A Theoretical Study of Structural, Electronics, and magnetic properties of GdX_3[X = In and Sn]: DFT

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ABSTRACT

In this article, we have investigated the electronic and magnetic properties of intermetallic materials such as GdIn3 and GdSn3. In the present study, a theoretical approach known as Density Functional Theory (DFT) was employed. The electronic structural properties of GdIn3 and GdSn3 compounds were evaluated in terms of lattice parameters (a_0, c_0), bulk modulus (B0), and first-order pressure derivative (B'0). The crystal structures of GdIn3 and GdSn3 exhibit a resemblance to the cubic L_{12} ($AuCu_3$) crystal structure, with a space group of pm-3m (no. 221). The metallic nature of $GdIn_3$ and $GdSn_3$ compounds is demonstrated by their electronic behavior, which is characterized by band structure (BS) and density of states (DOS). The metallic properties of this substance can be attributed to the presence of Gd-f orbital states, which also contribute to its magnetic character. All the parameters in this study are consistent with both the experimental and theoretical results.

Keywords: DFT, DOS, Electronic Properties, Magnetic Properties.

Introduction

Rare-earth intermetallic compounds frequently exhibit elevated melting points, rendering them well-suited for utilization in situations characterized by high temperatures. The ability to retain ductility even under extreme temperatures is significant for applications that entail mechanical stress in high-temperature environments. These compounds exhibit remarkable mechanical properties, such as exceptional strength and hardness, rendering them highly attractive for structural applications. Frequently, they exhibit a comparatively decreased density or specific weight, hence conferring benefits for weight-sensitive applications. Certain intermetallic compounds containing rare-earth elements have notable resistance to corrosion, a highly desirable characteristic for their utilization in situations with high levels of aggressiveness. These materials exhibit a diverse array of mechanical properties across varying temperatures, hence offering a broad spectrum of potential applications. Numerous intermetallic compounds containing rare-earth elements have intriguing electrical and magnetic characteristics, rendering them valuable for applications in electronic and magnetic devices. Due to their distinctive properties, intermetallic compounds containing rare-earth elements are utilized throughout several industries, encompassing aerospace, automotive, electronics, and materials research. Special emphasis should be placed on their significance in the advancement of specialized technologies through the creation of sophisticated materials

[3]. The electronic configuration of Gd-64 is exceptional $4f^7 5d^1 6s^2$ ($4f^8 6s^2$) now this configuration has 4f and 5d shell incomplete, so Gd and its compounds show magnetic properties due to 4f state and mechanical properties due to 5d state like transition metals [1,2]. It has lot of potential in multiple sectors like aviation, automobile, spintronics, electrical and electronics industries [4,5]. Rare earths have magnetic nature in intermetallic compound because they contain incompletely filled 4-f electron orbitals. When the temperature rises above room temperature these show ferromagnetic nature with high spin polarization [5]. We have thought of the chemical nature of rare earth elements, we found these have external electron arrangement, so these have shown similar properties. In rare earth elements have range from La ($4f^0$) to Lu ($4f^{14}$) and all elements of inner 4-f orbital have pairs and unpaired numbers. The comprehension and utilization of the electronic and magnetic characteristics of rare-earth elements and their compounds have resulted in significant technological progress in various domains, including electronics, telecommunications, energy generation, and storage [6-8]. In this paper, we have calculated structural properties of $GdIn_3$ and $GdSn_3$. This crystal structure belongs to cubic $L1_2$ $AuCu_3$ crystal type structure, and space group is Pm-3m (No. 221). The rare earth atoms (Gd) are in (0, 0, 0) position. The Wyckoff position of non-magnetic elements In or Sn (0, 1/2, 1/2) [5,9]. The structural properties of $GdIn_3$ and $GdSn_3$ have been studied by GGA approximation, K-point optimization by SCF for first Brillouin Zone (BZ) and the muffin tin radius (R_{mt}) (General 2-3 a.u. for rare earth elements) using the WIEN-2K code [10]. The Electronic properties in terms of Bs and DOS with help of DFT of $GdIn_3$ and $GdSn_3$. Full- Potential linearized augmented plane-wave (FPLAPW) + local orbital's (LO) method with interface with WIEN2K software [11]. The magnetic properties of $GdIn_3$ and $GdSn_3$ are magnetic momentum and magnetic types of material obtained by DOS with spin contribution of electron orbitals. The magnetic structures of $GdIn_3$ and $GdSn_3$ are very complex, it is changing properties on low temperature (Neel temperature 42K) [12-14].

