An evaluation of BiFeO₃ as a photovoltaic material

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A B S T R A C T

Keywords:

Photovoltaic effects
Ferroelectric
Semiconductors
Efficiency
Multi-gap

An analysis of BiFeO₃, focusing on its absorption properties, is carried out using experimental results from the literature and first-principles. In order to identify the different contributions to the absorption coefficient, the results have been split into inter- and intra-atomic contributions. Its potential as a photovoltaic material has been evaluated using both theoretical and experimental optical results. Because of the ferroelectric properties, we have considered two mechanisms for generating photocurrent: the traditional radiative and the ferroelectric or photovoltaic effects. The efficiencies, when ferroelectric photogeneration coexists with the traditional photovoltaic mechanism, are only slightly larger than when only the latter is considered. However, the increase in efficiency is significant with just multi-gap solar cells.

1. Introduction

Designing photocatalysts and solar-cell materials which respond to visible light irradiation for solar energy applications may be one of the most important challenges of the near future. Microscopically, this response is a consequence of their electronic and optical properties. A powerful complementary tool that allows these basic properties to be obtained and quantified, and which are barely accessible through experiments, is the first principles methodology.

Multiferroics, in which both electric and magnetic orders coexist in the same phase, are becoming of great interest, although these systems are rare in nature. Bi-based multiferroics are one of these systems and they have been studied extensively. In particular, BiFeO₃ (BFO) has attracted a great deal of interest. The spontaneous electric polarization, multiferroism, and static magnetoelectric coupling have been widely studied both experimentally and theoretically [1–5].

At room temperature, BFO is a G-type antiferromagnetic perovskite with a rhombohedral *R3c* structure (*n*° 161). The distorted FeO₆ octahedra are corner shared through oxygen, and the Bi atoms are not exactly in the middle of the FeO₆ octahedra owing to the off-center displacement of the Bi due to the presence of 6s lone pair electrons. Both types of distortion permit the development of a spontaneous polarization and give rise to the ferroelectric (FE) phase.

BFO has a direct band-gap of 2.6–2.7 eV [1,2] and has been previously shown to exhibit a conventional or radiative photovoltaic (R-PV) [2] and anomalous or FE-PV [6] effect. For FE-PV, it has been observed that a homogeneous short-circuited crystal exhibits a photocurrent in the direction of spontaneous polarization under uniform illumination [7]. As has been observed in bulk photoferroelectrics, the

increase in conductivity under illumination is greater at applied fields coincident with the direction of spontaneous polarization [2]. The anomalous PV effect, with an open-circuit voltage greater than the energy band-gap, has been observed in a number of FE materials. Furthermore, a new type of PV cell that carries out the charge carrier separation in the semiconductor with the bound surface charges of the FE has been described in the literature [8] where the non-equilibrium photoexcited carriers are effectively driven by the FE polarization.

The origin of the observed BFO PV properties is not quite clear. Large photovoltages have been observed in the opposite direction of the material polarization [6]. The photovoltage was attributed to the periodic domain walls acting both to separate and collect photoexcited carriers. The photocurrent in BFO has also been reported as being generated uniformly throughout the sample, consistent with an FE-PV effect [1].

The main experimental and theoretical research activities focus on exploring the origin of the observed BFO PV properties [1–5]. However, despite experimental and theoretical research activities, there is little analysis focusing on the effect of these properties in PV devices with a response to visible light. With the objective of evaluating the effect of the microscopic optical properties at the solar-cell device level, we will use first-principles and experimental data in our analyses. Firstly, we will use first principles to obtain the electronic and optical properties, in particular, the absorption coefficients. The results will be compared with other theoretical and experimental results in the literature. Later, using these theoretical absorption coefficients and optical data in the literature, we will evaluate the potential of BFO as a PV material: (i) using the traditional radiative PV effect and (ii) the combination of the traditional and the so-called bulk (or FE-) PV effect.

