Electronic, magnetic and elastic properties of new half-Heusler compounds *X*BaGa (*X=Li, Na, K* and *Rb*)

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The structural, half-metallic and elastic properties of the hypothetical half-Heusler compounds *XBaGa* (*X=Li, Na, K, and Rb*) were investigated using first-principles calculations within the generalized gradient approximation (GGA) and GGA+*mbj* based on density function theory (DFT). The absence of the transition-metal atoms makes these compounds important model systems for the study of origin and properties of half-metallic ferromagnetism of sp electron systems. It is shown that for all the compounds the ferromagnetic state is favorable than the non-magnetic state. 'It is also found that these compounds *i.e. KBaGa* and *RbBaGa* exhibit half metallic ferromagnetic properties with an integer magnetic moment of 2 μB per formula unit at their equilibrium lattice constants. The magnetic moment mainly originates from the spin polarization of p-like states of anion and partial involvement of cation *d*-like states (*Ba*). The individual elastic constants, shear modulus, Young's moduli, ratio B/G and the Poisson's ratio were also calculated. The compounds are ductile based on the ratio B/G, they may inherently be the least brittle materials.

1. INTRODUCTION

Half-metallic ferromagnets (there by HMF's) are considered ideal candidates for spintronic applications since they possess 100% polarization of carriers at Fermi level. The concept of HM was first established from electronic structure calculations of half-Heusler NiMnSb alloy by de Groot *et al.*; [1].

In general, HMF's can essentially be treated as hybrids of metals and semiconductors. In other words, the spin resolved bands have a special behavior *i.e.* Majority (minority) spin band shows

metallic-like behavior whereas the minority (majority) spin band shows semiconductor-like behavior with a gap at Fermi level EF. HMF's should satisfy the following two conditions. i) They should exhibit 100% spin-polarization at EF and it is due to existence of metallic and semiconducting nature in their opposite spin states, ii) The total magnetic moment/unit cell should be an integer.

Heusler compounds are a typical class of HMF's and have been intensively studied. this peculiar property (HM) is exhibited by several transition-metal based alloys [2-3] but lately, half-metallic ferromagnetism has been observed for several alloys which do not include transition-metal atoms, I-V, II-V, I-IV and II-IV compounds in ZB and rocksalt structures and some of them have been confirmed experimentally [4,5]. HMF was investigated using the first principles calculations in hypothetical half-Heusler phases such as NiVM (M= P, As, Sb, S, Se and Te) by Ming Zang et al [6] and GeKCa and SnKCa by Chen et al [7]. These facts motivated us to search for new ferromagnetic half metallic half-Heusler alloys without transition metals.

These compounds have the advantage of being energy-efficient for applications since they create weak external magnetic fields and thus lead to minimal energy losses. From the literature review on sp ferromagnets, it is observed that these materials are very promising candidates for spintronic applications since; the half-metallic gaps are wide, they have a small spin magnetic moment per formula unit and thus create small external magnetic fields, their equilibrium lattice constants are close to that of semiconductors and results of the ZB and RS structures suggest high values of Curie temperature [8].

Nowadays attention has also been drawn to potential sp-electron HMF in full-Heusler and half-Heusler structures. This is mainly because the Heusler-based materials have T_C much higher than room temperature [9]. High T_C is very important for application to spintronic devices since it stabilizes the half-metallicity of the material through a small reduction of the spin-polarization at room temperature. Therefore, it is of great interest to merge the magnetic properties of the sp-HM compounds with the properties of Heusler-type structure.

Therefore, it is important to search for new sp-electron HMF with half-Heusler (C1b)-type structure. Motivated by the above findings, in this work, the structural, electronic and magnetic properties of XBaGa compounds (X=Li, Na, K, and Rb), which may help to understand the potential applications of half metallic compounds. Density functional theory (DFT) which is a powerful tool for computational material sciences will be used to calculate properties like density of states, band structures, magnetic moment and other related properties like elastic constants and

curie temperature. We will use the program package Wien2k code [10] to perform electronic structure calculations which uses DFT. It is based on the full- potential linearized augmented plane-wave (FP-LAPW) method, one among the most accurate schemes for band structure calculations.

2. METHOD OF CALCULATION

Half-Heusler compounds are ternary with a 1:1:1 stoichiometry XYZ and crystallizes into non-centrosymmetric cubic (MgAgAs) C1b configureuration [11,14] using space group of F-43m [15].

Table 1 In equivalent site occupancies within the C1b-type structure for XBaGa(X= Li, Na, K and Rb).

	X position	Ba position	Ga position	Magnetic ground state
Type 1	4*d* (3/4, 3/4, 3/4)	4*c* (1/4, 1/4, 1/4)	4*a* (0, 0, 0)	NM
Type 2	4*d* (3/4, 3/4, 3/4	4*b* (1/2, 1/2, 1/2)	4*a* (0, 0, 0)	NM
Type 3	4*d* (3/4, 3/4, 3/4	4*a* (0, 0, 0)	4*c* (1/4, 1/4, 1/4)	NM

Generally, there are six modes in which X, Y, and Z atoms can be distributed above the three sublattices. The interchanging of atoms at a1 and a2 results at equivalent positions due to symmetry, which means that X, Y, and Z atoms can be prescribed at (a1, a2, a3), (a3, a1, a2), and (a2, a3,a1). Due to this, to form C1b structure, there are three possible arrangements (type 1, type 2, type 3) as given in Table 1. For volume optimization, we utilized a self-consistent full-potential linearized augmented plane wave (FP-LAPW) method [16], which depends on DFT instigated into the WIEN2K simulation package [17]. We follow the Perdew–Burke–Ernzerhof (PBE) generalized gradient approximation (GGA) for the electronic exchange–correlation interaction [18]. However, the density of states and the band structure were calculated by using mBJ (modified Becke Johnson) potential. A mesh of $12 \times 12 \times 12$, consisting on 72 special k points that were

taken in the Brillouin zone of irreducible wedge for the integrations within the modified tetrahedron method [19] corresponding to 2000k points in the first Brillouin zone. Sphere, orbital momentum is taken l_{max} = 10. For the convergence of the Eigen-value energy, the expansion of plane waves is organized by cutoff parameter $K_{max} \times R_{mt}$ = 8.0 where K_{max} shows the uttermost value of the reciprocal lattice vector used in plane wave function and R_{mt} represents the smallest muffin tin sphere radii.

