OPTICAL PROPERTIES OF $BaTi_{0,99}Sr_{0,01}O_3$ SOLAR CELLS: A MOLECULAR MODELİNG STUDY

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ABSTRACT

Nowadays, energy resources (oil, coal and natural gas) are limited, studies on turning to alternative or sustainable energies have increased in recent years. Among the sustainable energy sources, solar energy attracts the most attention. Researchers in many industries are engineering all kinds of better-performing materials, abourt solar cells The most important point in using solar energy is the efficient conversion of sunlight into electrical energy. I this study Sr doped BaTiO3 candidate has strong photorefractive sensitivity and large electrooptic coefficients, making it a suitable crystal for use as a semiconductor in photovoltaic systems. In this study, optical properties of BaTiO3 were calculated with Denstiy Functional Theory (DFT).

Keywords: energy resources, solar cells, optical properties, denstiy functional theory (DFT).

INTRODUCTION

The world has focused on carbon-free energy due to the gases that harm the environment as a result of the burning of fossil fuels and global warming. (Al Dahoudi et al., 2013) Figure 1.1 shows the projection of world energy demand until 2040 and the total demand until 2040, which increases linearly with a growth of 2.2% per year after 2020 (IEA, 2019).

It has been determined that the world needs approximately 30TW of energy by 2050 to maintain current economic growth (Asım et al., 2012). Since solar energy has many advantages among renewable energy sources, solar cell studies have gained momentum. The Sun emits 3.8 million EJ/year of light (Şen, 2009). It has the potential to meet approximately 10,000 times the world's annual energy needs. Therefore, photovoltaic (light-electricity conversion) devices that can directly convert sunlight into electrical energy are needed (Gong et al., 2012). Scientific studies to efficiently utilize solar energy, a renewable energy source, have gained momentum recently. One of the most striking photovoltaic effective semiconductor devices used to convert the rays coming from the sun into electrical energy is solar cells (O'regan and Grätzel, 1991; Lewis et al., 2005).

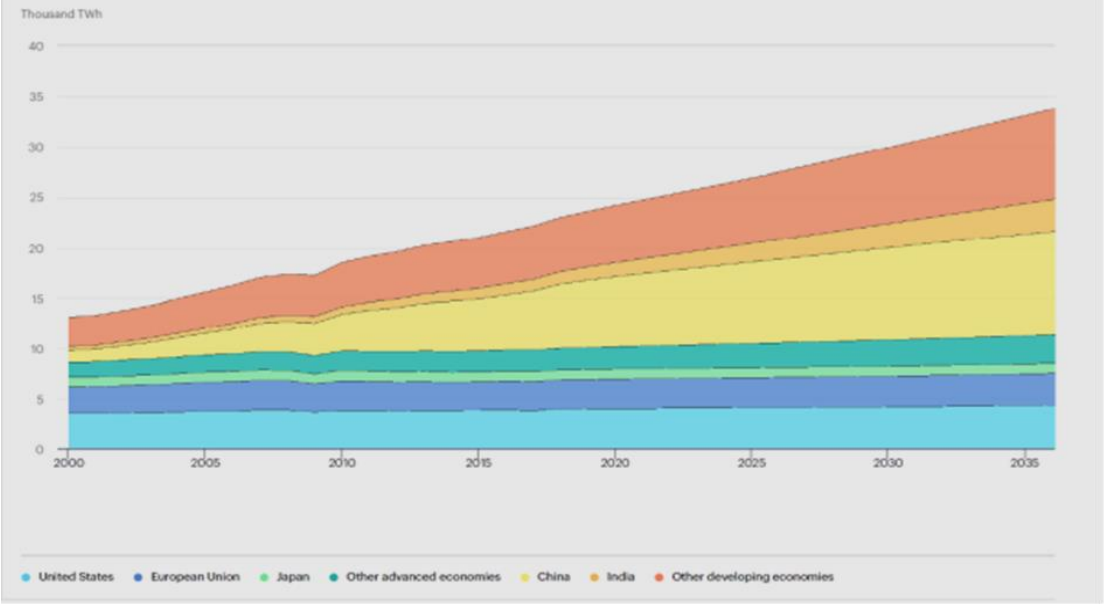

Figure 1. World energy demand projection until 2040 (IEA, 2019).

