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Study of Structural, Electronic, and Magnetic Properties of NdFeSi Compound

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Abstract
In this paper, we have calculated the structure and electronic and magnetic properties of the NdFeSi intermetallic compound with the help of WIEN2K software. It's based on a theoretical method called the full potential linearized augmented plane wave plus local orbital (FP-LAPW +lo) method based on density functional theory (DFT). The structural properties within the GGA approximation are in terms of the lattice constant, bulk modulus, first derivative of bulk modulus, and minimum volume. All these parameters were found to be almost equal to the experimental data. In this calculation, the electronic properties in terms of band structure, total and partial density of state (TDOS and PDOS) of the NdFeSi compound. The NdFeSi intermetallic compound shows a metallic nature, mainly due to the Nd-f state. In this paper, I focus on the magnetic properties of the NdFeSi compound. Because the magnetic moment of this compound is almost zero, in my calculation, the value of the magnetic moment is 7.02610 μB per unit cell and is ferromagnetic nature.

Keywords
DFT, Electronic properties, Density of state, Rare earth material

INTRODUCTION

The rare earth intermetallic compounds show many interesting properties related to research purposes. RETX type of rare earth intermetallic Compounds with a 1:1:1 stoichiometry of over 2000 compounds are available in materials science [3]. About 30 different types of crystal structures can be found in crystallography [4]. Rare-earth elements and 3-d transition metals are of significant industrial interest. In addition to being important from a theoretical perspective, rare earth intermetallic is also widely used. The most important application of rare earth intermetallic compounds is permanent magnets, heavy fermions, valence fluctuations, Kondo lattices, magneto-strictive materials, spin glasses, random anisotropy systems, hardness, ductility at room temperature, and high strength for industrial research [1]. These applications depend on the magnetic properties of the NdFeSi compound. Rare earth intermetallic is also important in several other topics as well. [2]. We know that Nd-Neodymium is a silver metallic element. And the magnetic moment is large. Fe-iron is paramagnetic in nature due to unpair electrons. And magnetic moment is almost zero. Similarly, Si is a semiconductor and shows that magnetic moment. In these compounds, the ternary rare earth iron silicide compounds, NdFeSi, were first synthesized [18]. now we have investigated the electronic and magnetic properties of RETX compounds. Welter et al. [7] reported the magnetic properties of some RFeSi compounds using neutron diffraction and magnetization data. They observed the ferromagnetic ordering of these compounds with the long-range ordering of magnetic moments along the c-axis. The NdFeSi compound is shown to have a ferromagnetic nature in several literature reviews at low Curie temperatures [5-6] but similar types of LaFeSi compounds are shown that paramagnet nature [7]. La

($4f^0$) to Lu ($4f^{14}$) on the periodic table are the rare earth elements. Each member of this series has both paired and unpaired electrons in the inner 4f orbital. Nd has a configuration electronic state of [Xe] 4f4 6s2, with 4f unfilled valence shell levels. Due to unfilled 4f electron orbitals, rare earth intermetallic compounds show magnetic properties. Because Nd is a heavy rare earth element and has a more magnetic moment compared to La($4f^0$). Due to magnetic properties are used for magnetic refrigeration (based on the magneto-caloric effect (MCE) technology), storage devices, and many more applications [8–10]. The NdFeSi, the compound shows a tetragonal CeFeSi-type crystal structure. Crystallography details of the NdFeSi compound [11-12] are shown in Table 1.

Table 1

Compound	Space Group	Lattice parameter (Å)	Nd	Fe	Si
NdFeSi	p4/nmm (129)	a_0=4.031 c_0=6.828	(0.25, 0.25, 0.67)	(0.75, 0.25, 0)	(0.25, 0.25, 0.20)

In this calculation, we have used the Wien2K software package, which is based on density functional theory (DFT) and implements the FPLAPW +lo method with the help of PBE-GGA [13–15]. The WIEN 2K program is a simulation tool that may be used to investigate the crystallographic, electronic, and magnetic characteristics of NdFeSi compounds. These alloys give researchers a chance to look at how rare earth concentration and unit cell expansion affect the magnetic characteristics of these alloys because La is isoelectronic with Nd but has an empty f shell and a bigger atomic size than Nd. The main focus of this work is to explore the impact of 4f localization on the structural, electronic, and magnetic properties of these alloys using GGA approaches to determine these parameters. The second motive for this work is to corroborate the experimental results that indicate iron has no magnetic moment in the NdFeSi compound and to examine the explanation for iron's nonmagnetic nature. This work's final purpose is to study the physical aspect of 4f-4f interaction. To the best of our understanding, no one has investigated the impact of rare earth concentration on the physical properties of these compounds.

