Investigation of self-consistent site-dependent DFT + U effect on electronic band structure and optical properties of SiFe$_2$O$_4$ spinel

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Abstract

The first-principle investigation of SiFe$_2$O$_4$ (SFO) spinel was performed with the help of a plane-wave pseudopotential technique within the generalized gradient approximation (GGA) and local density approximation (LDA) as implemented in Quantum Espresso Simulation package. The Electronic band structure and optical properties of SFO spinel-type material have been investigated and discussed in this paper. The calculated band structure reveals that SFO spinel-type material is a direct bandgap semiconductor. Using GGA + U and LDA + U the band gap value so obtained is 3.52 eV and 2.96 eV respectively. The contribution to valence and conduction bands due to different bands was analyzed on the basis of the total and partial density of state. The Optical properties of SFO spinel-type material have been calculated and discussed in detail. The real, $\varepsilon_1(\omega)$ and the imaginary, $\varepsilon_2(\omega)$ part of the complex dielectric constants is found to be 6.52 and 5.42 at energies of 3.44 eV and 6.21 eV respectively. The refractive index $n(0)$ and the reflectivity index $(R(\omega))$, at zero energy value were found to be 1.88 and 10% respectively. We found that SFO spinel-type material has good properties for optical devices.

1. Introduction

Transparent conducting oxides (TCOs) are materials that are characterized by high electrical conductivity and simultaneously very high optical transparency to visible light [1]. In 1907 the first report of TCOs (Cadmium Oxide, CdO) was published by Badekar [2], who used thermal oxidation of sputtered films of cadmium. From that time many researchers delve into the field of TCO so that new types of TCOs with broad range applications can be prepared. Some of the widely known used TCOs include In$_2$O$_3$:Sn (ITO), Sn$_2$O:F (FTO), ZnO:F (ZFO), as well as new TCOs in spinels, form such as; MgIn$_2$O$_4$, ZnGa$_2$O$_4$, ZnRh$_2$O$_4$, Zn$_2$TiO$_4$ [1, 3–5].

Spinel-type transition-metal oxides encompass a group of compounds having a general chemical formula of XM$_2$O$_4$, with M and X cations occupying two nonequivalent lattice sites: one with six octahedrally (O$_h$) coordinated oxygens and the other with four tetrahedrally (T$_d$) coordinated nearest-neighbor oxygen atoms [6]. Owing to the possibility of accommodating earths abundant transition metals in different oxidation states at the O$_h$ and T$_d$ sites, spinels such as the CuFe$_2$O$_4$, GaZn$_2$O$_4$, CuCo$_2$O$_4$ and SnMg$_2$O$_4$ offer an excellent opportunities for designing many technological applications which include: transparent conducting oxides (TCOs), [7–11], humidity sensors, magnetic materials for spintronics and storage devices, redox materials for solar-thermal water splitting, high surface-reactivity catalysts for water-gas shift reactions, electrodes in lithium-ion as well as sodium-ion batteries, and hydrogen generation for microbial systems [12–16]. In a ‘normal’ XM$_2$O$_4$ spinel-type oxide, all X cations occupy the O$_h$ sites while the M cations occupy T$_d$ sites, whereas, in an ‘inverse’ spinel-type, the O$_h$ sites are shared equally by X and M cations with the T$_d$ sites occupied only by X cations [17].
In the past few years, the use of first-principles methods to study the properties of the compounds of geophysical interest has greatly expanded and even comprehensive studies of the thermodynamical properties of some spinels are made available [9, 14, 18]. At the same time, the treatment of iron-containing minerals bears additional difficulties due to the possible presence of strong electron-correlation effects. Of these spinel oxides, the spinel SiFe$_2$O$_4$ (SFO) is particularly attractive due to its earth’s abundance as well as its robust physical and chemical properties. Although the SFO spinel-type had been studied experimentally by using different methods [19–21], yet, to the best of our knowledge, the theoretical information on the electronic properties of this important compound is narrowly reported [22, 23]. Consequently, In this paper, the electronic band properties, structure and optical properties of the SFO spinel-type material are systematically investigated using the self-consistent (sc) calculations based on the first principle (DFT) method, where other information such as the density of states (DOS), band structure, Fermi energy, bandgap type, density of states (DOS), width of the conduction and valence bands, etc can be obtained from DFT calculations.