The common areas of use of photovoltaic cells in the last 50 years can be summarized as follows:
i) in providing energy for remote locations (communication and weather observation systems, lighting and water pumping systems in developing countries, etc.).
ii) In providing energy for consumer products (electronic calculators, garden lighting, etc.).
iii) in providing energy for spacecraft (for satellites and space shuttles, etc.) (Lewis et al., 2005; ABF and Van Ryswyk., 2011).

$BaTiO_3$

From its discovery by Valasek in 1920 until 1943, ferroelectrics remained a theoretical interest because they have water-soluble and brittle structures(J.F.Scott et al.) . This situation began to change after the discovery of perovskite-structured $BaTiO_3$ in 1945. The simplicity of its structure has increased theoretical studies and its physical properties have created a great incentive for the production of electronic devices. $BaTiO_3$ is in the group of ABO3-type perovskite crystals and is among the ferroelectric materials with the most significant cubic symmetry. Particularly among ferroelectric perovskites, $BaTiO_3$ have technological applications in many different places such as waveguides in electro-optics, laser frequency doubling and high-capacity memory cells. In addition, ABO3 type perovskite crystals are in the material class with many physical properties such as superconducting, magnetoresistance and ferroelectricity. Another new application of perovskites has recently been found in hybrid organic-inorganic materials used in thin-film area-effect transistors . Due to $BaTiO_3$'s sensitivity to voltage, high dielectric constant and piezo-electric properties, it also enables its use as multi-layer capacitors (K. Uchino),thermistors (Karin et al.,) and opto-electronics (Lines et al.,). Additionally, due to the characteristic properties of $BaTiO_3$, it is also used as an electromagnetic wave absorber (Trainer et al.,) At the same time, polymer materials with high dielectric constant are also used as electro-magnetic wave absorbers (Hipel et al,.) . Therefore, it is very important to examine the dielectric behavior of $BaTiO_3$ at different frequencies. BaTiO3 has been used in some types of solar cells to accelerate electron transport in the electron transport layer. BaTiO3, a ferroelectric material, can be spontaneously polarized and also has an internal self-polarizing dipole moment. Internal measurable macroscopic electric field can be generated in ferroelectric materials to promote the separation and transport of photogenerated electron–hole pairs. It has been reported that pure-phase perovskite type BaTiO3 electrode was applied to dye-sensitized solar cells and a higher Voc was obtained than TiO2 electrode (Luo et al.,2020)
ABX_3 compositions are considered fcc if the small B cation occupies space at the octahedral interface in the fcc (face-centered cubic structure) array, with a larger cation and oxygen forming the fcc cage form derivative structure. Here, the closest neighbor of cation B is only oxygen (Heifets et al.,). To create efficient photoanode for solar cell applications, it is critical to understand how electromagnetic radiation is absorbed and charge is transferred to the photoanode semiconductor/electrolyte interface. (Vandana et al.,)

MATERIALS AND METHOD

Molecular Modelling

Modeling and simulation systems provide an opportunity to study the structural, mechanical, electronic, optical and thermodynamic properties of molecules and are extensively used to design the next electronic devices based on these materials (Hensen and Lamberts, 2012). Simulation programs are a modeling and simulation environment designed to enable researchers in materials science and chemistry to predict and understand the relationships of a material's atomic and molecular structure to its properties and behavior.

Optical properties were calculated with the PBE and GGA (Generalized Gradient Approximation) approach developed by Perdew, Burke and Ernzerhof (PBE) using the density functional theory (DFT) calculation method CASTEP modüle by Materials Studio. The supercells have been obtained as 2x2x2 .

RESULTS

In this section, the optical properties DFT results of the $BaTiO_3$ will be discussed.

Crystal structure

BaTiO3 perovskite that we are dealing with is cubic (space group Pm-3m). f Ba(1-x)SrxTiO3 are optimized. The lattice constants have calculated as a = b = c = 4.010 Å in our study. This lattice constant value has calculated approximately close in value with the experimentally reported 4.000 Å [8]. The differences between the value we have calculated and the experimental value is only 0.010 Å and is close to each other. This shows the closeness of this study to reality. A supercell was formed by shifting the stoichiometric structure 2x2x2. For the supercell a=b=c=8.020 Å and the volume is calculated as 515.849 A3 (S.Aksan 2024)