2. Methodology

We use the first principles density functional theory (DFT) [9,10] for obtaining the electronic and optical properties. In traditional DFT the interactions are treated using a mean field approach, which is not appropriate for suitably describing the electron self-interaction effects. Methods such as DFT+U incorporate an effective on-site Coulomb U factor in order to avoid the self-interaction problem partially [11–16]. The U value depends on several factors: (i) the choice of the orbitals into which the correction is applied; (ii) the method used for computing the orbital occupations; and (iii) the DFT+U implementation chosen [13–16]. In this work we use: (i) the DFT+U methodology and implementation described in references [13,14]; (ii) the generalized gradient approximation (GGA) from Perdew, Burke and Ernzerhof [17] for the exchange-correlation potential; (iii) the standard Troullier–Martins [18] pseudopotentials expressed in the Kleinman–Bylander [19,20] form; and (iv) a numerically localized pseudoatomic orbital basis set [21] for the valence wave functions. We use periodic boundary conditions, spin polarization, double-zeta with polarization localized basis sets, and the rhombohedral R3c structure with 172 special k-points in the irreducible Brillouin zone in all of the results presented. The positions of the cell atoms were relaxed by minimizing the quantum mechanical forces with the conjugated gradient algorithm. The convergence at the absolute energy minimum is considered when the forces on the atoms are less than $0.004 \text{ eV } \text{\AA}^{-1}$.

The complex dielectric function was later determined on the independent-particle approximation:

$$\epsilon_2(E) \sim \frac{1}{E^2} \sum_{\mu < \lambda} \int d\vec{k} |f_{\mu,\vec{k}} - f_{\lambda,\vec{k}}| |p_{\mu\lambda}|^2 \delta(E_{\lambda,\vec{k}} - E_{\mu,\vec{k}} - E)$$

where $E_{\mu,\vec{k}}$ and $f_{\mu,\vec{k}}$ are the single-particle energies and occupations of the μ band at $\vec{k}$ points in the Brillouin zone, and $p_{\mu\lambda}$ are the momentum matrix elements between the μ and λ bands at $\vec{k}$ points. The Kramers-Kronig relationships were used to obtain the other optical properties.

3. Results and discussion

3.1. Structure and electronic properties

The BFO experimental band-gaps reported in the literature are between 2.6 and 2.70 eV [1,2]. Theoretically, due to the well-known tendency of DFT calculations to underestimate the localization of the d-orbital electrons, the DFT+U method, including an effective Hubbard U in the Hamiltonian, has been used in previous studies in the literature [3–5]. The band-gaps reported are between 2.13 and 2.58 eV using different U values for the d(Fe) states and different DFT+U implementations and/or formalisms: 1.9 eV (U = 4 eV) [22], 2.58 eV (U = 5 eV) [3], 2.5 eV (U > 7 eV) [4], 2.13 eV (U = 4 eV) [5]. In this work we applied the orbital-dependent one-electron potential using the DFT+U formalism described in references [13,14]. The band-gaps obtained with U = 0 eV, U = 6 eV, and U > 8 eV are 1.71, 1.93, and 2.15 eV. Like other results, the band-gap increases with the increase in U and gets as high as 2.15 eV when U is greater than 8 eV.

It is interesting to stress that the experimental band-gaps are often obtained indirectly from optical absorption measurements by carrying out linear extrapolation or a fit of $(\alpha E)^p$, where α is the absorption coefficient for the photon energy E. The simplified model $\alpha E \sim (E - E_g)^{1/p}$ [1–3] is assumed implicitly. The band-gaps are calculated from the energy differences of the respective single-particle eigenvalue energies. Later, when α is calculated and the data fit the previous approximate model, the band-gaps obtained are around 0.1–0.3 eV larger depending on the fit or the extrapolation, and the energy range considered. Therefore, the difference between the theoretical and experimental band-gaps is ~ 0.1 – 0.3 eV lower if the band-gaps obtained from the simplified model (between 2.25 and 2.45 eV

Fig. 1. Imaginary part of the dielectric function $\epsilon_2(E)$ calculated theoretically ('Teo' label, GGA+U with U=8 eV) and a comparison with experimental data in references [1] ('e1' label) and [2] ('e2' label), and theoretical data from references [3] ('t1' label, GGA+U with U=5 eV) and [4] ('t2' label, GGA+U with U=7 eV).

with U > 8 eV) are used instead of the single-particle eigenvalue energies (2.15 eV with U > 8 eV). It is done on some occasions [3] in order to compare the theoretical and experimental band-gaps obtained (indirectly) from the simplified model.