Method of calculations

In this paper, we have used a computational methodology for studying different parts of crystalline materials, especially solids, the Full Potential Linearized Augmented Plane Wave Plus Local Orbital (FPLAPW+LO) method is a very good way to use computers to do electronic structure simulations. The proposed approach represents a refinement and expansion of the Linearized Augmented Plane Wave (LAPW) technology [15,16-17]. We have calculated the electronic and magnetic properties of compounds GdX_3 (X = In and Sn). We have chosen cutoff energy (E_{cut}) = 6.0 Ry, charge of crystal convergence =0.0001ec and K-point is 18 x 18 x 9 k points for SCF calculations, these parameters is help for analysis electronic, magnetic and thermodynamics properties. The muffin tin approximation is a widely employed technique in the field of quantum chemistry, which serves to accelerate the computational process involved in determining the electronic structure of a solid material. The process entails partitioning the spatial domain around each atom within a crystalline structure into two distinct regions. The first region, denoted as the "muffin tin," corresponds to an inner sphere centred at each atom. The second region comprises the interstitial space existing between the spheres. The electron's potential within the muffin tin is commonly considered to exhibit spherical symmetry and is typically represented by a simplified

potential model. The potential outside the muffin tin can be approximated by summing the contributions from all other atoms. The utilization of this approximation enables a substantial reduction in complexity when addressing the electronic structure problem, rendering it computationally viable to determine the electronic characteristics of extensive and intricate systems. If we need more plane wave, then we required large R_{MT}. There is large number of plane waves give more information in the calculation. But when we choose R_{MT} very large, surface charge would be leak. It is worth must be little given no centre charge ought to be spilled out. Its value should be very low, as there is no core charge leaking on its surface. If the charge leaks, the value of the R_{MT} is changed either to increase it or to decrease it. This has not charge leaking on its core surface. The value of R_{MT} is kept low so that more plane waves can remain in it. For the compounds GdIn3 and GdSn3, the RMT values employed were 2.50 atomic units for Gd, and 2.43 atomic units for In and Sn. The obtained values of RMT were deemed acceptable for the purposes of the computations. The Fermi energies for GdIn3 and GdSn3 were determined to be 0.56260 eV and 0.61689 eV, respectively, as shown in Table 3.

The magnetic moments of materials contain data regarding both the magnitude and direction of magnetization. The magnetic moment in this context is determined using spin-polarized calculations utilizing density functional theory (DFT) with the PBE-GGA [17] exchange correlation.

Results and discussion

Structural properties

In this study, we employed the Birch-Murnaghan equation of state (EOS) in conjunction with the Generalized Gradient Approximation (GGA) to determine the structural characteristics of the intermetallic compounds GdIn3 and GdSn3. The investigation of material properties under varying conditions is a widely employed methodology in the fields of solid-state physics and materials research. The Birch-Murnaghan equation of state is employed for the purpose of representing the correlation between the total energy (E) of a unit cell and its corresponding volume (V). The application of this method is particularly advantageous in the prediction of a material's response to variations in pressure. Within the given framework, the lattice constants (a_0) serve as the definitive lattice parameters of the crystal structure at equilibrium. The bulk modulus, denoted as B_0, is a parameter that quantifies the material's ability to withstand compression. The initial pressure derivative (B_0') offers insights into the variation of the bulk modulus in response to variations in pressure [18]. All calculated data shown in table 1. These results are very close to experimental data [19-23].

Bulk modules (B_0) are defined as degree of resistance of material to compression while bulk modulus is increase then degree of resistance is increase. Our conclusion is (B_o) $GdIn_3$ > (B_o) $GdSn_3$, bulk modulus value decreases from $GdIn_3$ < $GdSn_3$ and degree of resistance also decreases from $GdIn_3$ < $GdSn_3$ because of increase the values of lattice parameters, so lattice parameters increase in order (a_0) $GdIn_3$< (a_0) $GdSn_3$.

Bulk modulus and first order pressure derivatives experimental values are not found in literature, so my calculated data are considered as an expectation for these properties of $GdIn_3$ and $GdSn_3$.