3. RESULTS AND DISCUSSION

3.1. Electronic and magnetic properties

As we discuss the electronic and magnetic properties that merge form the XBaGa half-heusler compounds, we compare also the results obtained by the GGA and mBJ–GGA. First of all, we must note that the mBJ approximation affect only the band calculations. The overall band structure profiles for all the compounds are similar. In the energy band diagram, the lower most valence band arises from s-like states of anion Ga shown in figureure.3 and top most valence band is due to *np*-like states of anion with small admixture of d-like states of cation Ba. The anions create an s-band deep in energy, not shown here, which accommodates two valence electrons. The p-states of the anions can hybridize exclusively with the t2g d-states of Ga, which transform following the same symmetry group. These states lie high in the energy above the gaps for both spin directions, and thus the effect of the bands below the gaps is of anionic p-character. From the table 3, it can be observed that the positive value of HM gap for compounds KBaGa and RbBaGa illustrates the existence of true HM ferromagnetism. Also, it can be seen that Eg value decreases on increasing the size of the X (X=K, Rb) atoms, band overlap increases due to the
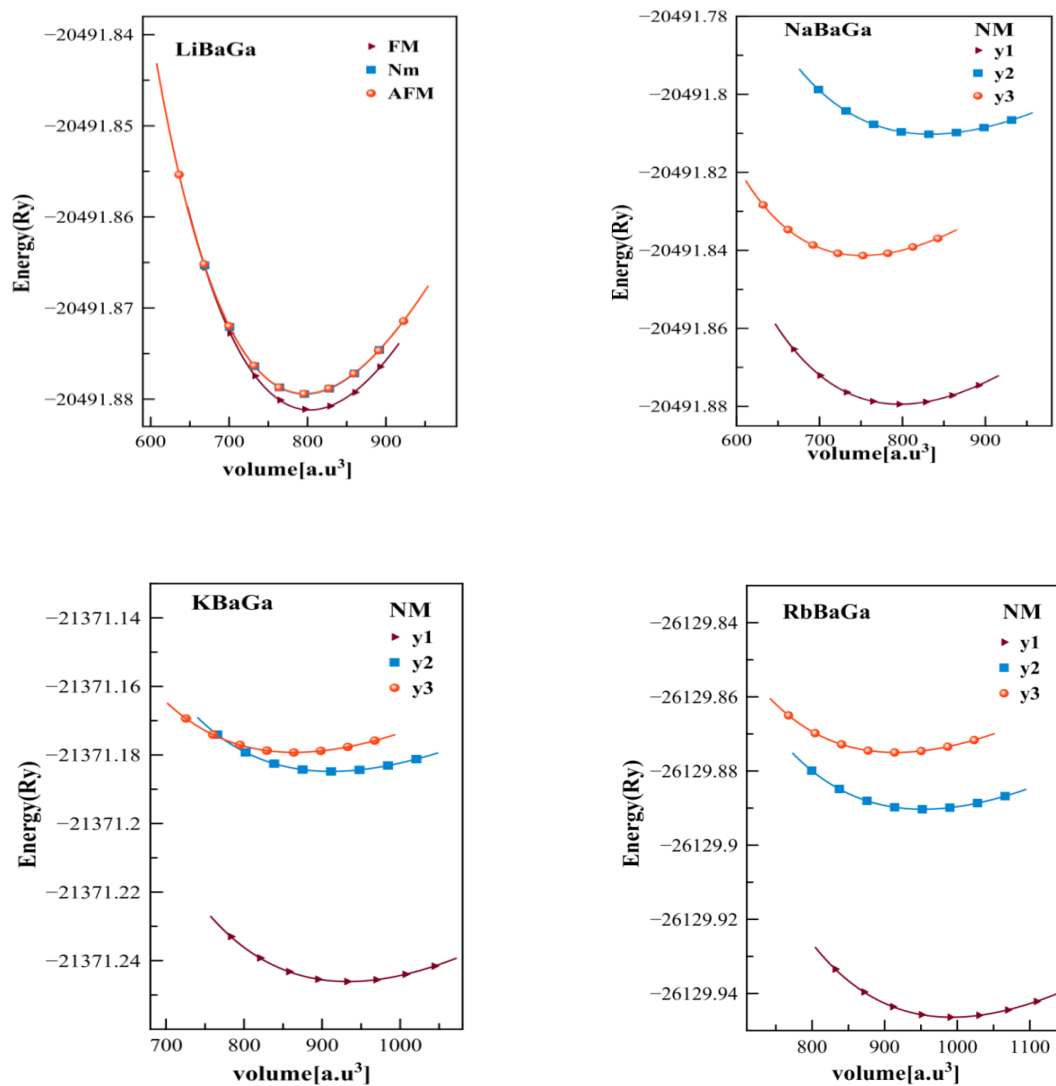
Figure 1 Total energy as a function of volume in the three atomic arrangements type (1), type (2) and type (3). The *curves* correspond to the FM state and origin of the total energy has been shifted to the energy minimum point of type (1) structure
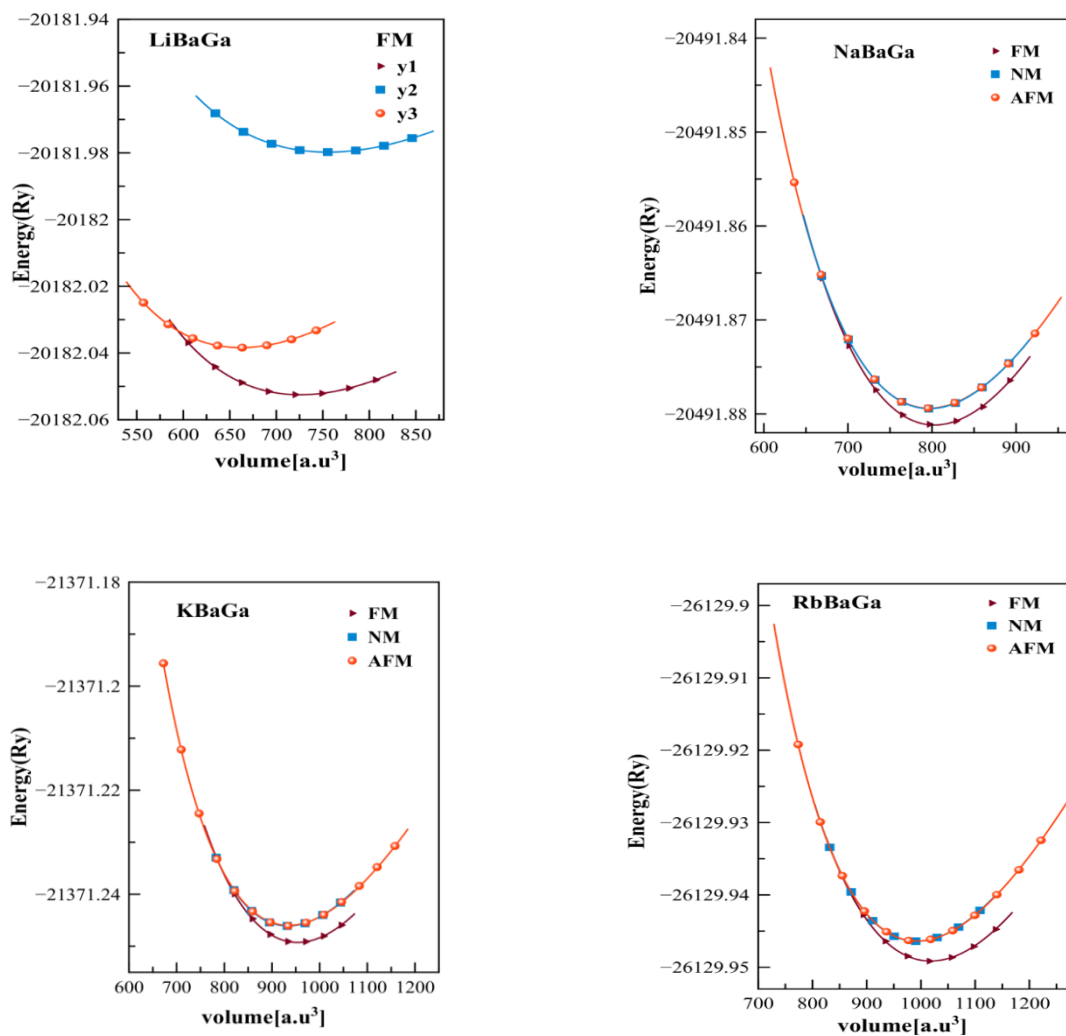
Figure 2 Total energy as a function of volume in the three magnetic states FM, AFM and NM. The *curves* correspond to the type (1) structure and the origin of the total energy has been shifted to the energy minimum point of FM state.

