



First principles calculations of optical and magnetic properties of SrFe₂O₄ compound under pressure



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ABSTRACT

In this research, the magnetic and optical properties of SrFe₂O₄ ceramic were studied. The calculations were performed by Full Potential Linearized Augmented Plane Wave method in Density Functional Theory framework with generalized gradient (GGA), GGA+U and modified Becke–Johnson approximations for the exchange and correlation functionals. The results show that SrFe₂O₄ is a ferrimagnetic ceramics with six different spin configurations. The Hubbard parameter was calculated ($U_{eff} = 4.5$ eV) by an ab initio method. The optical properties such as dielectric function, refraction index, electron energy-loss function, reflectivity, absorption coefficient and optical conductivity were investigated at zero up to 20 GPa pressure in *x*, *y* and *z* directions. The pressure coefficients of optical band, static dielectric constant, plasmon peak, static refraction index and the maximum of absorption were determined. Moreover, the pressure dependence of the static dielectric constant, plasmon peak, static refraction index, the maximum of absorption and the optical gap were investigated.

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1. Introduction

Ferrite powders are fabricated for dielectric and magnetic ceramic devices [1]. Mono ferrite strontium (SrFe₂O₄) has a spinel structure. This compound, like other ferrites has ferrimagnetic property. The general magnetic spinel formula is MFe₂O₄ where M is the divalent metal ion. The presence of Fe³⁺ prepares the unpaired electron spins and the part of the magnetic moment of a spinel [2]. SrFe₂O₄ has a framework structure of three-dimensionally linked FeO₄-tetrahedra corresponding to the ABW zeolite structure type. It has trivalent cations occupying the tetrahedral sites in combination with divalent cations residing in the voids of the framework [3].

Although J. Monteil et al. proposed the existence of non-stable SrFe₂O₄ in 1978 [4], the first attempt for making this compound was made by Vogel and Evans in 1979 [5]. They tested various molar ratios of SrO and Fe₂O₃ compounds and realized while reacting between the two parts in air, the summation of SrFe₆O₁₉, Sr₄Fe₅O₁₃ and SrFeO_{3-x} multiple phases is notable. The formation probability of any of these phases depends on the finalized reaction temperature and the ratio between Fe₂O₃ and SrO parts. Unfortunately, they didn't succeed in making SrFe₂O₄ compound

separately and almost no successful attempt was made after that until 1992, when P. Berthet et al. achieved SrFe₂O₄ compound with a pbc2 space group by considering 1:1 ratio between SrO and Fe₂O₃. But they weren't able to determine the exact location of atoms. On the other hand, their formed phase was not stable [6]. Less than a decade later, in 2001, Volker Kahlenberg et al. succeeded to build mono ferrite strontium with *P*2₁/*n* space group [3]. Other experimental work has been done on SrFe₂O₄ compound [7–9], but the current calculation is based on the Volker attempts. Very few experimental investigations have been performed on SrFe₂O₄ and to the best of our knowledge, there is no theoretical study to determine the optical properties of this compound. Thereupon, our work can be a first theoretical work in this direction.

Various properties, calculating for a compound are derived from its unique structure. Optical properties provide a proper basis for band structure studies. The purpose of this work is to produce a thorough ab initio calculation of the optical properties of SrFe₂O₄ compound.

The article is organized as follows: in Section 1, the method of calculation is explained and in Section 2, spin configuration and magnetic properties are investigated. In Section 3, the optical properties of SrFe₂O₄ at 0 GPa up to 20 GPa, in *x*, *y* and *z* directions by various approximations (GGA, GGA+U and mBJ) are studied. Finally, the conclusions are given in Section 4.

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2. Computational approach

The first-principles calculation of the optical excitations is performed by Full-Potential-Linearized Augmented Plane Wave (FP-LAPW) method [10] in the framework density functional theory [11], with various approximations by WIEN2k [12] package. The approximations of GGA [13,14], GGA+U [15] and mBJGGA [16] were used for the exchange correlation potentials. The structural properties of the mono ferrite strontium compound have been calculated experimentally by Volker Kahlenberg et al. in 2001 [3]. They reported that a mono ferrite strontium compound with the space group of $p21/n$ has a monoclinic structure. Experimental lattice constants equal to: $a = 15.33$ (a.u.), $b/a = 1.12$ (a.u.), $c/a = 1.34$ (a.u.) and $\gamma = 91.53^\circ$.

In these calculations, the valence electron configuration for Sr, Fe and O atoms are: [Kr]: $5s^2$, [Ar]: $4s^23d^6$, [He]: $2p^4$ respectively. By determining the amount of 0.0001 (e) as charge, 0.0001 (Ry) as energy and 1 (mRy/a.u.) as force convergence, with and without considering the spin polarization, self-consistent calculations achieved the desired convergence after 19 and 22 cycles respectively. The muffin-tin radiuses for iron, strontium and oxygen were chosen as 1.82, 2.28 and 1.61 (a.u.) respectively. The muffin-tin radiuses were chosen so that they encompass the majority of atomic charge in the spheres. In these calculations, considering the amounts of system energy per $RK_{\max}(R_{\text{mt}} \times K_{\max})$, k-point and G_{\max} , the amount of 7 was chosen as the optimal value for RK_{\max} , 14 (a.u.)⁻¹ for G_{\max} and the number of 1000 k-points (227 points in the irreducible part of the Brillouin zone) as a proper amount for this sake. Per the chosen amount of k-points, a K-mesh as $11 \times 10 \times 8$ was created. The calculations were done in four states of non-magnetic (NM), Ferromagnetic (FM), anti-Ferromagnetic (AFM) and Ferrimagnetic (Ferri). In Hubbard method, localized electrons in d and f orbitals are calculated using Hubbard sentence and non-localized electrons in p and s orbitals with LDA or GGA approximations [17]. The mBJGGA functional was developed to resolve the on-site correlation energy term and gives rise to more accurate band gaps [18].