Table 1

Lattice parameters, a_0, c_0 (Å), Bulk modulus, B_0 (GPa), Pressure derivative of bulk modulus, B_0' (GPa) equilibrium condition (at 0K) for GdX_3[X= In and Sn] using PBE-GGA.

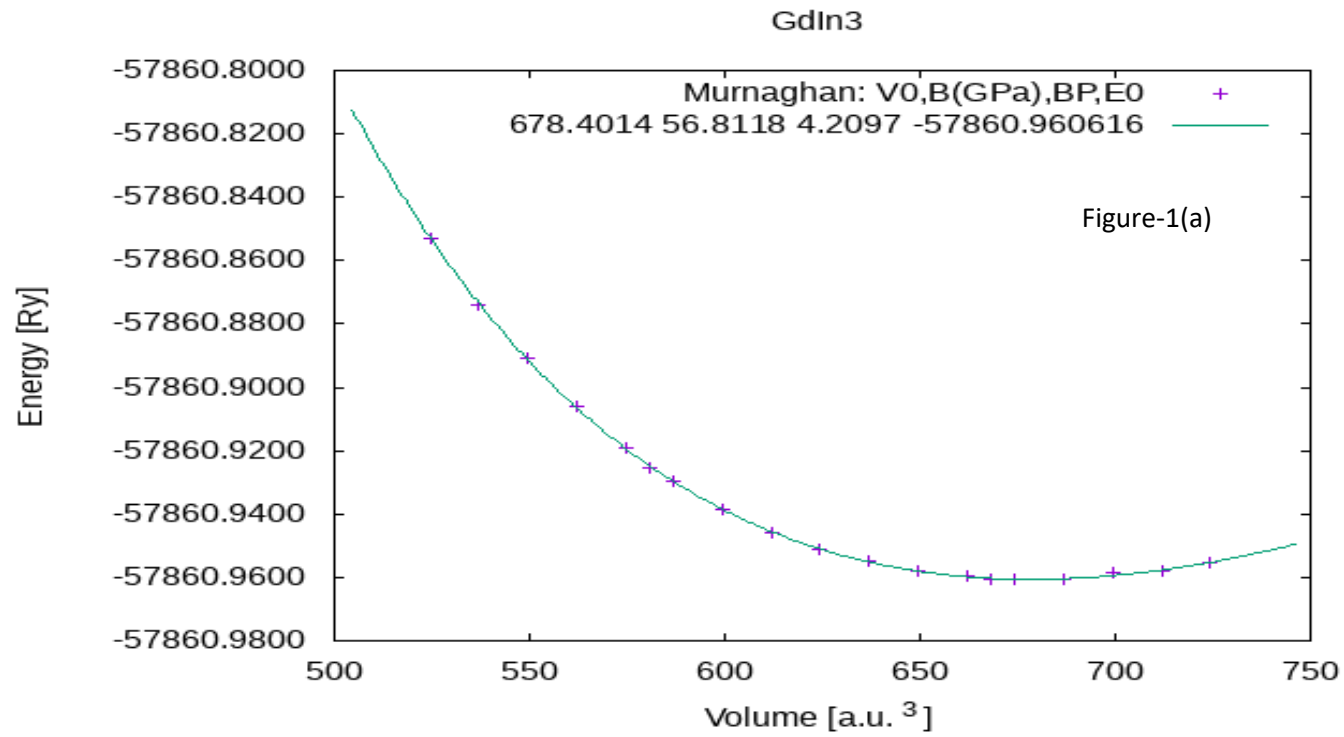
Compounds	a_0, c_0	B	B_0'
$GdIn_3$	4.523	52.9371	5.0193
$GdSn_3$	4.596	46.5392	5.8773

The energy versus volume curves for $GdIn_3$ and $GdSn_3$ are shown in Figs. 1(a) - 1(b). These figures are indicating stability of compound. We have obtained values from these curves which is Minimum energy values (E_0) -57860.960618 eV corresponding to minimum volume (V_0) 679.4430 a.u^3 for $GdIn_3$ and Minimum energy values (E_0) -59635.979756 eV corresponding to minimum volume (V_0) 714.2212 a.u^3 for $GdSn_3$ (shown in Table-2). These result lead to the conclusion that if the minimum energy of compound is increase, its minimum volume decrease. The GdSn3 is an itinerant compounds, while GdSn3 are trivalent similarly for GdIn3, results also shows Gd-lattice constants are contracted, which attributed to the lanthanide contraction, i.e., Left Europium ($4f^7 6s^2$) and Ytterbium ($4f^{14} 6s^2$), the atomic numbers are increase in lanthanide series then the atomic radius of lanthanide (La) series are decrease due to weak shielding effect of 4f shells electrons and It is confirms for both RIn3 and RSn3 [R=Gd] case.