Table 2 Lattice parameter, bulk modulus, and energy difference between FM and NM states, formation energy and Curie temperature of the different compounds.

Compound	VXC		a (Å)	B₀ (GPa)	B'	ΔE (meV)	T_C	ΔH (eV)
LiBaGa	GGA		7.548	17.024	3.802	0.002	210.48	-0.471
	(TB-LMTO) [20]	LSDA	7.383	21		0.0026		-0.351
NaBaGa	GGA		7.807	15.977	3.141	0.002	233.47	-0.430
	(TB-LMTO) [20]	LSDA	7.547	19				-0.242
KBaGa	GGA		8.268	12.412	2.664	0.003	315.72	-0.3944
	(TB-LMTO) [20]	LSDA	7.936	15				-0.544
RbBaGa	GGA		8.449	10.536	2.760	0.003	315.72	-0.3944
	(TB-LMTO) [20]	LSDA	8.124	14				-1.421

Weakened repulsion between anion Ga, cation X (X =K and Rb) and Ba which results in the decrease in Eg. Furthermore, the spin-polarized band structure of other compounds namely, LiBaGa and NaBaGa in figureure 3 shows that the top of the valence band in majority spin channel

slightly crosses E_F which make both the spin channels metallic in nature. In other words, these compounds are on the verge of being fully spin-polarized and these materials are called as nearly HMF materials. In this case the spin-splitting is not enough to push the minority spin states to higher energy and transfer the minority spin electrons to the majority spin channel to make it fully occupied. In the case of LiBaGa and NaBaGa it is very weak. It is shown from Table 3 that the spin-polarization energy is very low E (27m eV) for LiBaGa and NaBaGa. In the following and in order to find the stable phase of hypothetical XBaGa (X=Li, Na, K, and Rb) compounds in half-Heusler (C1b)-type structure, they adopt three possible arrangements noted type (1), type(2) and type(3) as shown in table 1, where X denotes Li, Na, K and Rb. The correct atomic arrangement and the magnetic ground states are determined by minimizing the total energy as function of volume. The total energy is minimized according to three atomic arrangements to see which one is the most favorable (see Figure.1). We performed a spin-polarized and spin-unpolarized calculation for every atomic configureuration to find the magnetic ground state, ferromagnetic (FM), anti-ferromagnetic (AFM), and non-magnetic (NM) state (see Figure. 2). From these results, one can confirm that the three compounds take the type (1) arrangement with a ferromagnetic ground state. The obtained results are summarized in Table 2. In the ferromagnetic state, the computed lattice parameters are overestimated [20] whereas the bulk modulus is underestimated for XBaGa (X=Li, Na, K, and Rb) [20], and generally it is found that the lattice parameter increases with increasing of the X atomic number in the formula. As a consequence, the bulk modulus decreases, yielding in a weaker hybridization between the atoms. The compounds with higher atomic number are more easily compressible than lower ones. The calculated formation energy (ΔH) value is given in Table 2. From the table2, it can be considered that XBaGa (X=Li, Na, K, and Rb) half-Heusler alloys have negative value of formation energy and that indicates they may be stable if they are synthesized experimentally, as per the stability of other works [20] and other possible binary and ternary phases [21–23].
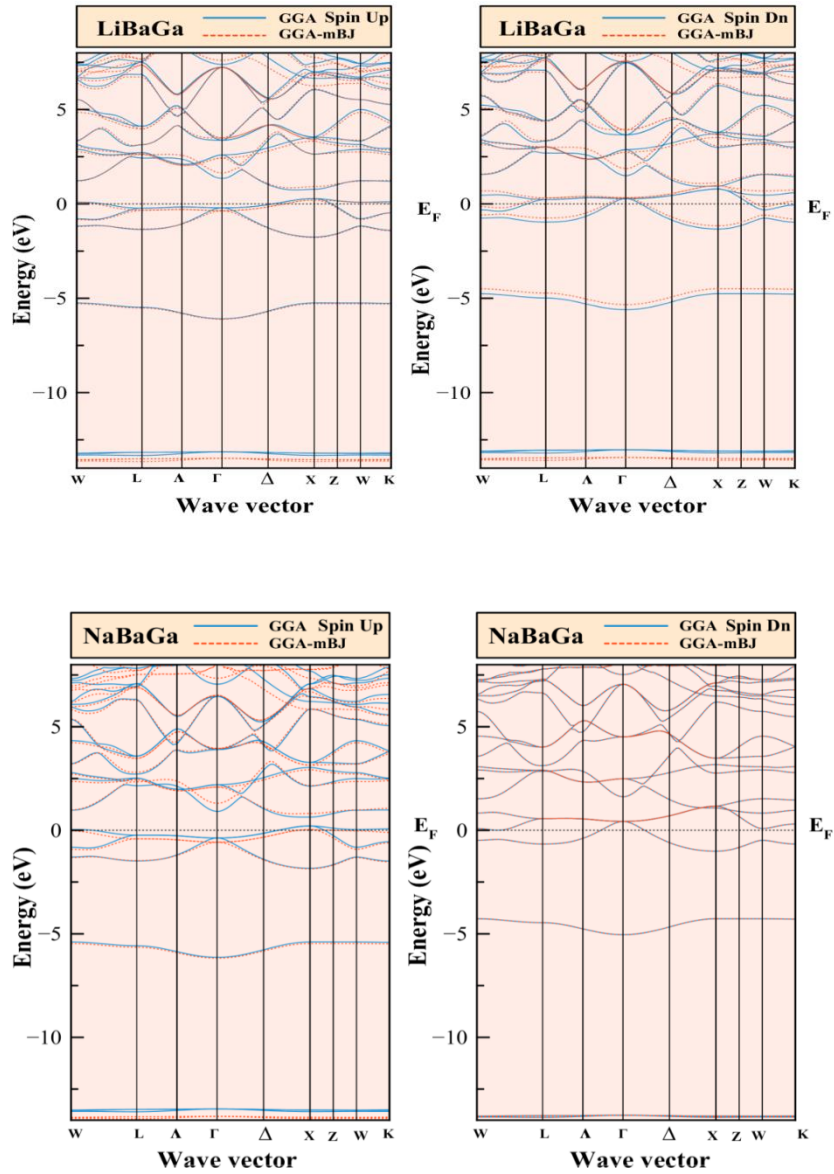
Figure 3 Band structure of ferromagnetic XBaGa at the equilibrium lattice constant in the type (1) structure. GGA and mBJ–GGA band structures are shown in *solid* and *dotted lines*, respectively.