In order to determine the atomic and orbital composition of the edges of the VB and the CB, we have calculated the projected density of states (PDOS) as a function of energy. A detailed analysis of the PDOS reveals that the states of the edge of the VB are derived mainly from the p(O) and s(Bi) states, while the CB edge states consist mainly of the p(Bi) states. These results are in accordance with other results in the literature [3,4].

3.2. Optical properties

The absorption coefficients (AC) have been obtained in order to analyze the potential of this compound as solar radiation absorbers. A good candidate for PV applications must have a high optical absorption of the sunlight spectrum. Firstly we have obtained the complex dielectric function in accordance with the methodology section. Our results of the imaginary part of the dielectric function are compared with other experimental [1,2] and theoretical [4,5] results in the literature in Fig. 1. The comparison shows that our results are within the range obtained experimentally. In particular, two absorption peaks located at 3.0–3.2 and 4.26–4.4 eV [1,2] are well reproduced via the imaginary part of linear dielectric function and the AC.

The optical properties on the independent-particle approximation depend on the square of the momentum operator matrix elements. We have split the momentum operator matrix elements $p_{\mu\lambda}$ into symmetrically non-equivalent species contributions such as $p_{\mu\lambda} = \sum_A \sum_B p_{\mu\lambda}^{AB}$, where $p_{\mu\lambda}^{AB}$ is the inter-species component that couples the basis set functions on different species atoms A and B. If A = B, it represents an intra-species component. With their square, the complex dielectric function and other optical properties can be split: $\epsilon_2 = \sum_A \sum_B \epsilon_2^{AB} +$ (terms involving three and four different non-equivalent species). From this analysis the largest contributions correspond to the Bi-Bi, O-O and Bi-O transitions. Transitions involving the Fe atoms contribute almost nothing to the optical properties.

In order to look into the contribution in greater depth from the atomic states, we have additionally split $p_{\mu\lambda}^{AB}$ into angular momentum contributions like $p_{\mu\lambda}^{AB} = \sum_{l_A} \sum_{l_B} (p_{\mu\lambda}^{AB})_{l_A l_B}$, where $(p_{\mu\lambda}^{AB})_{l_A l_B}$ is the contribution of the transition between the l_A shell-states (in A) and the l_B shell-states (in B). Then the complex dielectric function can be split as $\epsilon_2 = \epsilon_2(S) + T$, where $\epsilon_2(S) = \sum_A \sum_B \sum_{l_A \in A} \sum_{l_B \in B} (\epsilon_2)_{l_A l_B}^{AB}$ and T represents the terms involving three and four different non-equivalent species. The more important $(\epsilon_2)_{l_A l_B}^{AB}$ contributions to the absorption coefficient are

Fig. 2. (a) More important terms of the imaginary part of the dielectric function split into angular momentum contributions $(\epsilon_2)_{AB}^R$. (b) Complex dielectric function ϵ_2 and sum of the first and second terms $\epsilon_2(S)$ resulting in the splitting of ϵ_2 .

represented in Fig. 2. In decreasing order they are $(\epsilon_2)_{sp}^{BiBi}$, $(\epsilon_2)_{sp}^{OO}$, $(\epsilon_2)_{pp}^{BiBi}$, and $(\epsilon_2)_{sp}^{BiO}$. They correspond to the intra-species transitions $s(\text{Bi})-p(\text{Bi})$, $s(\text{O})-p(\text{O})$, and to the inter-species transitions $p(\text{O})-p(\text{Bi})$ and $s(\text{Bi})-p(\text{O})$. The other transitions, not shown in the Figure, make a very low contribution. As usual, we use the notation s , p , d , etc for $l = 0, 1, 2$, etc.

In the previous analyses, the third and fourth order terms (T) have been disregarded. In order to evaluate their contribution, the complex dielectric function ϵ_2 and the sum of the first and second terms resulting of the splitting $\epsilon_2(S)$ is represented in Fig. 2(b). The difference between these terms indicates the contribution T of the terms disregarded. From the Figure, although the contribution of the disregarded terms is larger for the two absorption peaks, the maximum contribution to the range the energies is less than the 15%. Therefore the approximation $\epsilon_2 \sim \epsilon_2(S)$ is justified.