To overcome the problem of standard DFT on underestimation of the bandgap which can lead, in extreme cases, to incorrect calculations of a system as metallic rather than insulating, many theoretical techniques, like the quantum Monte Carlo (QMC) approaches, optimised effective potential (OEP) method, dynamical mean-field theory (DMFT), and DFT + U (GGA + U/LDA + U) methods that are applied for the strongly correlated and localized 3d or 4f electrons in rare-earth and transition oxides, have been developed [24, 25]. For the purpose of this work, we employed the GGA + U and LDA + U techniques so that, the Fe 3d state is treated by using Hubbard extensions to approximate DFT energy functionals. This method will serve as a better choice and computationally less expensive for the correct prediction of fundamental energy bandgap closer to the experimental measurements. In addition, we investigated the optical properties of SFO spinel-type material via Random phase approximation (RPA) based on GGA + U + RPA.

Even though the electronic structure of solid-state materials at room temperature can be found from many experimental techniques as demonstrated by Ono and Zhang [26, 27] yet, it is anticipated that the DFT + U carried out in the present work, will provide more basic theoretical background and understandings of the ground and excited-state properties of the SFO spinel-type material.

2. Computational details

In the present calculations of the total energy and electronic band structure of SFO, we used plane wave self-consistent field (PWscf) code, distributed with the Quantum ESPRESSO (QE) simulation package [28] with ultrasoft pseudopotentials (USPPs). The exchange-correlation (XC) potential is approximated by Generalized Gradient Approximation (GGA), with Perdew–Burke–Ernzerhof (PBE) and Local Density Approximation (LDA) in the form of Perdew–Zunger (PZ) parameterization [29, 30]. The take into account, the on-site Coulomb interactions between 3d electrons, we used the value of the Coulomb integral $U = 5.3$ eV (following [31]) for Fe in the DFT + U calculations. The valance states of the atoms considered in the USPPs are as follows: Si:3s,3p, Fe:3s,3p, 3d, and O:2 s, 2p state. An automatically generated $8 \times 8 \times 8$ sampling k-point grid following the convention of Monkhorst and Pack [32] is used for Brillouin-Zone (BZ) integration yielding 721 k-points in the irreducible wedge of the BZ centered at $\Gamma$-point. The band structure calculations have been carried out following a path along the high symmetry points $\Gamma$-L-B$_1$/B-Z- $\Gamma$-X/Q-F-P$_1$/Z-L-P. The internal coordinates of these points are (0, 0, 0), (1/2, 1/2, 0), (1/2, 1/4, 1/4), (3/4, 1/2, 1/4), (1/2, 1/2, 1/2), (3/8, 0, −3/8), (5/8, 3/8, 0), (1/2, 1/2, 0), (5/8, 5/8, 1/4) and (3/4, 3/8, 3/8) in the first BZ, respectively as proposed by Wahyu and Stefani [33]. Wave functions are expanded in plane-wave basis sets up to a kinetic energy cut-off value of 600 Ry.

All calculations were performed using the optimized structural parameters obtained in this work as shown in figure 1. We obtained equations of state (EOS’s) for SFO using some volume points, fitted the total energies to the Birch-Murnaghan EOS [34], and derived the equilibrium energy and volumes, bulk modulus derivative (B’), and bulk moduli (B$_0$). Optical properties of SFO spinel-type material were performed using Yambo code at the level of GGA + U within random phase approximation. GGA + U is chosen because the gap obtained with it is closer to the experimental result [35–37]. The complex dielectric function $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$ is an important function that describes the optical properties of a material. Using equation (1) the real part ($\varepsilon_1(\omega)$) was calculated by employing the Kramers-Kronig relations while the imaginary part ($\varepsilon_2(\omega)$) of the complex dielectric function is obtained by summing transitions from valence (occupied) to conduction (unoccupied) states (with fixed k) over the BZ as shown in equation (2) [38].