Majority and minority spins are shown in the left and right panel, respectively. The Fermi level is set to zero.
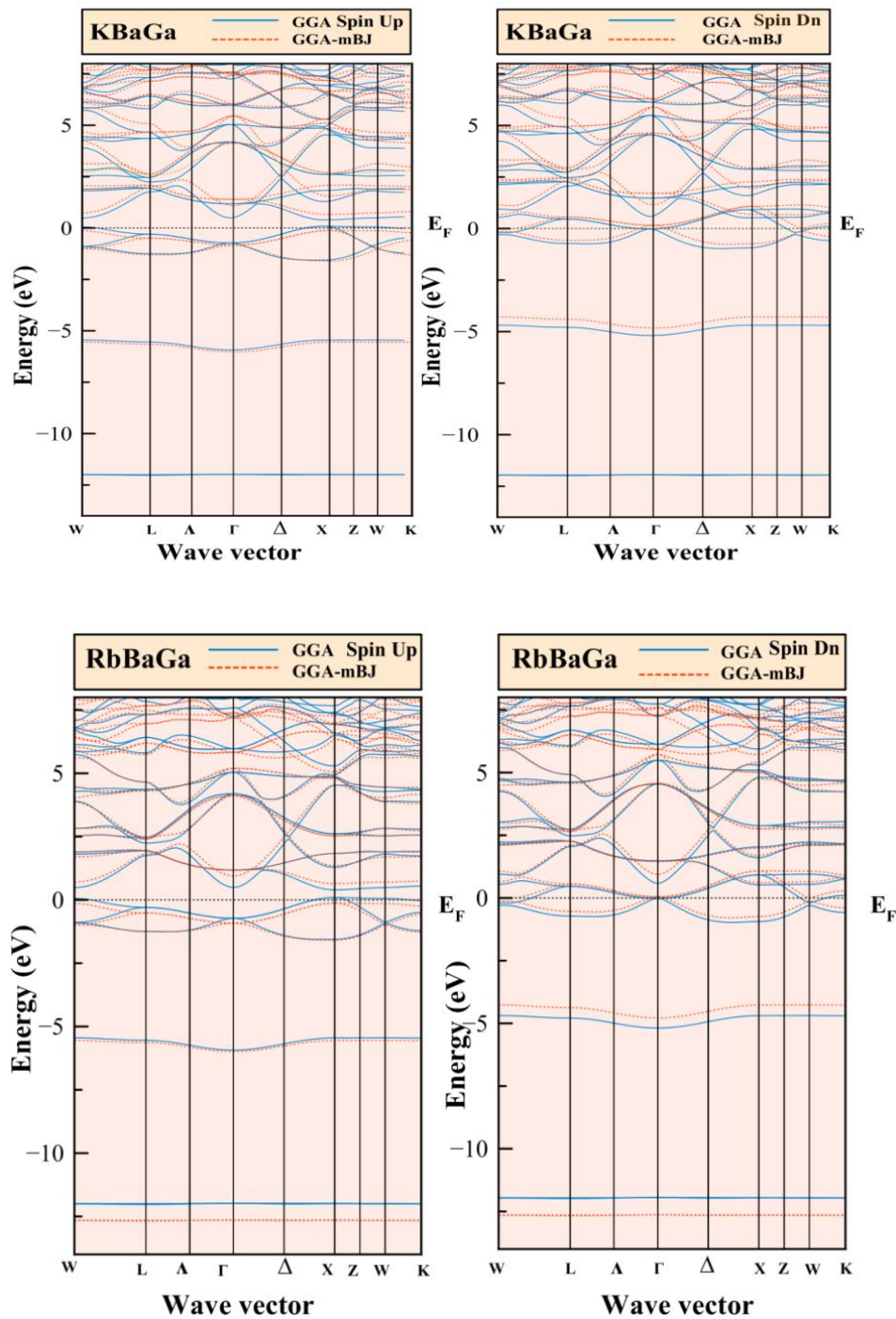
Figure. 3 continued

Table 3 Total magnetic moment Mtot (µB*)* of compounds XBaGa and local magnetic moments (µB*)* of Ba, Ga, and X atom. MI (µB*)* is the magnetic moment of the interstitial region, band gap E_{BG} (eV).and half-metallic gap E_{HM} (eV) in the spin up channel

Compound	VXC	M_X (µB)	M_{Ba} (µB)	M_{Ga} (µB)	M_I (µB)	M_{tot} (µB)	E_{BG}(eV)	Bande transition	E_{HM}(eV)
LiBaGa	GGA	0.115	0.450	0.165	0.354	1.086			
	mBJ–GGA	0.168	0.632	0.216	0.485	1.50			
	(TB-LMTO) LSDA[19]	0.038	0.132	0.310	0.019	0.500			-0.667
NaBaGa	GGA	0.099	0.609	0.212	0.459	1.381			
	mBJ–GGA	0.146	0.914	0.275	0.641	1.977			
KBaGa		0.122	0.838	0.260	0.532	1.742			

GGA								
mBJ–GGA	0.122	1.048	0.282	0.546	2.0	0.779	X→X	0.116
RbBaGa GGA	0.104	0.882	0.268	0.496	1.752			
mBJ–GGA	0.110	1.090	0.291	0.574	2.00	0.769	X→X	0.126

When there is an exchange   between the magnetic moments of neighboring atoms, a magnetic order on a macroscopic scale may form at low temperatures. The sign of the coupling will determine the characteristics of the coupling, either parallel to each other (i.e. ferromagnetism) or anti-parallel to each other (i.e. anti-ferromagnetism). The critical temperature increases when the coupling is stronger [23].