3.3. Solar cell efficiencies

The overall solar cell efficiency is essentially the product of the efficiencies corresponding to the processes: (i) absorption, (ii) charge separation and transport, and (iii) collection at the contacts. The first process depends only on the material absorption properties. The other two processes usually determinate the basic structure of the device and depend on contacts, transport properties, interfacial barriers, doping, manufacture, etc. The absorption efficiency will be evaluated in this study. This efficiency is a first filter: if it is small then the semiconductor is not a good candidate for solar cell devices independently of the other efficiencies. At a later stage, the other processes, dependent on the device structure, should be optimized for each case.

There are several ideal assumptions generally used in the specific literature [23–26] to obtain solar cell maximum absorption efficiencies: the cell operates at 300 K, any non-radiative recombination is suppressed, the carrier mobilities are infinite (no ohmic losses), and the illumination comes from an isotropic gas of photons from the spectrum of a 5760 K black body reduced by the factor 46200 (BB spectrum).

Another important approximation is to assume that the solar cell absorbs all incident photons above the band-gap. It implies that the absorption coefficient is a step function: zero for energies of less than the energy band-gap and constant for energies above the band-gap. In this way the dependence of the efficiency is simplified from the absorption coefficient to the band-gap energy. Then the band-gaps are used as an evaluation criterion of the potential for solar cell applications [23–26]. The functional form of the absorption coefficients with respect to the photon energy is not considered in these analyses. In part it is due to the simplification of the calculation and the difficulty in obtaining absorption coefficient (theoretical or experimental) results with respect to energy band-gap results.

In order to avoid this simplification when maximum efficiency is obtained, the absorption coefficients obtained from first-principles and from experimental data will be used instead of band-gap energies as the evaluation criterion for the solar cell efficiency. As a consequence, the efficiencies depend on the thickness w of the device. For obtaining the absorption coefficients from experimental data, we previously carried out a spline interpolation of the imaginary part of the dielectric function [1] and the absorption coefficient [2] of the experimental data in these references.

The absorption coefficients have been obtained from the dielectric function for both theoretical and experimental data using the Kramers-Kronig relationships, except for data from reference [2] where the experimental result is the absorption coefficient. They have later been used to obtain the maximum efficiencies for several solar concentrations (Fig. 3). To avoid differences in the absorption range of energies, and to compare the results, the theoretical absorption coefficient is scaled to the experimental energy. Only for very thin cells ($< 0.15 \mu\text{m}$) are there small differences between the results. From the results in the figure, solar cell devices of only a few microns in thickness have efficiencies of around 15.5% and 17.5% for the concentration factor of the sunlight $f_c = 1$ (without concentration) and $f_c \sim 46200$ (maximum concentration). They are far from the maximum overall efficiency ($\sim 31\%$ and 41% for $f_c = 1$ and $f_c \sim 46200$, and $E_g = 1.1\text{--}1.3 \text{ eV}$ respectively [23–26]). In order to compare it with the AM1.5 spectrum normalized to 1000 W m^{-2} , a concentration factor f_c of the BB spectrum is approximately equivalent to a concentration factor of $1.35 f_c$ of the AM1.5 spectrum.

There are alternatives to increasing the limiting efficiency of single-gap solar cells. For example, to take advantage of the FE-PV effect [7], an additional mechanism that can generate photocurrent in FE semiconductors. In this case the current generation is due to the FE polarization instead of optical transitions between the valence band (VB) and conduction band (CB) with the traditional radiative (R-PV) mechanism.

Fig. 3. Efficiency η (%) as a function of the cell thickness w using the absorption coefficients obtained from calculations ('t' label), and experimental data in references [1] ('e1' label) and [2] ('e2' label). The thin and thick lines correspond to the light concentration factor $f_c = 1$ (without concentration) and maximum concentration ($f_c = \text{max} \sim 46200$).