$$\varepsilon_1(\omega) = 1 + \left(\frac{2}{\pi}\right)\int_0^\infty \frac{\omega'}{\omega'^2 - \omega^2} \int d\omega'$$

$$\varepsilon_2(\omega) = \frac{1}{2\pi} \int \frac{\omega'}{\omega'^2 - \omega^2} \int d\omega'$$
where $P$ represents the Cauchy principal value, $c_k$ and $v_k$ are the Bloch functions for the unoccupied and occupied states. The symbols $\omega$ and $k$ denote the frequency of incident radiation and momentum operator respectively while the total energy is given by an integral part of equation (2).

The results obtained from equations (1) and (2) were used to calculate other frequency-dependent complex dielectric functions such as the extinction coefficient ($k(\omega)$), conductivity ($\sigma(\omega)$), reflectivity index ($R(\omega)$), absorption coefficient ($\alpha(\omega)$), electron loss function ($L(\omega)$) and the refractive index ($n(\omega)$) as given in the equations (3)–(8) [38, 39].

3. Results and discussion
3.1. Structure parameters
Firstly, in order to avoid certain errors and obtain correct results for electronic and optical properties, complete geometry optimization of the spinel structure for both lattice parameters and atomic coordinates is performed. The optimized structural cell parameters of the SFO are listed in table 1. The lattice parameter, $a_0$, of SFO and the total energy (lowest value of the parabolic energy-volume curves as illustrated in figures 1(a) and (b)) of the unit cell in the SFO spinel-type material are varied due to variation of volume, $V_0$ where, the calculated lattice
parameters and volumes when compared with experimental results show a small and consistent decrease (<11%), while values of $B_0$ and $B'$ obtained from the EOS fitting show an underestimation of less than 10%. These deviations are due to the use of GGA/LDA in our DFT calculations and is a well-known consequence of, LDA calculations which underestimate the lattice parameters relative to the experimental values while GGA typically produce larger lattice parameters than the LDA, in some cases so much higher than they overestimate the lattice constants [24]. In this work, we observed that the use of GGA and LDA in our calculation miscalculate the lattice parameter by 4.85% and 10.32% respectively. However, incorporating the U scheme tends to decrease the error in the lattice parameter relative to bare GGA/LDA results. The calculated lattice parameter with the inclusion of the U corrections is interestingly close to the experimental results as shown in table 1. This confirmed that the inclusion of the U corrections in the DFT calculations of correlated and localized 3$d$ or 4$f$ electrons in rare-earth and transition oxides is significant for predicting reliable lattice parameters as it gives an excellent equivalent with experimental results.

3.2. Electronic properties

The calculated bands energy and total density of state (TDOS) structure curves of SFO are presented in figures 2(a)–(d) using the GGA/LDA and GGA + U/LDA + U. The electronic bands energy in figures 2(a) and (c) appear to illustrate no energy gap at the Fermi level, thus, standard DFT failed to predict the insulator properties of SFO spinel-type material despite the fact that, it was found to be an insulator experimentally. In order to understand the characteristics of electronic band states of SFO and to correct this problem, another approach is needed to be able to investigate the properties conscientiously. In this work, we have used DFT + U approximation to resolve the bandgap of SFO. The calculated bandgap based on DFT + U with different approximations is reported in table 2. Some of our results agreed well with that of the experiment. The detailed knowledge of the electronic structure of SFO is important in assessing its potential applications in optical and optoelectronic devices. In figures 2 (b) and (d) the valance band maxima (VBM) and the conduction band minima (CBM) from both GGA + U and LDA + U lies at the same symmetry point F. This indicates that SFO has a direct energy bandgap. The calculated band gaps for the SFO material are 3.52 eV and 2.96 eV using GGA + U and LDA + U respectively. The bandgap obtained using the GGA + U is closer to the experimental value of 4.22 eV which was obtained using spectroscopic technique relative to LDA + U [41, 42]. The slight incongruities noted between the bandgap value obtained from GGA + U and the experimental is usually attributed to some physical aspects.