The magnetic moment determines the magnetic nature of a material. The calculated magnetic moment of *XBaGa* is listed in the Table-3. It is note that Ba atom had the prominent contributions to the total magnetic moment of *XBaGa*. The calculated magnetic moments of *XBaGa* do not properly fit with Slater-Pauling rule[23,24] of half-metallicity, $M=N_v - 24$, where N_v is the number of valence electrons in a unit cell and M is the magnetic moment. It is expected, any compound of *XBaGa* is not completely half-metallic We notice they have relation between the magnetic moment ant curie temperature, the magnetic moment increases with curie temperature. Temperature of a ferromagnetic material is called the Curie temperature (*T*c) and that of an anti-ferromagnetic material, the Neel temperature (*T*N). To understand the origin of ferromagnetism, the spin-polarized total and partial density of states of XBaGa compounds in half-Heusler (C1b)-type structure are calculated at their equilibrium volume and are shown in figureure 4 From the

total DOS histogram, it is observed that for KBaGa and RbBaGa compounds, there is spin-splitting of energy states around E_F and it indicates the presence of ferromagnetism with the majority spin states exhibiting semiconducting property and minority spin states exhibiting metallic property. Hence it proves the existence of true half-metallicity in these compounds. The spin-polarization property at the Fermi of a material can be calculated by the using the density of states at the Fermi level for the corresponding spin defined as [25]

$$P = \frac{N_\uparrow(E_F) - N_\downarrow(E_F)}{N_\uparrow(E_F) + N_\downarrow(E_F)}$$

where $N_\uparrow(E_F)$ and $N_\downarrow(E_F)$ are the density of states at the Fermi level for spin-up and spin-down, respectively. If the spin-up (or spin-down) contribution to the density states at the Fermi level is zero, a material will be 100% spin-polarized. For the d-like orbital character, P will be high but low for s-like or s+d-like orbital character [25].

The calculated spin-polarizations (P) of XBaGa are listed in the Table-4

The highly spinpolarized materials are very important for spintronic device applications.

Table 4 The calculated density of sates at the Fermi level for spin-up $N_\uparrow(E_F)$ (states/ eV f.u.) and spin-down $N_\downarrow(E_F)$ (states/ eV f.u.), as well as the polarization in %.

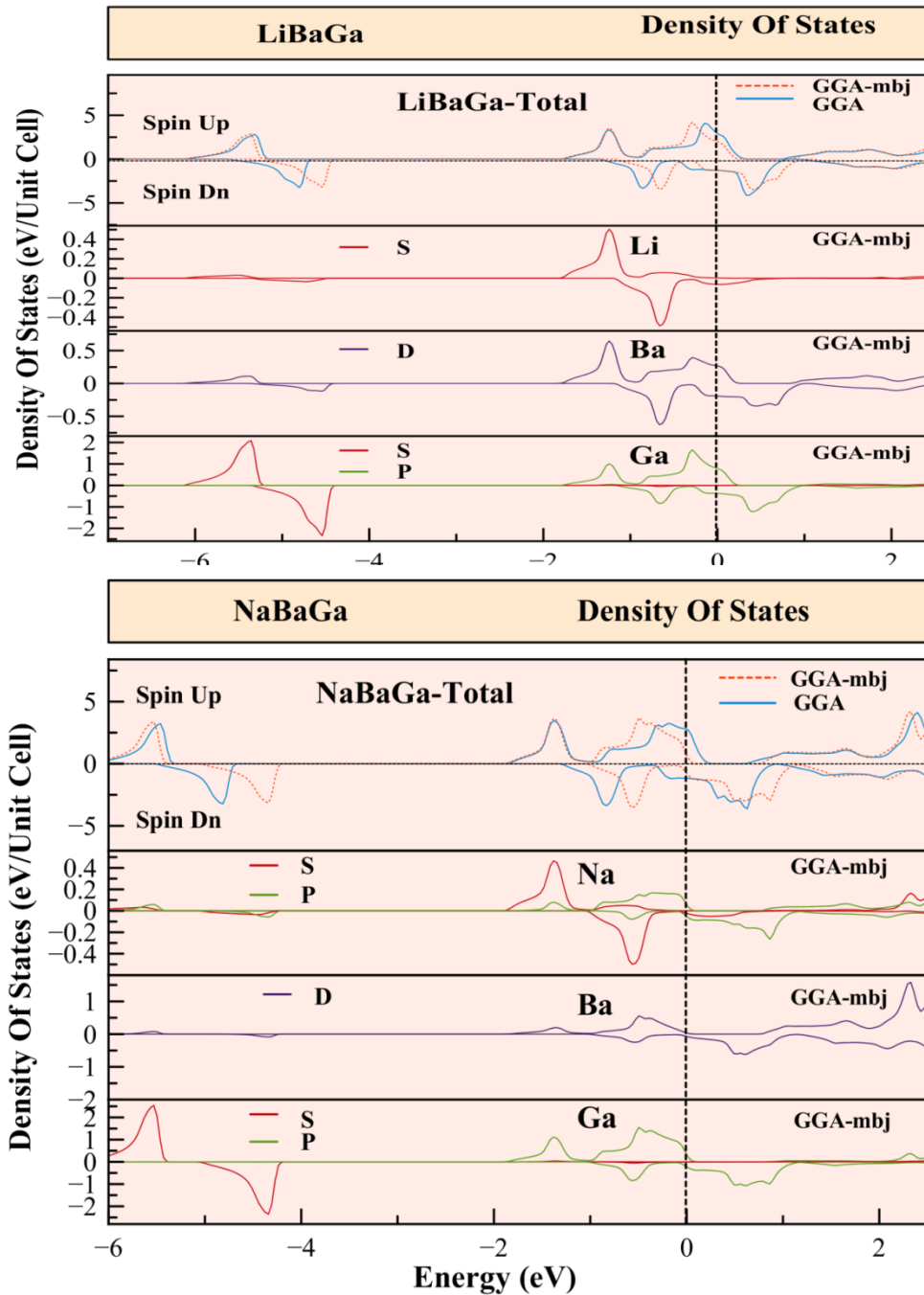| Compounds	GGA			GGA-mbj		
	$N_\uparrow(E_F)$	$N_\downarrow(E_F)$	P%	$N_\uparrow(E_F)$	$N_\downarrow(E_F)$	P%
LiBaGa	2.7831	1.3089	36.02	1.7698	1.2736	16.30
NaBaGa	2.8222	1.1732	41.27	1.0755	0.5795	29.96
KBaGa	2.5101	0.9162	45.24	0	0.32	100
RbBaGa	1.9664	0.9783	33.55	0	0.228	100