METHOD OF CALCULATIONS

The WIEN 2K program is a simulation tool that is used for the investigation of some properties in this paper [16]. Kohn-Sham DFT is implemented using the FPLAPW +lo, which has been modified to determine the properties of materials [16]. In the context of DFT, it often coincides with the treatment of the whole potential and charge density without any shape approximation as well as the equal treatment of the valence and core electrons. The name "all-electron full-potential linearized augmented plane-wave method" is frequently used to describe this (FLAPW) [16]. Because of these things, it is one of the most accurate ways to use DFT, and it can be used on all crystalline materials, no matter what they are made of. The structural, electronic, and magnetic characteristics of NdFeSi compounds have been estimated using these techniques. With the aid of the Birch-Murnaghan equation [2.1 and 2.2] (EOS) with PBE-GGA method.

$$E_{total} = E_0(V) + \frac{B_0 V_0}{B_0'(B_0'-1)}\left[B_0\left(1-\frac{V_0}{V}\right)+\left(\frac{V_0}{V}\right)^{B_0'}-1\right] \qquad [2.1]$$

$$E_{total} = E_0(V) + \frac{9B_0V_0}{16}\left\{\left[\left(\frac{a_0}{a}\right)^2-1\right]^3 B_0' + \left[\left(\frac{a_0}{a}\right)^2-1\right]^2\left[6-4\left(\frac{a_0}{a}\right)^2\right]\right\} \qquad [2.2]$$

DFT is an important technique that has been used to perform first-principles total energy calculations with the help of the FP-LAPW+lo method. these methods to investigate how the NdFeSi compound affects the structural, electronic, and magnetic properties of the NdFeSi crystallographic data. The ground state structural properties have been calculated using the GGA parameterization scheme, as suggested by Wu and Cohen (WC), and their deviance from Vegard's rule has been explored. The electronic and magnetic characteristics of our material have also been examined using the Engel-Vosko (EV) GGA functional. In this paper, the structural, electronic, and magnetic characteristics of NdFeSi compounds have been investigated using these techniques.

RESULTS AND DISCUSSION

Structural Properties

We created the NdFeSi compound's unit cell structure with the help of the VESTA software [17], as shown in Fig. 1. The crystal structure and lattice parameter displayed in Table-1 have been computed using the Birch-Murnaghan equation of state (BM-EOS) and WIEN 2K software. Additionally, we determined that the lattice parameter was in strong accord with literature studies. The Birch-Murnaghan equation of state has been used to calculate the structural properties of the NdFeSi intermetallic compound.

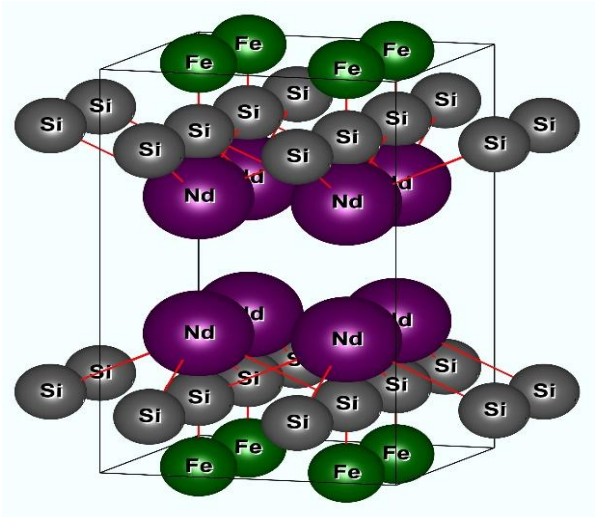

Fig. 1 Unit cell structure of NdFeSi generated by VESTA

The computed values of the structural characteristics for the intermetallic complex NdFeSi are displayed in Table 2. The NdFeSi compound's calculated values came the closest to matching the experimental values [18-26]. Bulk modulus is an important property of materials in material science. The bulk modulus of a material refers to its degree of compression resistance. The degree of resistance grows in value along with the bulk modulus value. The bulk modulus for the NdFeSi compound is displayed in Table 2. There is no information about the bulk modulus and first-order pressure derivatives of the NdFeSi compound in the scientific literature. We calculated data that is regarded as having expected values. Figure -2 depicts the energy versus volume curves for unit cells made of the NdFeSi material.