Table 2

Minimum energy, E_{min}, (Ryd), Fermi energy,E_F (eV), unit cell volume, V_0 (a. u. ^3), (at 0K) for $GdIn_3$ and $GdSn_3$ using PBE-GGA.

	$GdIn_3$	$GdSn_3$
E_{min}	-57860.960618	-59635.979756
E_F	0.56260	0.61689
V_0	697.4430	714.2212



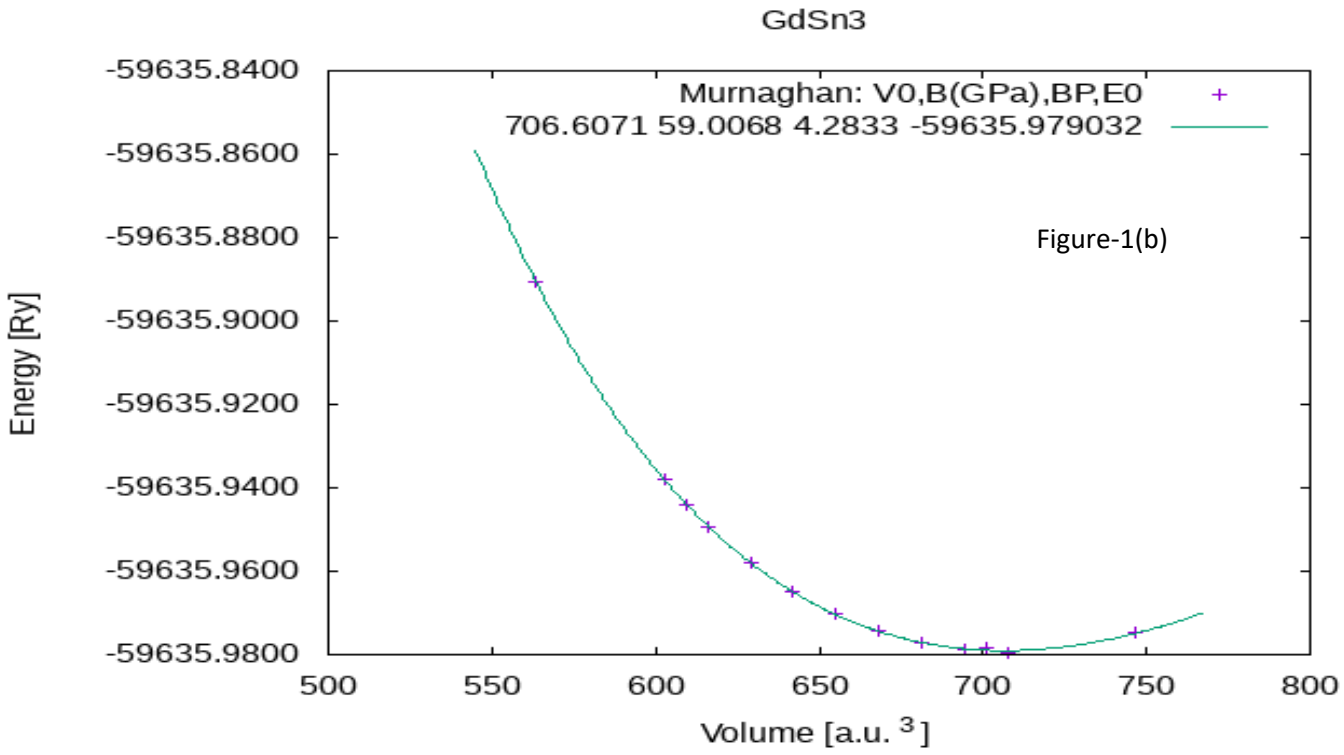


Figure 1: Variation of total energy with volume of 1(a) $GdIn_3$, 1(b) $GdSn_3$, compounds in AuCu3 structure.