Figure 4 Total and orbital spin density of states (DOSs) of ferromagnetic XBaGa at the equilibrium lattice constant in the type (1) structure. GGA and mBJ–GGA spin DOSs are shown in *solid* and *dotted* lines, respectively. The Fermi level is set to zero.
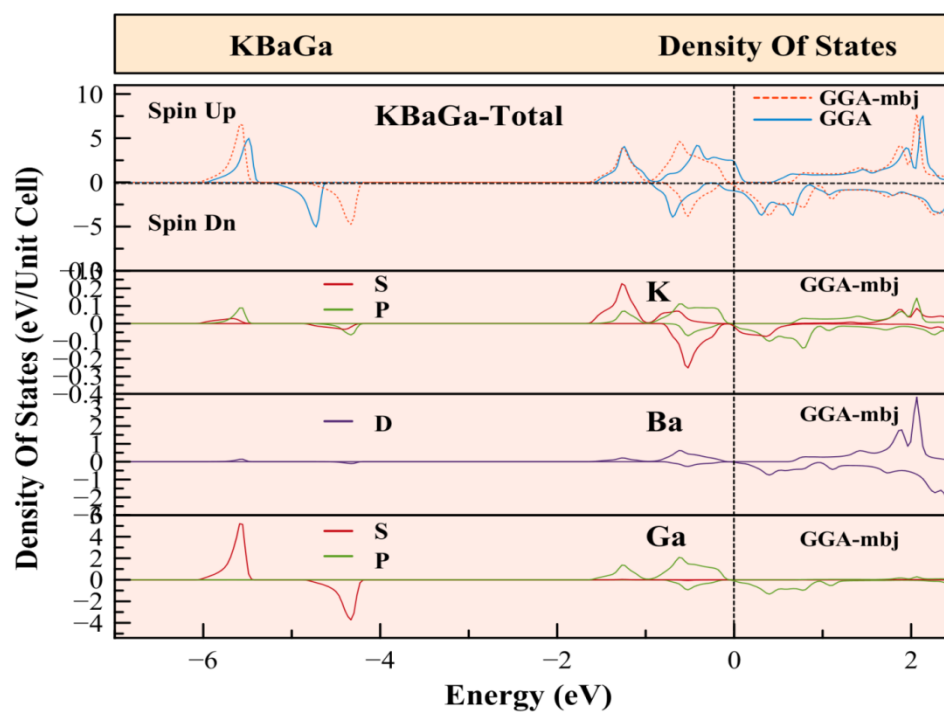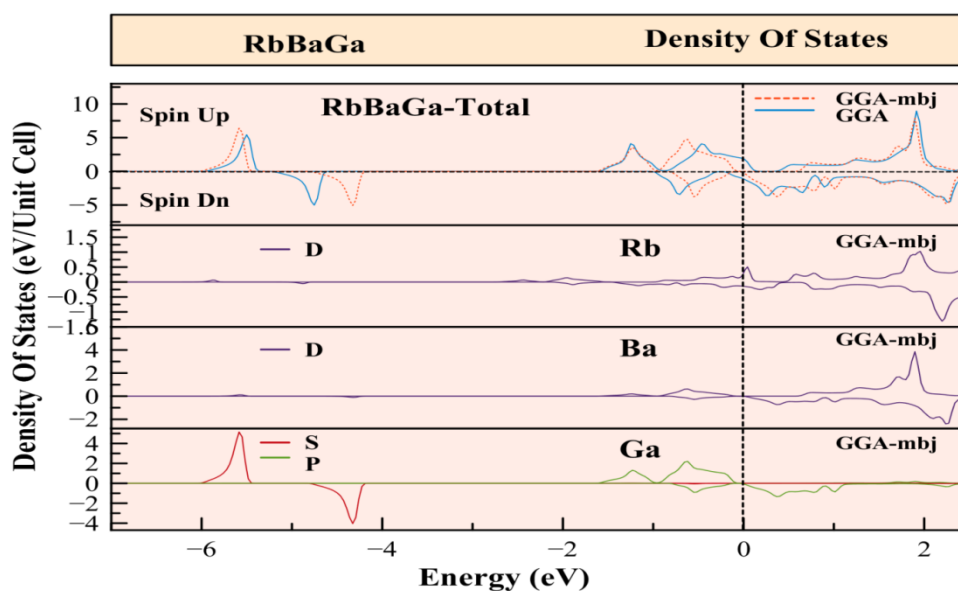
Figure.4 continued