These curves show that the NdFeSi compounds are stable, with a minimum volume (V_0) of 749.9931 a.u.^{3} and corresponding minimum energy values (E_0) of -44771.811751 eV. The conclusion is that the NdFeSi compound's minimum energy and volume both increase with each other.

Table 2

Compounds	Lattice parameters		Bulk modulus	Pressure derivative of bulk modulus	Fermi Energy
	a_0	c_o	B_o	B_0'	E_F
NaFeSi	4.069	6.918	103.7584	4.3393	0.64630
Exp.	4.031[a]	6.828[a]	-----	-----	-----

[a] Ref. [18]

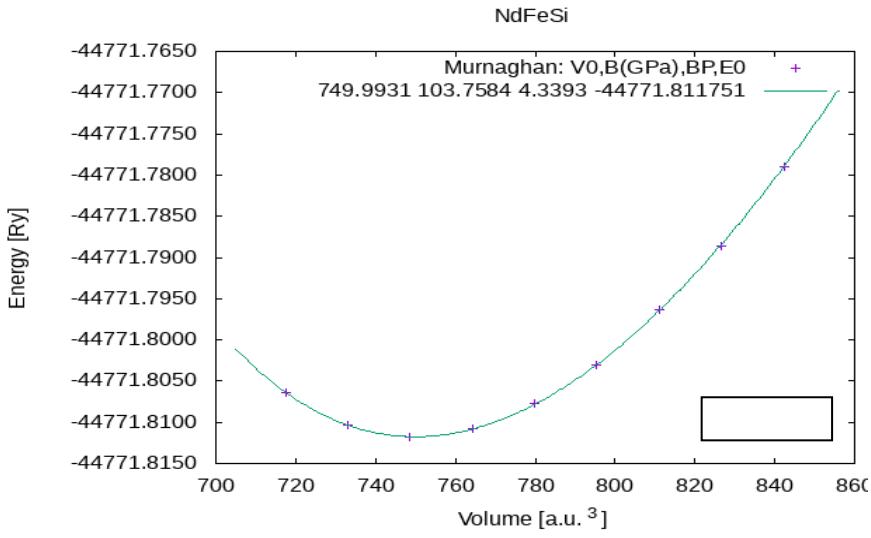

Fig. 2 Variation of total energy with unit cell volume of NdFeSi compound

Electronic Properties

The electronic properties have been calculated with help of GGA approximation. In this study, we compute the electronic band diagrams for the majority and minority spin channels of the NdFeSi compound. In band diagram, fermi level located at origin, shown in Fig 3(a-b). Most of the band in shown Fig. 3(a) is between -10.0 eV and 0 eV for the spin-up channel. In Fig. 3 (b), most of the band lies from approximately -9.5 eV to 0 eV. These figures directly indicate that both bands are overlapping with each other. As a result, we can say that the NdFeSi compound indicates a metallic nature. These metallic properties are primarily due to the electronic states of Nd-f state.