Electronic Behavior:

We discuss electronic properties in terms of band structure (BS) for $AuCu_3$-type $GdIn_3$ and $GdSn_3$. we have calculated the BS of $GdIn_3$ and $GdSn_3$ compounds for both along with high symmetry Brillouin zone direction using GGA approximation. Where Fermi level is situated, origin as shown in Figures 2(a)–2(d) for both compounds. In band diagrams most of bands lies from -9 eV to 0eV spin below the Fermi level for GdIn3. Similarly, most of the band lies from -11eV to 0eV in both spins below the Fermi level for $GdSn_3$. Which indicates from band diagrams that compound is metallic character. Because in band diagrams valance bands and conduction bands overlap among themselves. This result is mainly responsible for Gd -4f ([Xe] $4f^7 5d^1 6s^2$) electronic shell is half filled. The result is clear our compound has metallic nature.

We discuss the total and partial density of state shown in figure 3(a)–3(d) for $GdIn_3$ and shown in figure 3(e)–3(h) for $GdSn_3$ compound. For $GdIn_3$ [figs. 3(a) and 3(b)] compound, we can see total density of state along with spin up and spin down state, there are two sharp peaks approximately belong to -5.0 eV below the Fermi level and +1.0eV above the Fermi level. In fig. 3(a), -5.0 eV sharp peak, most responsible for Gd-f electronic shell with minor role of

In-s electronic shell [fig.3(c)]. In Fig.3 (b), +1.0 eV sharp peak most responsible for Gd-f electronic shell with minor role Gd-d([Xe] $4f^7 5d^1 6s^2$) and In-p([Kr] $4d^{10}\ 5s^2\ 5p^1$) electronic shell. The sharp peak we get is due to the hybridization of the Gd-d, and In-p electronic shell [fig. 3(d)] along with Gd-f shell. Similarly, For GdSn3 [figure 3(e)–3(h)] compound, all configurations are same, only small different is The sharp peak we get is due to the hybridization of the Gd-d, and Sn-p electronic shell [fig. 3(h)] along with Gd-f shell. which Gd-4f electronic shell is main responsible for total and partial density of state variation in curves for GdIn3 and GdSn3. We find Fermi energy (E_F) for $GdIn_3$ and $GdSn_3$. shown in Table-2. According to our result, this compound has shown metallic nature.