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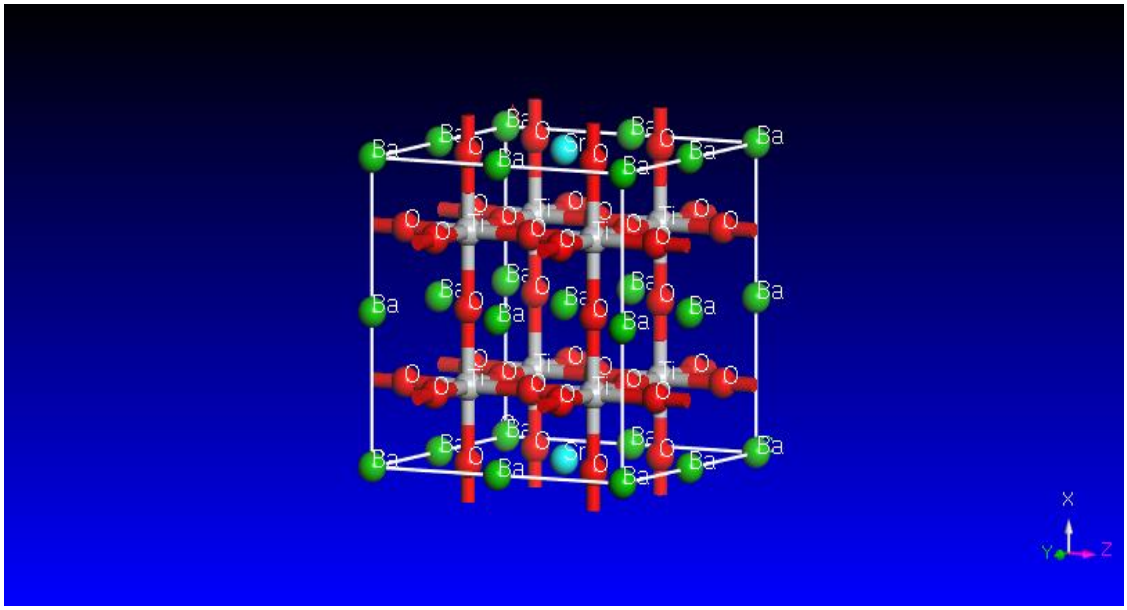

Figure 2. $BaTi_{0,99}Sr_{0,01}O_3$ Super cell cyrstal structure.

Pseudo atomic calculation performed for O 2s2 2p4 Converged in 22 iterations to a total energy of -423.8174 eV Pseudo atomic calculation performed for Ti 3s2 3p6 3d2 4s2 Converged in 30 iterations to a total energy of -1566.4933 eV, Pseudo atomic calculation performed for Sr 4s2 4p6 5s2 Converged in 21 iterations to a total energy of -836.1744 eV Pseudo atomic calculation performed for Ba 5s2 5p6 6s2 Converged in 23 iterations to a total energy of -692.4315 eV.

Band structure

Most important aspects of solid state physics is the study of electronic structure, that explain a material properties such as electrical conductivity, electronic thermal conductivity, electronic and optical properties, The band structures of the cubic, phases using GGA functionals are shown in Figure3.

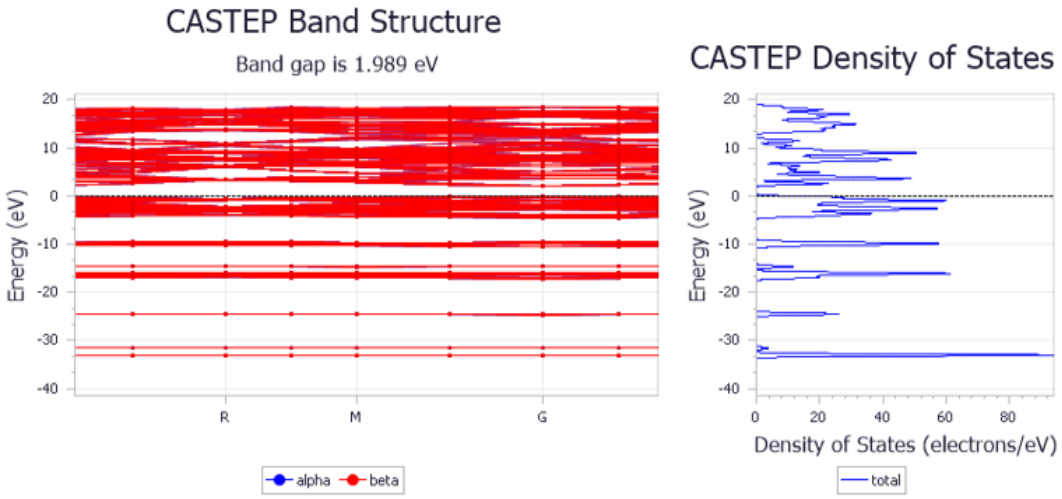

Figure 3. $BaTi_{0,99}Sr_{0,01}O_3$ Band Structure.

