Research Article

Density Functional Theory based investigation of Structural, Electronics and Magnetic Properties of Rare Rarth (Er) doped ZnGa Compound

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Abstract

The electronic and magnetic properties of the intermetallic compound ErZnGa were investigated using density functional theory (DFT). This chemical crystallizes in a hexagonal $CaIn_2$-type structure and is a member of the space group $P6_3/mmc$ (No. 194). Parameters of Structure: The anticipated lattice constants (a_0, c_0), bulk modulus (B_0), and its first-order pressure derivative (B_0') demonstrate significant agreement with empirical and previously documented theoretical values, hence confirming the accuracy of the used computational method. The electrons localised in the 4f orbitals of erbium (Er) are crucial in determining the magnetic response of ErZnGa and significantly influence its magnetic properties. Electronic qualities: The density of states (DOS) and band structure of the molecule were thoroughly examined in order to assess its electronic qualities. Understanding these properties is necessary to evaluate the material's potential use in electrical and magnetic devices. The findings derived from calculations align with the existing experimental and theoretical data, demonstrating the dependability of the used approaches. All things considered, this study contributes to our understanding of the interplay between ErZnGa's electrical and magnetic properties, paving the way for more research into its possible technological applications.

Keyword: Structural properties; intermetallic materials; Density Functional Theory.

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Introduction

RTX-type trivalent rare-earth intermetallic compounds exhibit a wide array of intricate mechanical, chemical, and physical characteristics. In this context, R denotes a rare-earth element, T signifies a transition metal, and X symbolises a p-block element. Almost 2000 different combinations of RTX-type compounds have been identified and studied [1]. These materials provide a variety of options for research and education, which makes them significant to materials science. Consistent with this research direction, the binary compound $ErCu_2$ was altered to produce the ternary intermetallic compound ErCuGa, which crystallises in the KHg_2-type structure inside the space group Imma [2–5]. A new ternary compound called ErCuGa is produced by partially replacing Cu atoms with Ga atoms in a 1:1 ratio [6]. By focusing our study on ErZnGa, a ternary compound that has structural and chemical characteristics with ErCuGa, we have expanded on this foundation. However, there is presently no comprehensive literature on the electrical and magnetic properties of ErZnGa. Despite its structural similarity to ErCuGa, nothing is known about the fundamental physical properties of ErZnGa. The crystallographic properties were analysed using X-ray powder diffraction, revealing that the compound crystallises in a $CaIn_2$-type hexagonal structure within the space group $P6_3/mmc$ [7–8]. The main objective of this study is to theoretically analyse the electronic and magnetic properties of the ErZnGa compound, including an exploration of its band structure, total and partial density of states (DOS), and magnetic moment. We used density functional theory (DFT) with full-potential augmented plane wave and localised orbital (FP-LAPW+lo) techniques [9].

Computational Approach

The calculations were performed using the WIEN2k software, which use the linear augmented plane wave (LAPW) method extensively [10]. To ensure accurate convergence of the energy eigenvalues, the basis set was expanded under the condition RMT × Kmax = 7, where RMT represents the minimum muffin-tin radius of the atomic spheres inside the unit cell, and Kmax indicates the maximum vector magnitude for the plane wave expansion. The valence wave functions of the atomic spheres were expanded to a maximum angular momentum quantum number of lmax = 10. The Fourier expansion of the charge density was performed up to the reciprocal lattice vector Gmax = 12. The tetrahedron method was used for Brillouin zone integration using a dense k-point mesh of 1000 points, yielding a high level of accuracy in the electronic structure simulation. Muffin-tin radii (R_{MT}) of 2.00, 2.43, and 2.43 bohr were used for Er, Zn, and Ga, respectively, and were found to be suitable for producing reliable results. The computed Fermi energy of the system was 0.4307 eV, as shown in Table 1. In connection with its magnetic characteristics, the material's magnetic moment was also calculated. By implying their use in spintronic devices, these magnetic properties indicate a promising path for the advancement of state-of-the-art spin-based electronic technologies.

Result:

Structure Properties

The structural features of the ErZnGa compound have been obtained by experimental lattice parameter optimization. According to the most current report, the molecule has crystallized in the cubic B1-phase, in the space group P63/mmc, with a0 = 4.393 and c0 = 7.048 Å [7]. For Er, Zn, and Ga, their corresponding atomic positions are 2a (0, 0, 0), 2b (0.33, 0.66, 0.71), and 2c (0.33, 0.66, 0.28) [7]. The ErZnGa compound's crystal structure was obtained using the xcrysden program, as shown in figure 1. A software program called Xcrysden was created to visualize crystalline and molecular structures. In addition to allowing interactive manipulation via rotation and other methods, it permits the overlay of structures. The GNU/Linux operating system powers the program. Birch-Murnaghan's equation of state has been used to calculate geometry and structural parameters, as has been explained in references [11–12]. Correlation between the system's total energy and the unit cell's volume is part of the technique. Figure 2 shows the stable structure of the minimal ground state energy in the ferromagnetic phase. Through the integration of both theoretical and experimental data, the lattice constant was optimized. Table 1 presents the computed ground state parameters, including bulk modulus (B_0), lattice constant (a_0), pressure derivative of bulk modulus, and total energy.