Firstly, the renowned limitation of the DFT is the use of approximations to treat the exchange-correlation energies in the DFT calculations (where the approximations do not fully replicate the exact exchange-correlation interactions in the compounds). Nevertheless, GW approximation has been employed for the subsequent calculations of the fundamental band gap and other optical properties of the material. The GW method has been repeatedly used by many researchers and provide an accurate description of the band gaps of semiconductors and insulators as well as reproducing the bandgap trends as reported in more complicated hybrid (exact) functional or computationally expensive methods [36, 37, 45]. Second, due to the pre-conditions adopted in the DFT formalism where the ground and excited states properties calculations of the materials are performed at temperature, $\theta = 0 K$, and this, is much lower than the temperatures at which the experimental properties of many materials were measured [46].

Consequently, this may perhaps lead to additional discrepancies that are observed between the DFT calculated and the experimental band gap values of SFO as depicted in figures 2(b) and (d). It is worthy to note that, the calculated energy band gaps of the studied material (SFO) lie between 2.69 eV to 3.60 eV and this indicates that, SFO may be efficiently utilized as ideal transparent materials (TM) [1, 23].

The PDOS (partial density of states) for the Si, Fe, O atoms of the bulk SFO spinel-type material are investigated through the GGA + U and LDA + U as illustrated in figures 3(a) and (b). The PDOS plots in figure 3 clearly display that there is an energy range (below the fermi, $E_f$ as well as above it) where the DOS

### Table 1. Optimized Lattice parameters ($a_0$), Total Equilibrium Energy ($E_0$), volume ($V_0$), bulk moduli ($B_0$), and bulk modulus derivative ($B'$) from Murnaghan’s EOS.

| Method   | $a_0$ (Å) | $V_0$ (Å^3) | $B_0$ (GPa) | $B'$ | $E_0$ (Ry) |
|----------|-----------|-------------|-------------|------|-------------|
| GGA      | 5.683     | 876.22      | 235.7       | 4.37 | −1273.812   |
| LDA      | 5.563     | 825.80      | 221.3       | 4.42 | −1273.622   |
| GGA + U  | 5.736     | 896.03      | 275.3       | 4.34 | −1273.178   |
| LDA + U  | 5.583     | 836.91      | 263.7       | 4.11 | −1272.919   |
| Experiment (31) | 5.895 | 920.868     | 181         |      | 168.9 [40]  |
|          |           |             |             |      | 5.7 [40]    |
remains at zero, hence, confirming that the SFO spinel-type is an insulator [41]. Furthermore, the PDOS plots in figure 3 reveal two main regions one in the VB and the other in the CB of the SFO spinel-type using both GGA + U and LDA + U. The first region below fermi (−0.94 eV to −7.20 eV) consists of the contributions by the Fe-3d, O-2p, Si-3s and Fe-3p states using GGA + U while for LDA + U is from −0.55 eV to 8.15 eV which consist of Fe-3d, Si-3s, O-2s and O-2p states. The conduction band region from (2.58 eV above fermi) is mainly contributed by the Fe-3d, O-2p, Fe-4s states using the GGA + U and that of LDA + U from 2.41 eV above the fermi consist of Si-3s, Fe-3d, O-2s and O-2p states. Notably, the mixed nature of the density of states suggests strong hybridization among the states of cations and anions. From figures 3(a) and (b), it can be clearly observed that there are significant contributions of the Si-3s and O-2s states in both GGA + U and LDA + U. Thus, the PDOS plots offer additional information such as the degree of the various contributions from the different states due to the different elements in the SFO spinel-type and this will complement the experimental results of this material that were previously reported.