3. Magnetic properties

The calculations were carried out first by using the experimental data for lattice constants, then by comparing the energy of different volumes of the unit cell, the most stable state was recognized and the optimal structural parameters were found. The theoretical lattice constants were obtained as: $a = 15.33$ (a.u.), $b/a = 1.12$, $c/a = 1.33$, and $\gamma = 91.53^\circ$ by GGA approximation and $a = 15.34$ (a.u.), $b/a = 1.12$, $c/a = 1.33$, and $\gamma = 91.53^\circ$ by GGA+U approximation. Since SrFe_2O_4 has magnetic properties, it was studied in non-magnetic (NM), ferromagnetic (FM), anti-ferromagnetic (AFM) and ferrimagnetic states respectively in various approximations such as GGA and LDA.

For the non-magnetic state, the calculations were performed without considering spin polarization while they require additional considerations for the magnetic states. The different spin configurations of iron atoms create various magnetic states. For instance, in the ferromagnetic state all of the iron atoms are oriented up or down direction. Six different possible spin configurations were considered for iron atoms (Fig. 1) to analysis the ferrimagnetic and antiferromagnetic states. The configurations are shown in Table 1. The difference between these two states is related to occupation number and the magnetic moment of iron atoms. After optimization, it was found that SC5 state with the lowest cohesive energy is the most stable spin configuration for both antiferromagnetic and ferromagnetic states.

The energy–volume curves of SrFe_2O_4 in all four mentioned state are shown in Fig. 2. SrFe_2O_4 has metallic and half-metallic

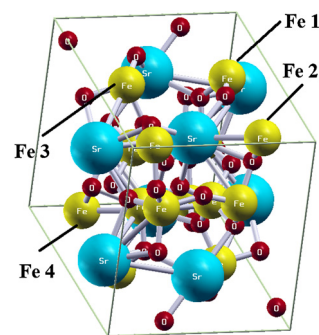


Fig. 1. The unit cell structure of SrFe_2O_4 .

Table 1

Six spin configurations for four iron atoms in SrFe_2O_4 .

No. or number of Iron atoms	1 2 3 4	1 2 3 4	1 2 3 4
Spin configurations	$\uparrow \downarrow \uparrow \downarrow$	$\downarrow \uparrow \downarrow \uparrow$	$\uparrow \uparrow \downarrow \downarrow$
Energy	-4.8932 eV	-4.3597 eV	-4.9465 eV
The name of spin configurations	(SC1)	(SC2)	(SC3)
No. or number os Iron atoms	1 2 3 4	1 2 3 4	1 2 3 4
Spin configurations	$\downarrow \downarrow \uparrow \uparrow$	$\uparrow \downarrow \uparrow \downarrow$	$\downarrow \uparrow \uparrow \downarrow$
Energy	-4.9453 eV	-4.9734 eV	-4.9735 eV
The name of spin configurations	(SC4)	(SC5)	(SC6)

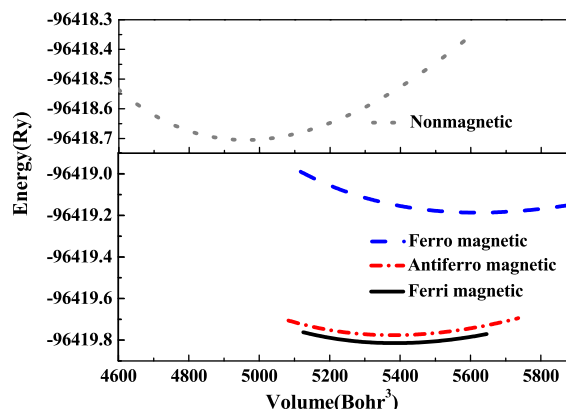


Fig. 2. Energy–volume curves of SrFe_2O_4 compound in four states of NM, FM, AFM and ferrimagnetic.

properties for NM and FM respectively, whereas AFM and ferrimagnetic states show semi-conductive behavior. According to the cohesive energy and energy–volume curve of system, it is obvious that the compound has the most stable state with ferrimagnetic order. Six different spin configurations were considered for iron atoms to analysis the ferrimagnetic state. Above-mentioned configurations and their energies are shown in Fig. 1. The SC5 state with the lowest amount of energy is the most stable state. The magnetic moment of SrFe_2O_4 was not reported experimentally but other magnetic spinel compounds such as NiFe_2O_4 , CoFe_2O_4 , Fe_3O_4 [19–21] and MnFe_2O_4 [19] have magnetic moment equal to 2, 3, 4 and 5 μ_B respectively. In addition, the cognate compounds of SrFe_2O_4 like BaFe_2O_4 , MgFe_2O_4 , and CaFe_2O_4 have the band gaps between 1.32 to 2.2 eV [22]. The magnetic moment of SrFe_2O_4 is possibly close to one of the mentioned compounds.

Low spin magnetic moment and band gap obtained from GGA approximation, suggest that GGA is not a proper approximation to explain the magnetic or electronic properties of this compound; therefore, we used other approximations such as GGA+U and mBJGGA. First, we need to determine the value of the Hubbard parameter (U) to investigate the spin configurations with GGA+U approximation. In the LDA+U method an orbital dependent field

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