Density of states (DOS)

Most of the electronic and optical properties of crystalline solids are connected explicitly to the structure of the DOS, including the contribution of each atom to bonding-antibonding states, conductivity, magnetic order, optoelectronic properties.

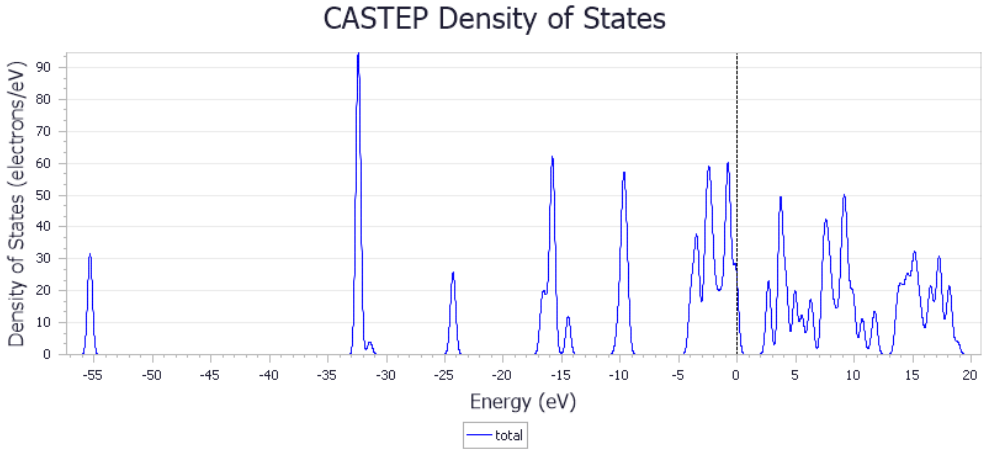

Figure 4. DOS of $BaTi_{0,99}Sr_{0,01}O_3$

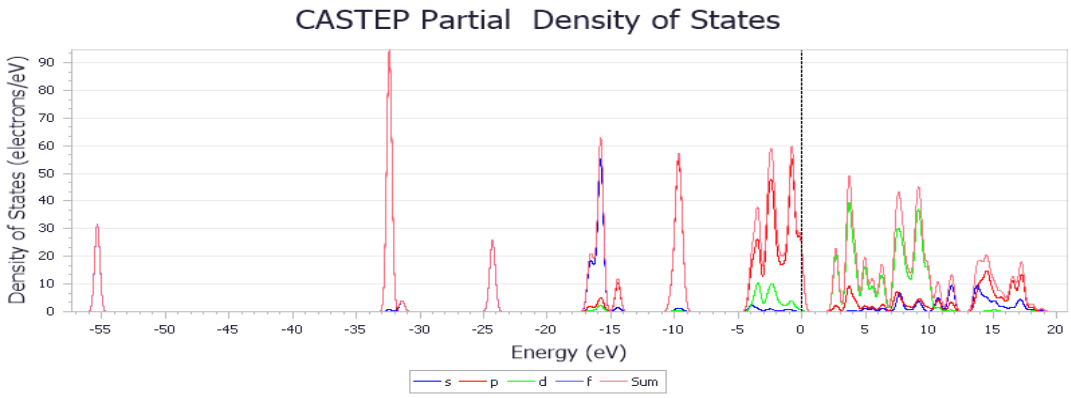

Figure 5. PDOS of $BaTi_{0,99}Sr_{0,01}O_3$

Fermi level implies that $BaTi_{0,99}Sr_{0,01}O_3$will exhibit electrical conductivity. It has been computed the PDOS of Ba, Ti, and O atoms in order to better understand their role in TDOS and chemical bonding. I can be seen electronic distribution in the upper valence band (VB) near Fermi level (EF) (0 to −5 eV) mainly attributed to the O-2p states, which is common for most of the oxide semiconductors. The Ti-3d states also contribute to form the upper valence band hence there is a strong hybridization occurred between O-2p and T-3d states it is contributed with the others. (Vandana et.al). It has been computed the optical properties such as their complex optical properties