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), Fermi energy (E_F in eV).

Compounds	a_0	c_o	Bo	B_0'	E_F
ErZnGa	4.573	7.206	71.2734	1.5519	0.4307
Exp. -	4.393[7]	7.048[7]	-----------	-----	---------

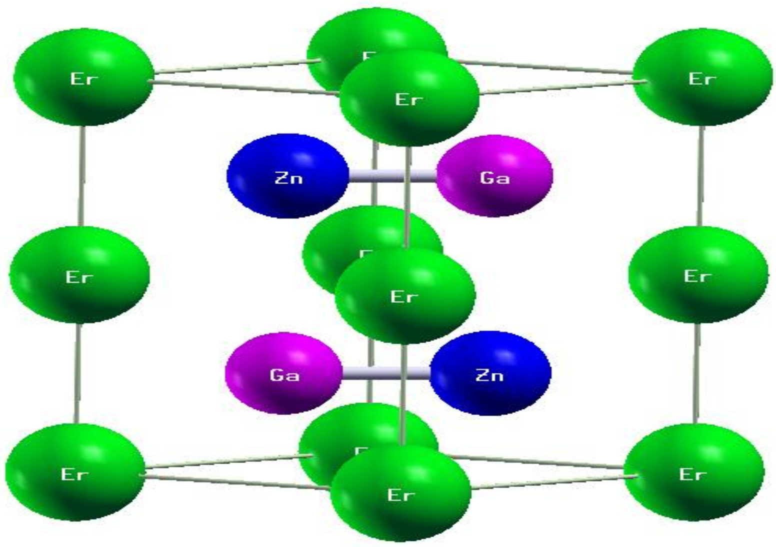

Figure-1 Unit cell structure of ErZnGa

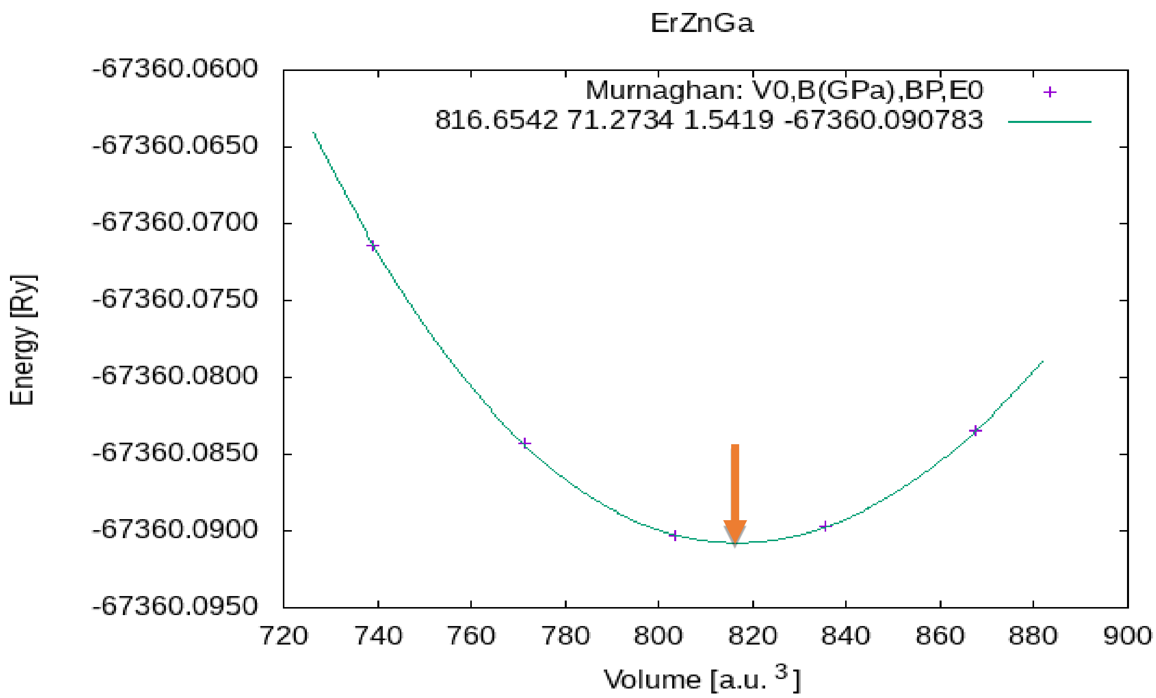

Figure-2 Energy Vs. volume curve with using murnaghan equation of state.