From the PDOS diagram, it can be seen that the spin-polarized states near EF is mainly due to anionic Ga *p*-like states which is slightly hybridized with n*d*-like states of cation Ba. In these compounds, there are no localized *d* electrons, hence there is no room for double exchange or *p-d* exchange mechanism which is responsible for magnetism in transition metal-based compounds. The strong spin-polarization of 2*p*-like states of anion around E_F in the titled compounds is mainly due to the hybridization of anionic 2*p*-like states with *nd*-like states of cation (Ba) and it is responsible for magnetism in these compounds. Due to this bond formation, the top of the valence band (three) are fully occupied in majority spin states whereas, minority spin states are partially occupied. Therefore, the majority spin states in these compounds exhibit semiconducting nature with a band gap around the Fermi level and metallic nature in minority spin states. This can be understood from the electronic arrangement. There are six valence electrons in XBaGa compounds (X: *ns*1; Ba: *ns*2; Ga: *ns*2, *np*1) which contributes to the bond formation and magnetism in these compounds. In this X and Ba (cations) donate their *ns*-like electrons to *np*-like states of Ga (anion). Out of these six electrons, two electrons occupy the Ga-*ns* state in the lowest energy (not shown in figureure) and the three electrons fully occupy the majority spin states near the Fermi level. The remaining one electron partially fill the corresponding minority spin states near the Fermi level introducing two holes which provides the total magnetic moment of 2.0 B/f.u. Here, we come to the magnetic properties of these half-Heusler compounds. As shown in Table 3, the magnetic moment calculations show that total magnetic moment per formula unit for the two compounds KBaGa and RbBaGa are integral. The integral total magnetic moment, which is a typical

characteristic of HM ferromagnets, obeys the Slater-Pauling rule for the half-Heusler alloys. We can see that the major contributions to the total magnetic moments come from Ba atoms, while the Ga and X (X=Li, Na, K, Rb) atoms can be regarded as minor. Furthermore, from Table 3, it can be seen that the compounds namely LiBaGa and NaBaGa at their equilibrium volume, possess non-integer magnetic moment [26–29] which indicates the presence of ferromagnetism. It means that there is spin-polarization of energy states around E_F, however it is not 100%. Hence, these compounds exhibit nearly HMF.

3.2 Elastic properties

The results of the structural and elastic properties are summarized in Table 4 and should provide good predictions of the structural and elastic properties when no experimental data are available. These results are consistent with the results of ref. [19]. Thus, the FP-LAPW method using the GGA approximation is an appropriate and effective method for studying the structural and elastic properties To verify these results of the elastic constants and bulk modulus it is easy to see that the conditions for mechanical stability for cubic crystals are verified: $C_{11} - C_{12} > 0$, $C_{11} > 0$, $C_{44} > 0$, $C_{11} + 2C_{12} > 0$, $C_{12} < B < C_{11}$ [30].

From the Cij constants of a compound, some of its important properties such as the stiffness, brittle ductility nature and type of chemical bonding can be estimated. Numerous macroscopic elastic moduli parameters such as the shear modulus G, Young's modulus E, Poisson's ratio m, anisotropy factor A and the Pugh's B/G ratio were calculated and presented in Table 5. For the XBaGa compounds, the corresponding value of *v* is about 0.269, 0.282 and 0.379, thus indicating a strong ionic contribution in the intra-atomic bonding for this compound. According to Pugh's empirical criterion, [31] a high and low B/G ratio may be associated with a ductile and brittle nature for a particular compound, respectively, and the critical value separating ductile and brittle materials is around 1.75. For the XBaGa compound, the calculated value of the B/G ratio is about 1.834 to 1.967, thus indicating that the investigated compound can be classified as a ductile material. The elastic anisotropy [32] of a crystal is an important factor, since it provides information about the possible formation of micro cracks or other structural defects that occur during crystal growth. For a material with perfect elastic isotropy, $A = 1$, the difference $(A - 1)$, be it positive or negative, is a measure of the degree of elastic anisotropy of the material.

Table 5 Calculated elastic constants (C_{11}, C_{12} *and* C_{44}, *in GPa*), Young's modulus (*E, in GPa*), shear modulus (*G, in GPa*), Poisson's ratios (m, dimensionless), anisotropy factor (A) and *B/G* ratio for the XBaGa (*X=Li, Na, K, Rb*) compounds using the FP-LAPW method within the GGA.

	C_{11}	C_{12}	C_{44}	B	G	E	v	A	G_v	G_R	B/G
LiBaGa	29.069	13.7423	10.7678	18.496	4.865	13.418	0.379	1.510	9.313	0.416	1.834
NaBaGa	26.1957	9.0899	6.8950	14.791	7.516	15.005	0.282	0.806	7.558	7.474	1.967
KBaGa	25.3791	6.0874	5.6416	12.517	7.0041	15.303	0.112	0.584	7.2433	6.7649	1.787
RbBaGa	19.5240	4.6209	4.0328	9.588	5.225	2.684	0.269	0.541	5.512	4.938	1.835

4. CONCLUSIONS

In this paper, we have performed first principles calculations based on spin density functional theory to shed light on the magnetic and electronic structures of sp-electron HM in a series of new half Heusler-based, half metallic materials XBaGa, the main results obtained were the stability of the HM with respect to the lattice contraction and make these compounds promising candidates for spintronics applications. The p–p hybridization is shown to be essential for the formation of spin polarization and magnetic moment is mainly carried by the anions. It is shown that for all the compounds the ferromagnetic state is favorable than the non-magnetic state. 'It is also found that these compounds *i.e. KBaGa* and *RbBaGa* exhibit HMF property with an integer magnetic moment of *2 μB* per formula unit at their equilibrium lattice constant, These properties show that these compounds are good candidates for possible application in diluted magnetic semiconductors, spin injectors, and other spintronics applications. As for the elastic properties the value of the unidirectional elastic constant C_{11}, which is related to the unidirectional compression along the principal crystallographic directions, is higher than that of C_{44}, indicating that these compounds

present a weaker resistance to the pure shear deformation compared to the resistance to the

unidirectional compression.

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