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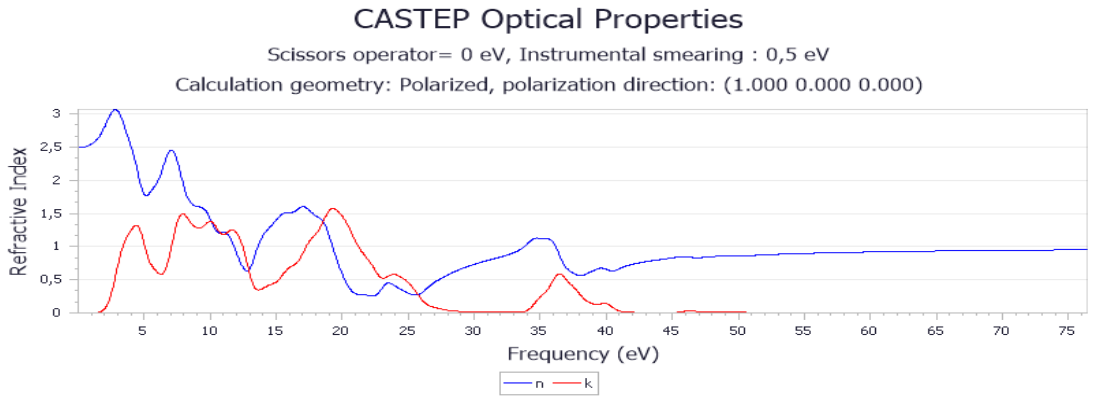

Figure 6. Refractive index of $BaTi_{0,99}Sr_{0,01}O_3$

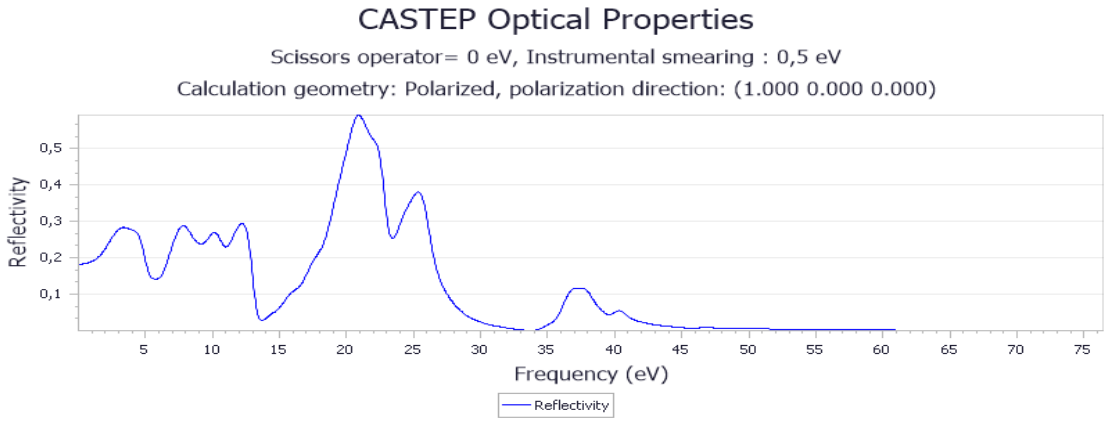

Figure 7. Reflectivity of $BaTi_{0,99}Sr_{0,01}O_3$

The frequency-dependent optical reflectivity R(ω) for BaTiO3 material is shown in Fig. 6 Fig. 8 absorption coefficient α(ω) indicates that it begins to absorb incident light at photon energies of for the GGA approximations. In consideration of this, it can be said that Sr doped BaTiO3 is a good candidate for use as an absorber layer in solar cells. For GGA approximations, the absorption coefficient approaches to its maximum value at around 20 eV.