Electronic and Magnetic Properties

The spin-resolved band structure and density of states have been graphed, and the electronic characteristics have been computed using the GGA method. Using the GGA approach, the band structure and density of states have been visually shown using the lattice constant that was determined using GGA calculation. These diagrams usually provide a good grasp of a substance's electrical properties. To understand the obtained results, the GGA approach was used to create band structure plots, which are shown in figure 3, and density of state plots, which are shown in figure 4. The origin is thought to be the location of the Fermi level. The band profiles support these compounds' metallic characteristics by demonstrating a strong overlap between the valence and conduction bands (shown in figure 3) and the absence of a band gap at the Fermi level.

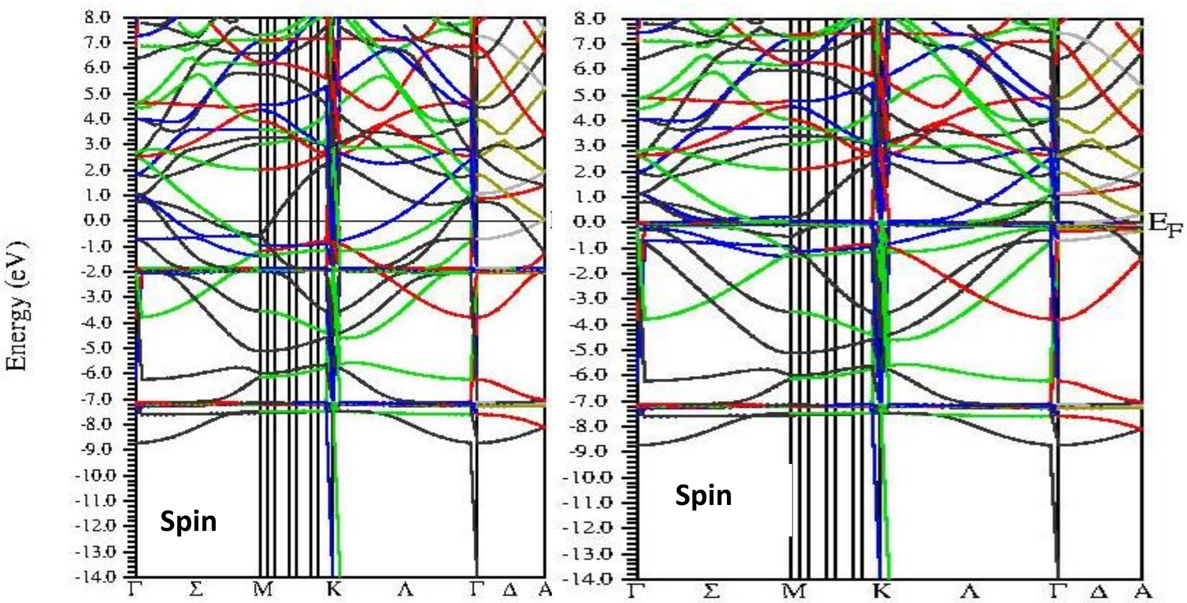

Figure-3

This work established the equilibrium lattice constant and total density of the ErZnGa compound using the GGA technique. The states linked to the 'f' orbitals of erbium exhibit a little displacement; yet, the band structures demonstrate significant similarities between the two spin states. The Zn-d states comprise the lowest energy band, ranging from about -8.0 eV to -3.0 eV. The flat band located in the conduction band at the Fermi level mostly results from the existence of erbium's 'f' states. The examination of the band structure indicates that the ErZnGa combination has a predominant metallic character due to the existence of Zn-d and Ga-s states at the Fermi level. The cumulative magnetic moment determined for this chemical is shown in Table 2. The density of states (DOS) at the Fermi level (EF) for the aforementioned molecule was computed using the GGA technique under ambient circumstances, revealing a value of 0.4307 for both majority and minority spin states.

Table 2

Calculated spin magnetic moments (μ_B) of ErZnGa using PBE-GGA.