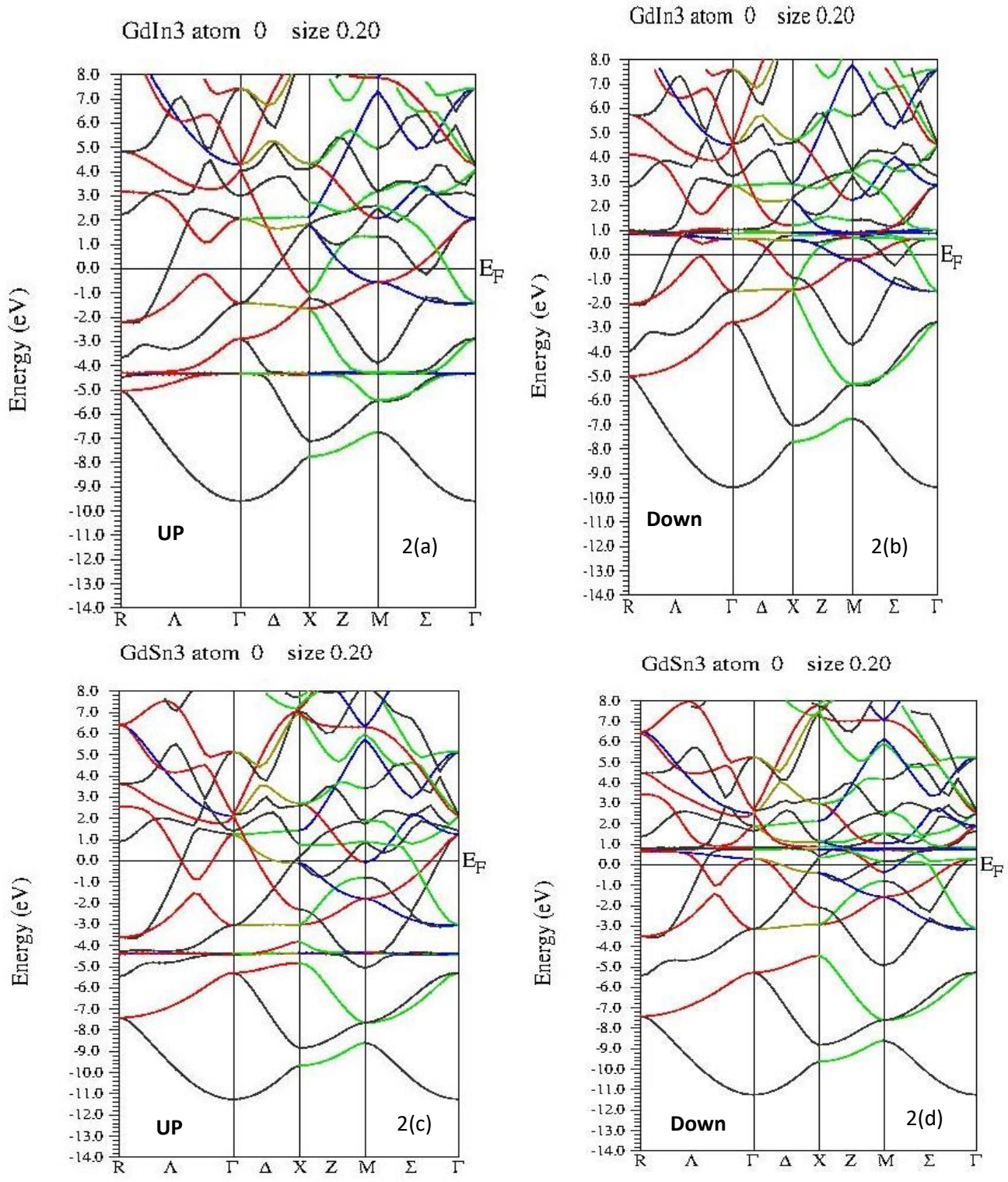


Figure 2: Electronic band structures of (a) $GdIn_3$ for spin up, (b) $GdIn_3$ for spin down, (c) $GdSn_3$ for spin up, (d) $GdSn_3$ for spin down using GGA approach in both spins.