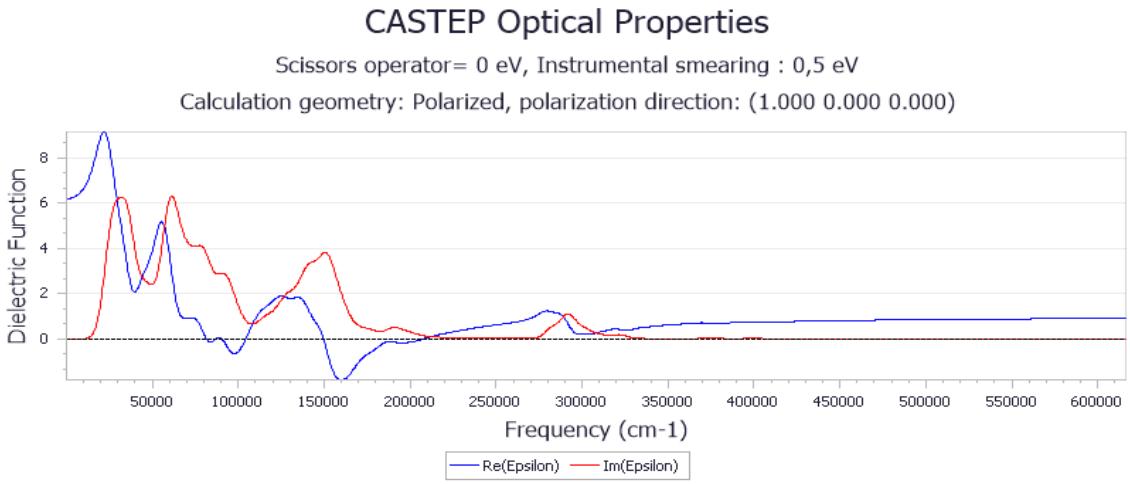

Figure 8. Dielectric Function of $BaTi_{0,99}Sr_{0,01}O_3$

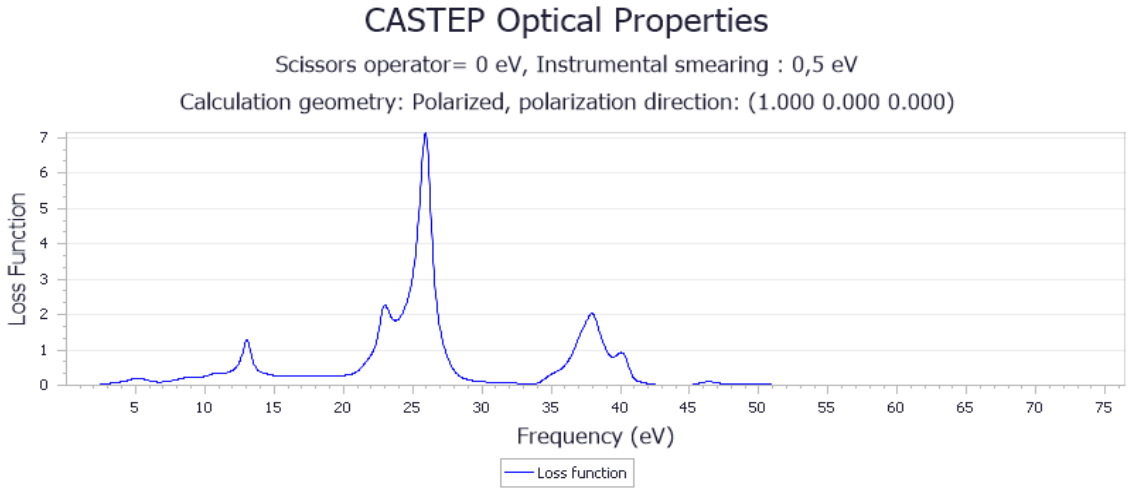

Figure 9. Loss Function of $BaTi_{0,99}Sr_{0,01}O_3$

The electronic transition from the Ti-d to Ba-d states may include many absorption peaks . Dielectric function affects reflectivity of the material. The amount of light energy reflected from the material surface serves as a general estimation of reflectivity . The reflectivity of BaTiO3 materials is GGA approximation shows the predicted refractive index n(ω) for BaTiO3. The transparency of the material is measured by the refractive index. Since they are closely related to the refractive index spectrum n(ω) which follows the real component of the dielectric function εr (ω). The photon energy at 0 eV, the maximum refractive spectra for GGA. Therefore, two important properties are seen in the refractive index n(ω) spectrum of BaTiO3. When the refractive index is greater than one, the photons entering into the material are slowed down by their contacts with electrons, more photons are decelerated while passing through the material, for a higher refractive index .Generally, any process that raises the electron density of the material also increases the refractive index.(vandana Et al.)