3.3. Optical properties

As stated in equation (1), the complex dielectric function ($\varepsilon(\omega)$) shows the optical response of the material at all photon energies. The real part ($\varepsilon_1(\omega)$), of the dielectric function, gives the energy stored in material while the imaginary part ($\varepsilon_2(\omega)$) is connected to the absorption behavior of the medium together with the electronic band structure of the material. We have shown in figure 4 (a and b) how $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ of the complex dielectric

|                           | GGA + U | LDA + U |
|---------------------------|---------|---------|
| This work                 | 3.52    | 2.96    |
| Experiment                | 4.22 [41, 42] |
| Others                    | 2.21 [43], 2.52 [44], 1.49 [22] |

Figure 2. Calculated Bands Energy and TDOS: (a) GGA (b) GGA + U (c) LDA (d) LDA + U.
function of the SFO spinel-type varied with photon energy ($E$). The corresponding value $\varepsilon_1(0)$ at $\omega = 0$ for SFO spinel-type material is given in table 3. After $\omega = 0$ the magnitude of $\varepsilon_1(\omega)$ start to increase with increasing photon energy, and the values of $\varepsilon_1(\omega)$ where the peaks of the $\varepsilon_1(\omega)$ spectra occur and the corresponding values of the photon energy for the SFO spinel-type material are also listed in table 3.

Furthermore, within the energy range of 9.58–17.82 eV the spectra of $\varepsilon_2(\omega)$ is negative and this indicates that this material shows metallic behavior in this photon energy range, which becomes reflective towards the incoming photons. The plot of $\varepsilon_2(\omega)$ in figure 4(b) demonstrated the variation of the frequency-dependent absorptive part of the complex dielectric function with photon energy while the threshold energy of the $\varepsilon_2(\omega)$ spectra are also listed in table 3. The calculated $\varepsilon_2(\omega)$ show that the optical absorption edge occurred at 3.52 eV, which is sometimes called optical bandgap. This value corresponds to the energy bandgap of the material under investigation, which characterizes the interband transition between maxima of the valence band and minima of the conduction band. It is worthy to note that, the different peaks in figure 4(b) are as a result of the electronic interband transitions and the origin of the different peaks can be related to the partial density of state plots.

Figure 3. The calculated Partial Density of State (PDOS) for the Si, Fe, O atoms in the bulk SFO using (a) GGA + U and (b) LDA + U.

Figure 4. Calculated Complex Dielectric Plots of the (a) Real part (b) Imaginary part.
displayed in figures 3(a) and (b). For example, the first peak is due to the transition of the electrons from the Fe-3d state in the CB to the Si-2p state in the VB. Equally, the second and third peaks are due to the electrons transition from the Fe-3d state to the Fe-3d and O-2p states. Some of the values of the energies at the different peaks of the $\varepsilon_1(\omega)$ spectra and the corresponding peak value of the $\varepsilon_2(\omega)$ are enumerated in table 3. The optical complex refractive index, $n(\omega)$ which is given by

$$n(\omega) = \omega_p^2 \epsilon_0 \mu_0 \epsilon_2(\omega)$$

where the ordinary refractive index and the extinction coefficient are represented by $n(\omega)$ and $k(\omega)$ respectively (1).

These optical parameters are important in the design of transparent conducting oxides (TCOs) devices (1). We can clearly observe from the plot of frequency-dependent refractive index, $n(\omega)$ in figure 5(a) that, its magnitude gradually rises with energy from the zero energy $\omega = 0$, $\lambda = \infty$ depicted value 1.88 and reach its highest value $n(\omega)$ maximum 6.51 corresponding to photon energy of about 4.36 eV. It is observed that the values of $\varepsilon_1(\omega)$ at $\omega = 0$ obey the following relationship of $n(\omega) = (\varepsilon_1(\omega))^{1/2}$. The value obtained for the refractive of SFO spinel-type material with inclusion of the electron-hole effect is slightly higher than that of silica glass (1.45) but similar to other members of compounds (1.72) that exist in spinel form. The variation of the $k(\omega)$ (extinction coefficient) with the photon energy is exhibited in figure 5(b). The threshold energy was found to be 3,21 eV, beyond this value the $k(\omega)$ gradually increases to a maximum value of 1.42 at an energy value of 12.62 eV. The values of the different peaks of in the plot indicate that the maximum behavior of this material where further increase in the energy brings a considerable decrease in the magnitude of the extinction coefficient $k(\omega)$.