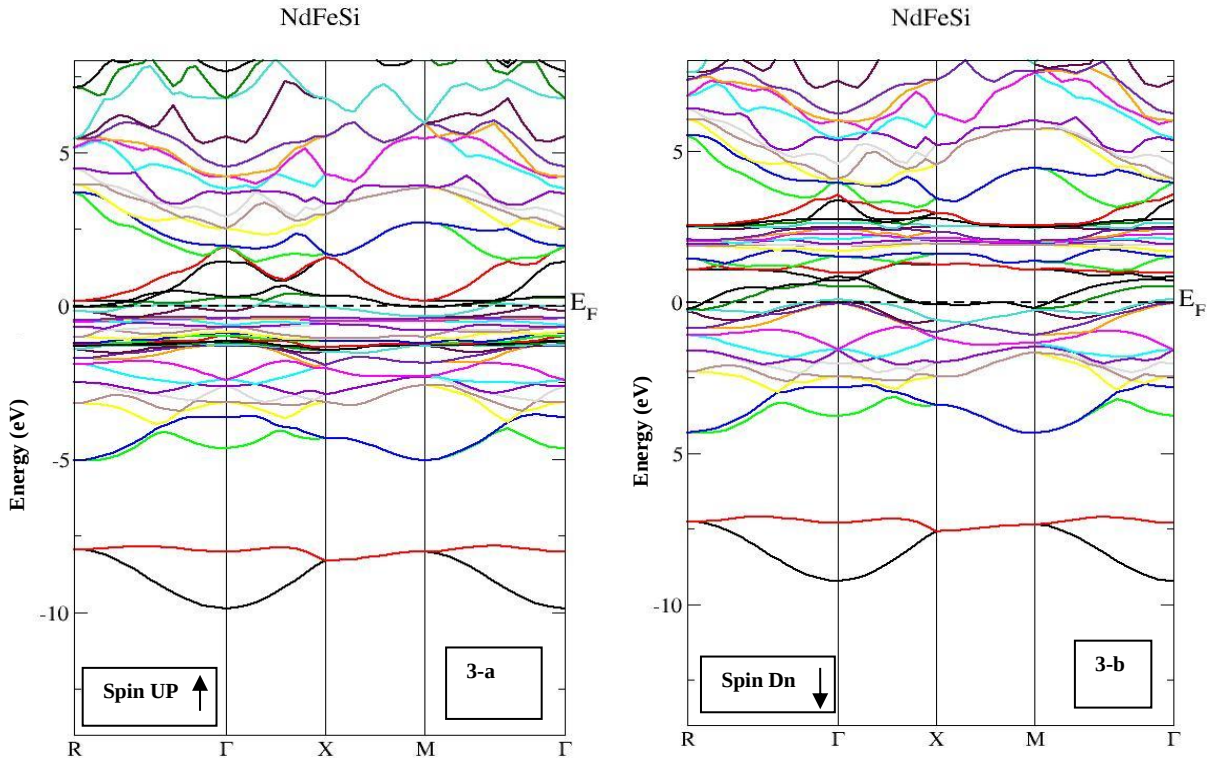

Fig. 3 Electronic band structures of (**a)** NdFeSi for spin up, and **(b)** NdFeSi for spin down, using GGA approach

We have total density of states and partial density of states for the compounds to learn more about the electronic behaviour. The total and partial density of states for NdFeSi compounds are shown in Figs. 4(a-h). Two sharp peaks are shown in the spin down channel and below the Fermi level in Fig. 4(a). About -7.1 eV for the spin-up channel, below the Fermi level, is the location of the first sharp peak. At about -0.62 eV, the spin-up channel's other strong peaks that are still present are below the Fermi level. The spin-down channel above the Fermi level also has one sharp peak, which is roughly at +2.0 eV. The high peak at -0.62 eV is mostly caused by the Nd-f electronic states, with a small amount of help from the Fe-d electronic states. While Nd-p, Si-s, and Nd-p electronic states also contributed slightly to the steep peak seen at -7.1 eV, Si-s electronic states account for most of it. Nd-f states are the primary cause of the strong peaks measured at 2.0 eV. The variation in the total and partial density of states curves has also shown that NdFeSi's Nd-4f electronic shell is the primary cause of the observed variation. Table 2 provides information on the NdFeSi Fermi energies (E_F). The metallic character of the NdFeSi compound.

Magnetic Properties

The magnetic moment of the NdFeSi compound has also been determined using the GGA approach presented in Table 3. No literature has ever mentioned the magnetic moment of the NdFeSi compound. It is known that the NdFeSi compound total magnetic moment, which is attributed to the Nd-f electronic shell, is mostly composed of the Nd3+ ions on their own and the Nd-4f electronic shell.

Table 3

Spin magnetic moments (μ_B)	
Interstitial region	1.23229
Nd	3.40766
Fe	-0.51018
Si	-0.00057
Total	**7.02610**

CONCLUSIONS

In this paper, we have investigated the structural, electronic, and magnetic properties of the NdFeSi compound. In this calculation, we have used a computational technique that is full potential linearized augmented plane wave method (FPAPW) with the help of WIEN2K software. The first-order pressure derivative (B_0'), bulk modulus (B_0), lattice constants (a_0), and unit cell energy (E) vs volume (V) curves have all been used to analyses structural properties. Lattice parameters have been calculated as is a_0=4.069 Å and c_0=6.918 (Å) and minimum volume (V_0) of 749.9931 a.u.^{3} and a corresponding minimum energy value (E_0) of -44771.811751 eV. All determined parameters have been found to be in respectable agreement with the experimental data. The density of states (total and partial) for electronic properties based on spin-polarized band structures has been computed. The metallic and magnetic properties of NdFeSi are supported by our electronic calculation profile. The Fermi energies (E_F) were calculated to be 0.64630 eV in this calculation.