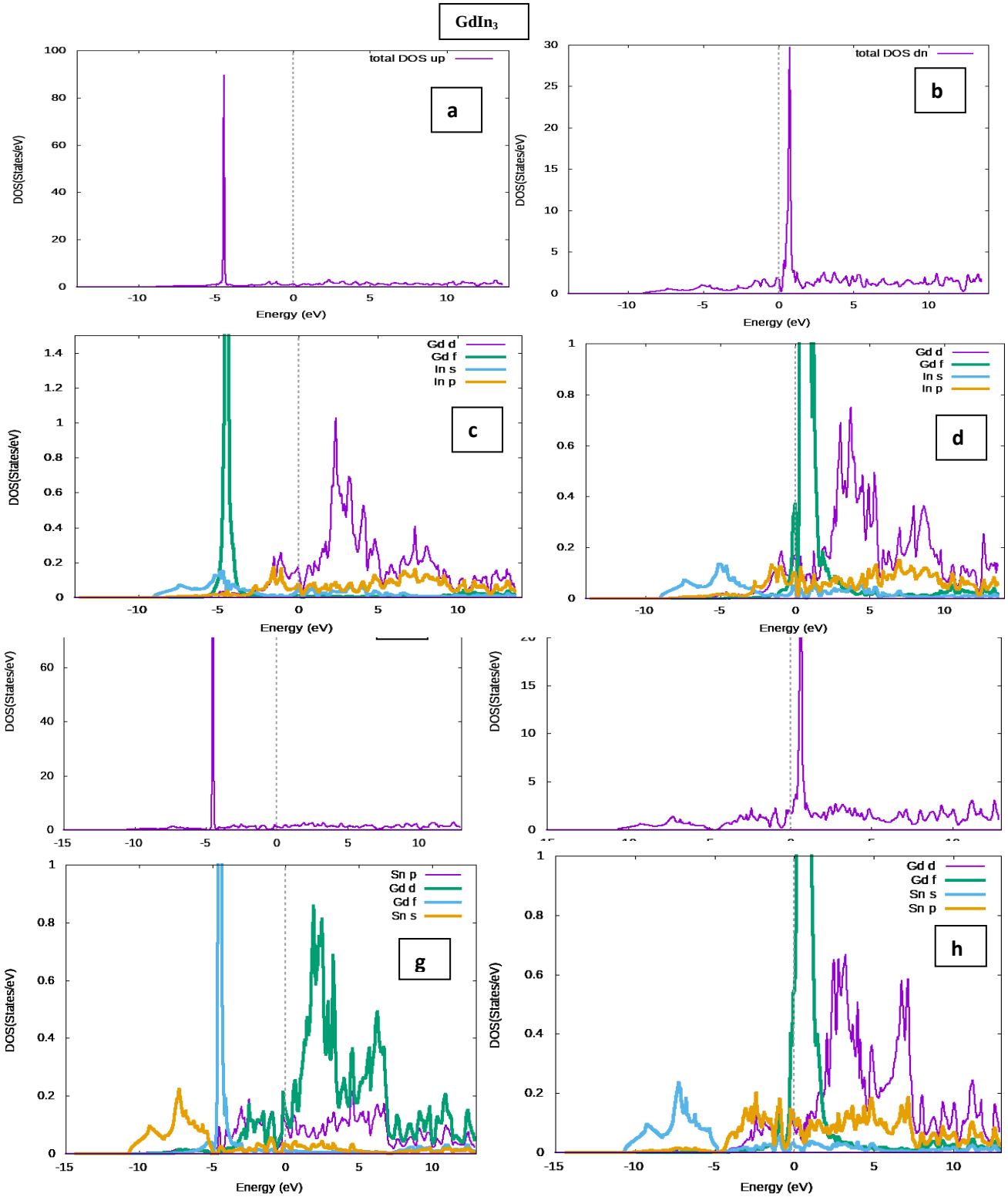


Figure-3 Total density of states of (a) $GdIn_3$ in spin-up, (b) $GdIn_3$ in spin-down and partial density of states of (c) $GdIn_3$ in spin-up, (d) $GdIn_3$ in spin-down and Total density of states of (e) $GdSn_3$ in spin-up, (f) $GdSn_3$ in spin-down and partial density of states of (g) $GdSn_3$ in spin-up, (h) $GdSn_3$ in spin-down.

Magnetic Properties:

This study investigates the magnetic properties shown by the substances $GdIn_3$ and $GdSn_3$. The intermetallic complexes $GdIn_3$ and $GdSn_3$ consist of the rare earth element gadolinium (Gd). Gadolinium is renowned for its robust magnetic characteristics, rendering it a subject of interest for diverse applications such as implementation in magnetic materials and utilization as contrast agents in the field of medical imaging. The magnetic moments of these compounds would be contingent upon the computational methodology and parameters employed in the calculations. In general, magnetic moments are computed for the complete unit cell and can be further analyzed to determine the contributions from individual atoms. The magnetic moment of an atom, as used in these computations, pertains to the comprehensive magnetic moment linked to the atom within the crystal lattice. The interstitial zone is commonly used to denote the voids or gaps inside the crystal lattice structure, where the presence of a certain atom may be absent. (All values shown in Table-3). Total magnetic moment of $GdIn_3$ and $GdSn_3$ compound is dominated by contribution of individual moment of Gd^{3+}. Gd-4f electronic shell responsible for the magnetic moment.

Table 3

Calculated spin magnetic moments (μ_B) of GdX_3[X= In and Sn] using PBE-GGA.

	$GdIn_3$	$GdSn_3$
Interstitial region	0.05023	0.02439
Gd	6.93514	6.83974
In or Sn	-0.03136	-0.02689
Total	6.89129	6.78347

Conclusions

DFT calculation of structural, electronic, and magnetic properties of GdX_3 (X = In and Sn) compounds. Advanced computational methods, namely Density Functional Theory (DFT) employing the full potential linearized augmented plane wave method (FPAPW) and the local orbital method (LO), are being utilized to determine the structural properties of $GdIn_3$ and $GdSn_3$ molecules. The aforementioned methodology represents an advanced strategy that enables precise prognostications of material characteristics by leveraging principles derived from quantum mechanics. As previously said, your interest lies in the computation of the structural characteristics, namely the total energy (E), in relation to various parameters such as volume (V), lattice constants (a0), bulk modulus (B_0), and the first-order pressure derivative (B_0'). These characteristics play a critical role in describing the behavior of materials under varying situations. These all results are very close to experimental data. We are calculated electronic properties in terms of electronic charge density, band structures, total density of state and partial density of state, Result is clear our compound have metallic nature. We are calculated magnetic properties in terms of magnetic moment. According to

result our compound shows magnetic nature and Gd-4f electronic shell responsible for the magnetic moment.

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