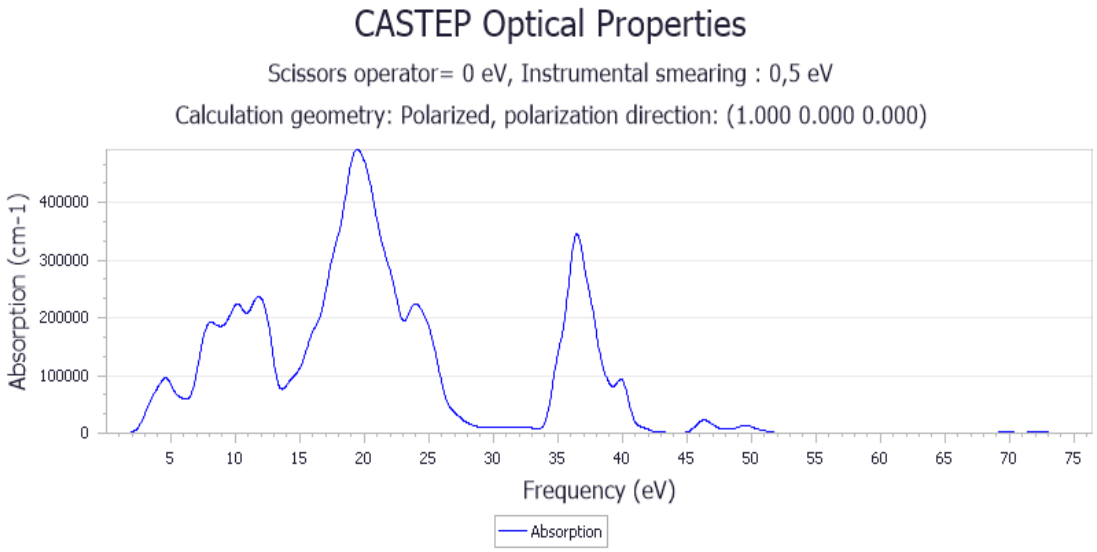

Figure 10. Absorption of $BaTi(1-x)SrxO_3$

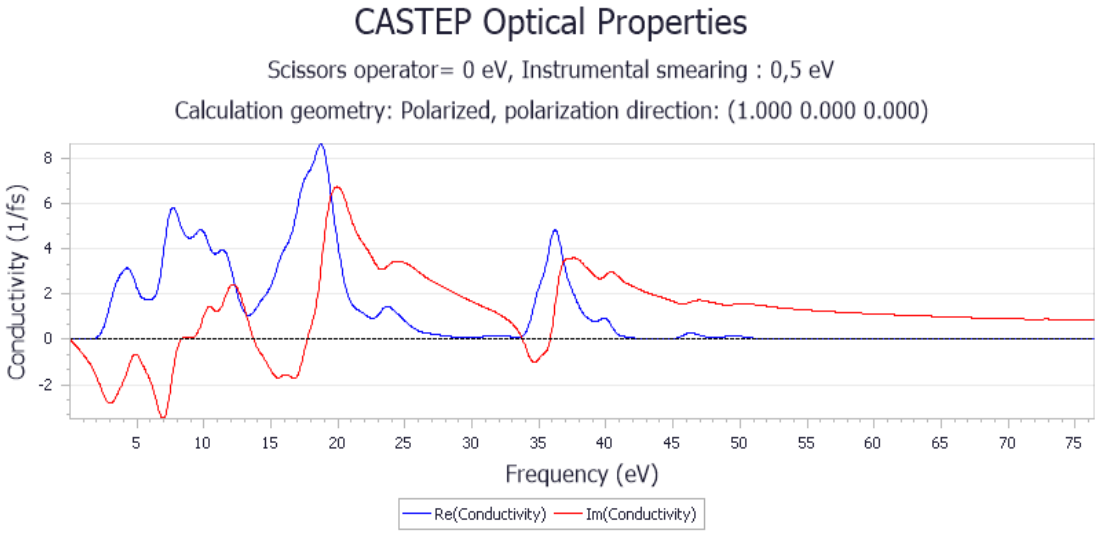

Figure 11. Conductvity of $BaTi(1-x)SrxO_3$

CONCLUSION

This study described the optical properties of Sr doped BaTiO3 perovskite solar cell material using density functional theory. The other theoretical results were found to be consistent with the analyzed structural parameters. the electronic and optical properties of BaTiO3 According to GGA exhibits indirect bandgap and semiconducting behaviour. It's characteristics are tuned, correspondingly by GGA approximation. The behavior of the materials properties seen in the plots of absorption coefficients versus energies in the UV region. A detailed comparisons of the optical characteristics of the GGA systems were performed by including complicated dielectric function, absorption spectrum, reflectivity and refractive index.

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