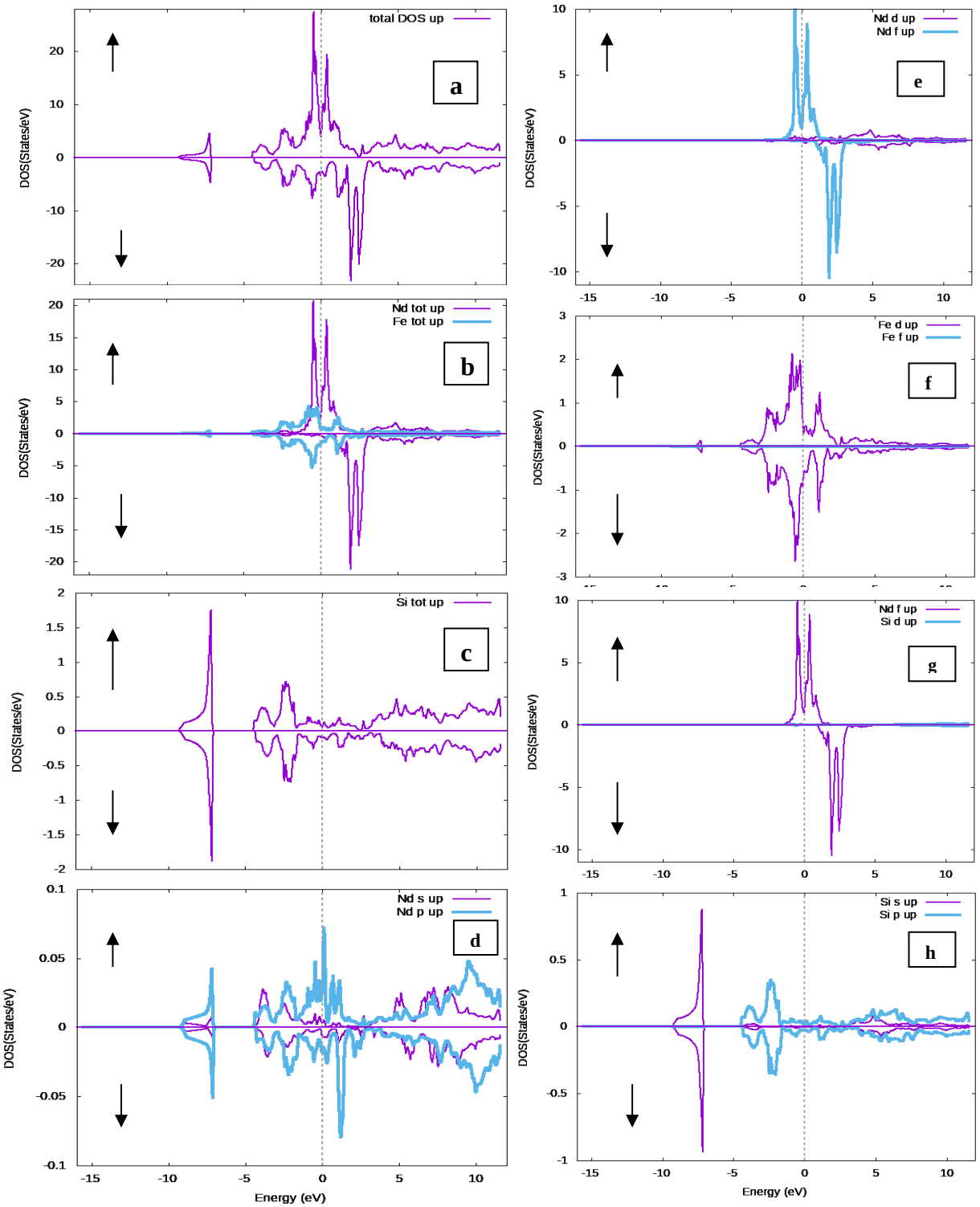

Fig. 4 Density of states(DOS) of **(a)** NdFeSi-total DOS for spin up and spin down, **(b)** Nd-total and Fe- total DOS spin up and spin down, **(c)** Si-total DOS for Spin up and spin down, **(d)** Nd-s partial DOS and Nd-p partial DOS for spin up and spin down, **(e)** Nd-d partial DOS and Nd-f partial DOS for spin up and spin down , **(f)** Fe-d partial DOS and Fe-f partial DOS for spin up and spin down **, (g)** Nd-f partial DOS and Si-d partial DOS for spin up and spin down, **(h)** Si-s partial DOS and Si-p partial DOS for spin up and spin down

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