The variation of the optical conductivity $\sigma(\omega)$ of SFO spinel-type with the photon energy is also displayed in figure 6(a). The threshold energy is 3.76 eV and above this value, the optical conductivity increases with an increase in the photon energy until it reaches a maximum value of $4.53 \times 10^{16} \Omega \text{cm}^{-1}$ at a photon energy of
9.86 eV. Figure 6(d) displayed the optical absorption coefficient, $\alpha(\omega)$ of the SFO spinel-type material. Within the energy range between 0.0 eV to 3.28 eV, the $\alpha(\omega)$ is zero, and this indicates an absence of interaction between the medium and the incident photon. It was well known that this range of energy agrees that of infrared (1.24 meV to 1.7 eV) as well as that of visible (1.7 eV to 3.3 eV) region of the solar spectrum. In addition, the nonexistence of interaction between the incident photon and the material suggests that the material is transparent to the incident radiation within the 0.0 eV to 3.28 eV range. Beyond this photons energy range, the magnitude of the optical absorption coefficient starts to increase and this shows an interaction between atomic charge and photons in the medium, therefore, photons are absorbed in the medium, in figure 6 we can note that the $\alpha(\omega)$ reaches its maximum value of $380.8 \times 10^6$ cm$^{-1}$ corresponding to photon energy of about 12.25 eV. Similarly, this energy range lies within the UV range of the solar spectrum thus predicts that the medium absorbs maximum photons in the UV region. Therefore, the transparency for the visible region of solar spectrum and absorbance of photons in the UV region make SFO spinel-type material useful in some devices that employ the use of TCOs such as flat panel displays and window layers in solar cells. Importantly, we observed from our calculation that there is a consistent trend for the threshold energies corresponding to $\varepsilon_1(\omega)$, $\sigma(\omega)$ and $\alpha(\omega)$ spectra.

The calculated real ($\varepsilon_1(\omega)$) and imaginary ($\varepsilon_2(\omega)$) part of the complex dielectric function ($\varepsilon(\omega)$) and the various optical parameters ($\varepsilon(\omega)$, $\sigma(\omega)$, $\alpha(\omega)$ and $\varepsilon_1(\omega)$) investigated the SFO spinel-type material with the better k-points mesh within a photon energy range of 0.0 eV – 20 eV did not result in any noticeable change in the trends or magnitude when compared with the spectra of various optical properties displayed in figures 5(a) and (b), as well as 6(a, b, c and d) for the studied material and this, confirms the reliability and convergence of the computed optical properties of the material studied.

4. Conclusion

In summary, we have explored the electronic, structural and optical properties of SFO spinel-type material using first-principles pseudopotential method based on DFT $+$ U. The investigated electronic bandstructure reveals that the SFO spinel-type material is a direct bandgap semiconductor material. We found the bandgap value in this work to be 2.96 eV and 3.52 eV using LDA $+$ U and GGA $+$ U respectively as compared to other experimental results 4.22 eV. However, we found that the bandgap calculated with GGA $+$ U is close to experimental value when compared to that of LDA $+$ U. From the plots of the TDOS and PDOS, it is found that the top of the VB is mainly formed by Fe-3d and O-2p state. Also, the optical nature of SFO spinel-type material
is exposed with the help of calculating optical parameters such as complex dielectric function, index of refraction, absorption coefficient, energy loss function, reflectivity and extinction index for radiation up to 20.0 eV. The computed static complex dielectric constants have the value 6.52 and 5.42 of $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ respectively. Our results suggest that SFO spinel-type material is a potential candidate for some optoelectronics materials.

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