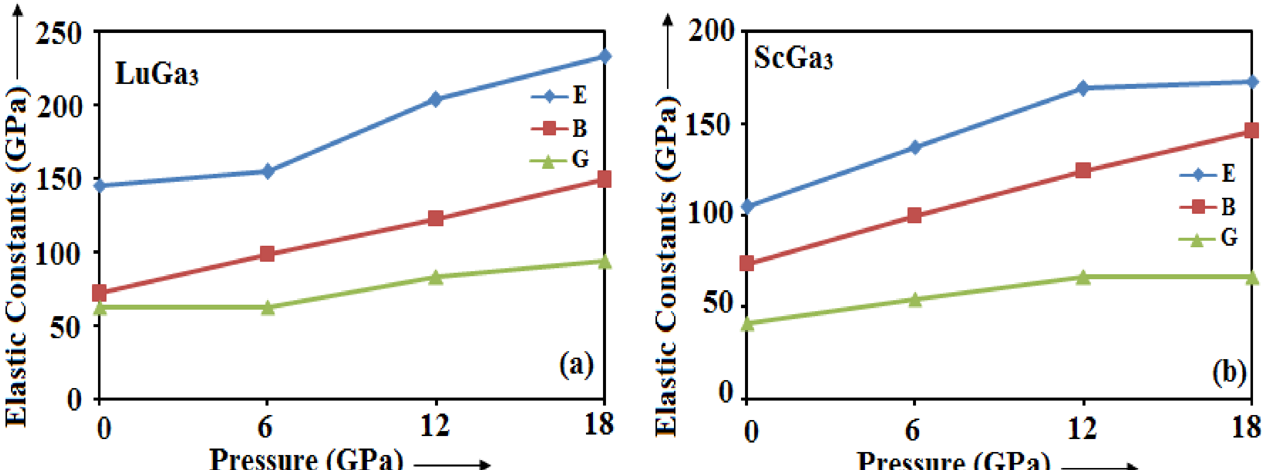

Figure 7 pounds in AuCu$_3$

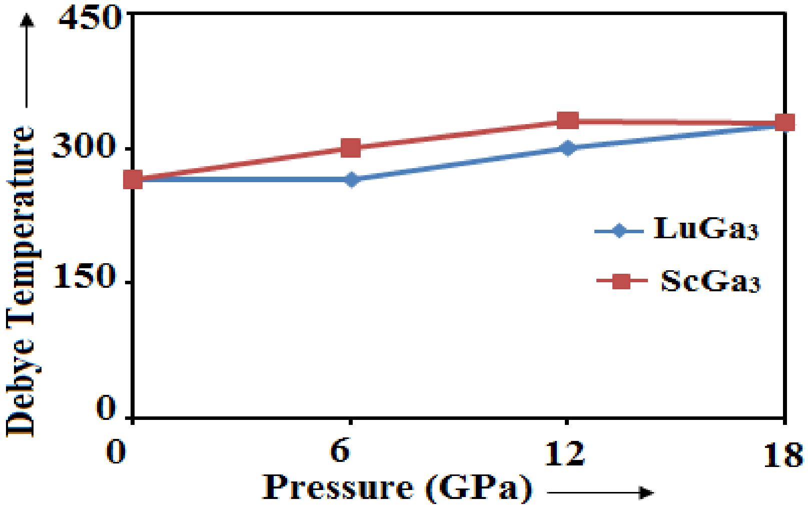

Figure 8: Variation of Debye temperature with pressure of RGa$_3$ compounds in AuCu$_3$ structure

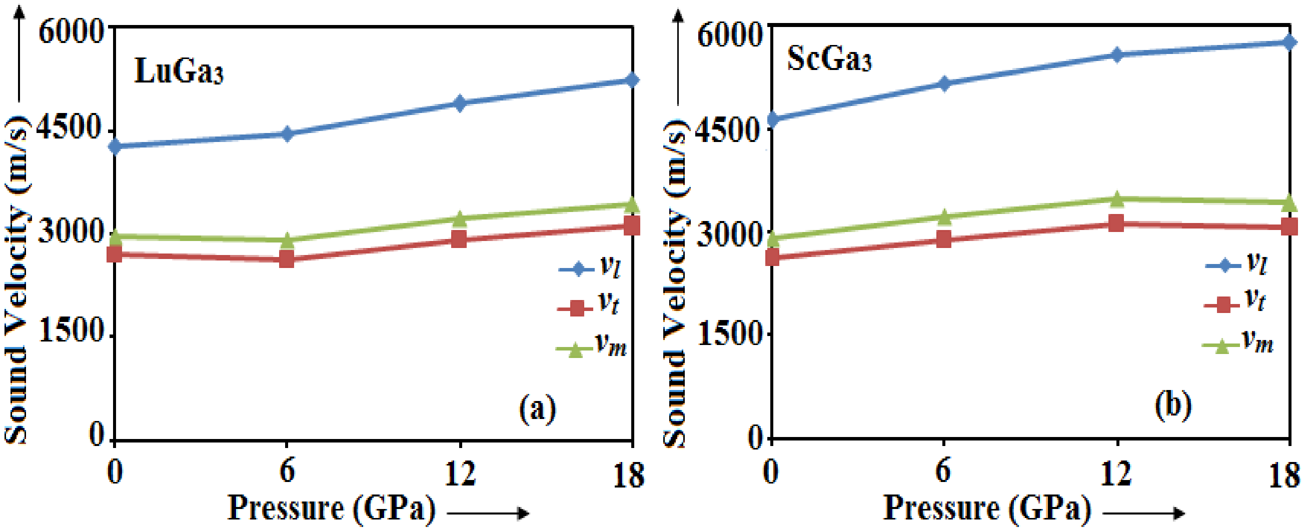

Figure 9: (a) – (b) Variation of longitudinal (v_l), transverse (v_t) and average (v_m) sound velocities with pressure of RGa$_3$ compounds in AuCu$_3$ structure