Fig. 4. Efficiency η (%) as a function of the gap number with $E_g = 2.5$ eV. $\eta_1(f_c = 1)$ and $\eta_1(f_c = \text{Max})$ are the radiative single-gap efficiencies without concentration and with maximum concentration respectively. η_{max} is the maximum efficiency if the radiative recombination is suppressed. The horizontal lines correspond to the maximum overall efficiency for single-gap solar cells ($\sim 31\%$ and 41% for $f_c = 1$ and $f_c = \text{Max} \sim 46200$). The lines between the gap numbers have been added for visual effect.

With $f_c = 1$ and after the polarization was positively oriented to maximize the FE driving force, a conversion efficiency of 8.1% for FE $\text{Bi}_2\text{FeCrO}_6$ (BFCO) thin-film solar cells in a multilayer configuration has been reported [27].

In order to evaluate different alternatives, the radiative single-gap efficiencies without concentration $\eta_1(f_c = 1)$ and with maximum concentration $\eta_1(f_c = \text{Max})$, the maximum efficiency if the radiative recombination is suppressed (η_{max}), and the maximum overall efficiency for single gap solar cells ($\sim 31\%$ and 41% for $f_c = 1$ and $f_c = \text{Max} \sim 46200$) are represented in Fig. 4 at $E_g = 2.5$ eV.

The maximum theoretical current that can be obtained from a material with $E_g = 2.6$ eV is $J = 11 \text{ mA cm}^{-2}$. It is assumed that only one electron is extracted to an external circuit for every incoming photon (quantum yields = 1). This limit corresponds to completely suppressing the emitted current because of the radiative recombination. If the two mechanisms (R-PV and FE-PV) coexist, the maximum voltage will be limited by the E_g . Therefore the maximum efficiency under these conditions is $\eta_{\text{max}} \sim 19\%$ (Fig. 4 for single-gap semiconductor). The efficiency obtained with the R-PV mechanism and maximum sunlight concentration ($\eta_1(f_c = \text{Max}) \sim 17.5\%$) is close to this upper boundary. However, they are far from the maximum overall efficiency ($\sim 31\%$ and 41% for $f_c = 1$ and $f_c \sim 46200$).

Furthermore, another alternative for increasing the limiting efficiency is to use multi-gap semiconductors with optimum band-gaps larger than for single-gap solar cells [23–26]. These materials have intermediate bands (IB) between the traditional VB and the CB. Therefore, a photon with a lower energy than the single-gap energy (between the VB and CB) can generate additional carriers, from VB-IB and IB-CB transitions, increasing both the current and the efficiency. We have obtained the maximum efficiencies at $E_g = 2.5$ eV using a generalized multi-gap model [23–26] (Fig. 4). It can be observed in the figure that, from the double-gap solar cells, the efficiencies exceed the limits of the single-gap solar cell ($\sim 41\%$ for maximum concentration). Then these materials could be interesting for PV when used as an absorbent in solar cell devices.

In summary, the coexistence of the R-PV and FE-PB effects does not significantly increase the efficiency for BFO as regards the traditional R-FV. In fact, for single-gap solar cells, the efficiencies are far from the maximum. However a large increase in efficiency can be obtained by inserting an IB into the BFO semiconductor host.

4. Conclusions

Using first-principles theory we have microscopically studied the BFO electronic and optical properties. Our theoretical results reproduce the experimental data on the linear dielectric function and absorption coefficients very well. The absorption coefficients have been split into inter- and intra-species contributions in order to identify the different contributions to the absorption. From the results, the largest contribution is from the intra-species transitions $s(\text{Bi})\text{-p}(\text{Bi})$, $s(\text{O})\text{-p}(\text{O})$, and to the inter-species transitions $p(\text{O})\text{-p}(\text{Bi})$ and $s(\text{Bi})\text{-p}(\text{O})$.

The BFO potential as a single-gap solar cell has been evaluated to obtain the maximum efficiencies considering the traditional PV effect, and the combination of both traditional and FE-PV effects. The FE-PV effect only increases the potentiality of the FE material slightly with respect to the traditional PV effect. Therefore BFO has little potential as a sunlight absorber in single-gap solar cell. In order to increase the efficiency it is necessary to increase the absorption of the solar spectrum, which can be achieved with multi-gap solar cells with IBs in the BFO band-gap.

Acknowledgments

This work has been supported by the National Spanish project INVENTA-PV (TEC2015-64189-C3-1-R MINECO/FEDER).

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