	ErZnGa
Interstitial region	-0.13968
Er	2.43466
Zn	-0.00757
Ga	0.00240
Total	4.71929

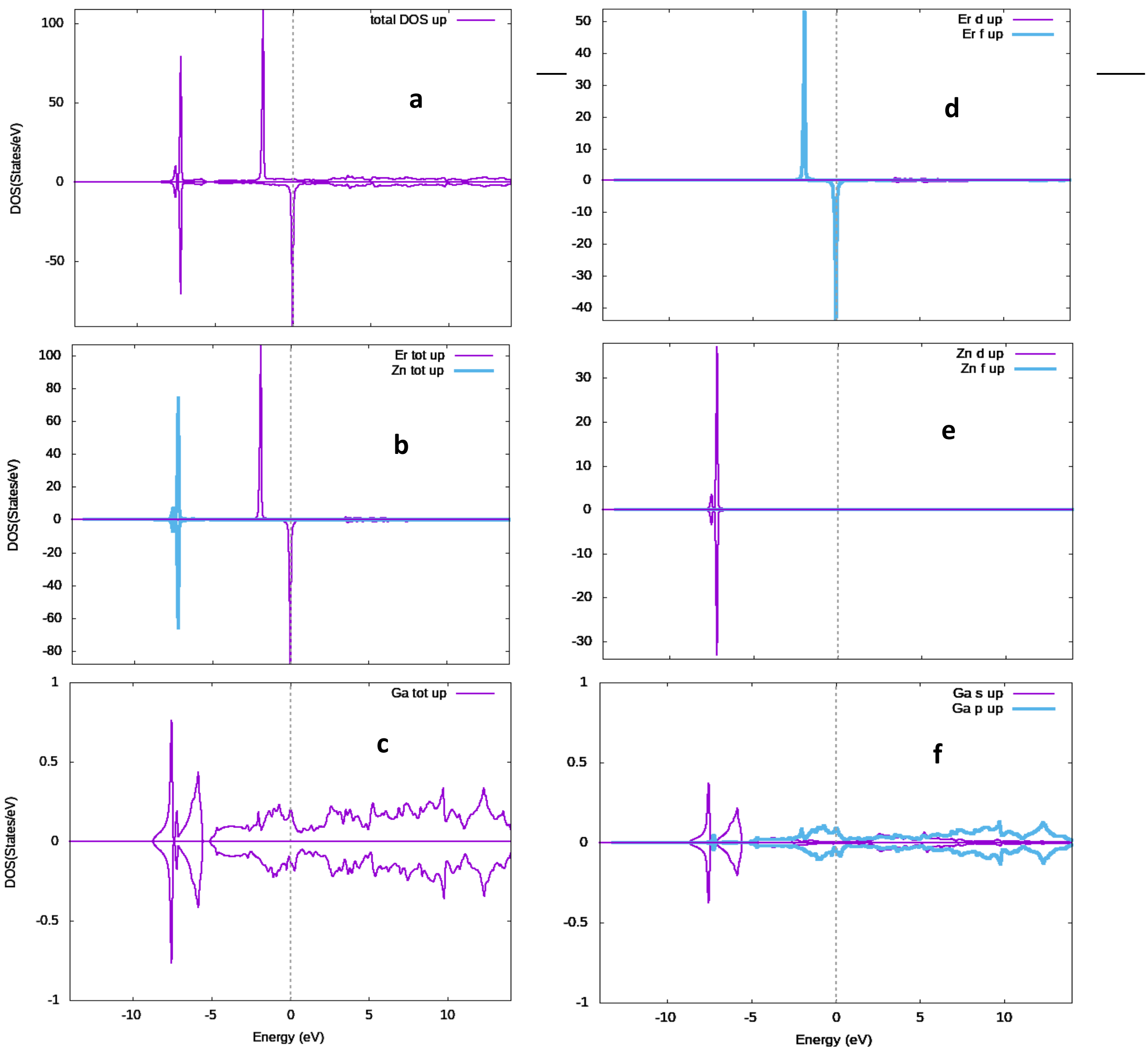

Figure-4 shown that DOS and PDOS are following (a) Total DOS for ErZnGa, (b) Er total and Zn total DOS, (c) Ga total DOS, (d) Er-d and Er-f PDOS, (e) Zn-d and Zn-f PDOS, and (f) Ga-s and Ga-p PDOS

Conclusion

In the present work, the FP-LAPW approach is used to thoroughly analyze the electrical and structural features of ErZnGa in the framework of density functional theory. The PBE-GGA technique is used to approximate the correlated energy exchange. Good agreement with experimental data is shown by the structure characteristics. The material exhibits no band gap, according to the band structures of these compounds. This indicates that the density of state and metallic character of the ErZnGa compound are confirmed by this compound. Er-element-based magnetic compound confirmation is known as a magnetic property.

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Conflict of interest: Nil
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