



Original Research Article

Investigation of Structural, Electronic and Optical Properties of SrTiO_3 and $\text{SrTi}_{0.94}\text{Ag}_{0.06}\text{O}_3$ Quantum Dots Based Semiconductor Using First Principle Approach

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ABSTRACT

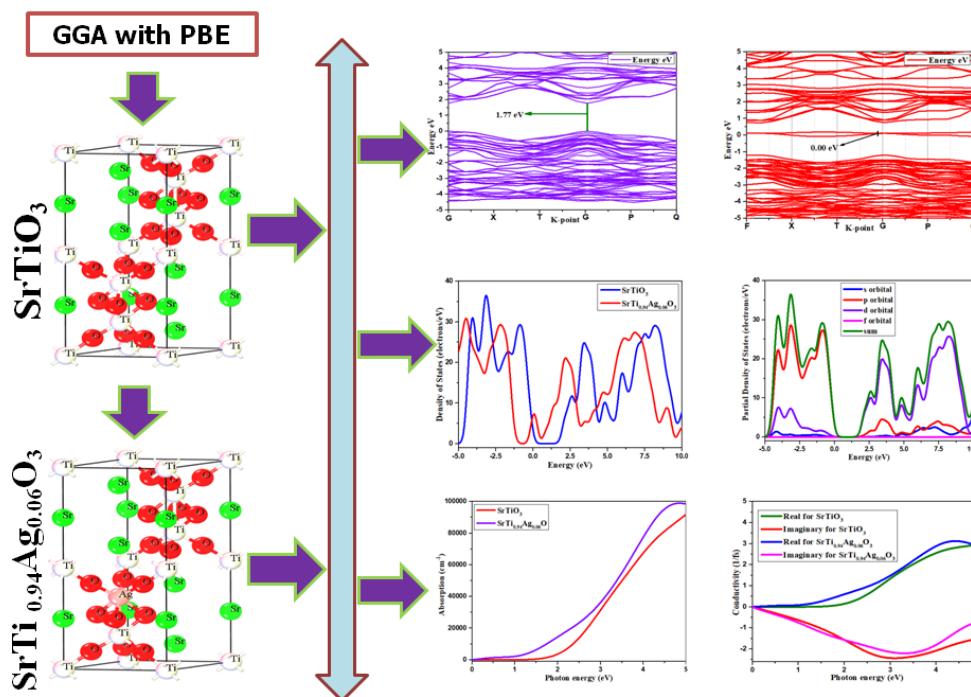
Due to the legitimate crystal size of SrTiO_3 , in this work, a synthesized compound was introduced and structurally characterized as the quantum dots. The crystal of SrTiO_3 was designed using computational tools. There is no obtainable information for hypothetical and conceptual studies, and computational studies. First, using the CASTAP code from material studio 8.0 the structural geometry was optimized using the generalized gradient approximation (GGA) with the hybrid functional, Perdew-Burke-Ernzerhof (PBE) to calculate the electronic structure, geometry, and optical properties for the SrTiO_3 . The crystal size of the optimized structure was 2.0 nm for both SrTiO_3 and $\text{SrTi}_{0.94}\text{Ag}_{0.06}\text{O}_3$, which stays in quantum dots. With the help of GGA with PBE, the band gap was recorded at 1.77 eV, and for evaluating the nature of 5s, 4p, and 3d orbitals for a Sr atom, 4s, 3p and 3d orbitals for Ti atom, 5s, 4p, and 4d orbitals for Ag atom and 2s, and 2p orbitals for O atom for SrTiO_3 are obtained. Density of state(DOS) and the partial Density of state(PDOS) of $\text{SrTi}_{0.94}\text{Ag}_{0.06}\text{O}_3$ were replicated. The optical properties, like absorption, reflection, refractive index, and conductivity, were replicated, dielectric function and loss function was computed. By replacing the Ti atom on SrTiO_3 6% Ag atom was doped to elaborate the demeanor nature, and because of this 0.00 eV band gap was obtained having a molecular formula by $\text{SrTi}_{0.94}\text{Ag}_{0.06}\text{O}_3$, as well as the optical conductivity and optical absorption was soared compared with parent SrTiO_3 .

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GRAPHICAL ABSTRACT



Introduction

During this digital era, a wide technological advancement in electronics is increasing, like the speed of light. This field of electronics is much more dependent on semiconductor materials because most of the applications used in these fields, such as IC, LCD/LED, BJT, MOSFET, transistor, resistor, photovoltaic solar power are quite impossible to make without semiconductor materials [1-3]. It is also an essential fact that for the development of the national economy and national security, every country uses high-speed computing, large-capacity data communication, storage, processing, electronic devices, which also depend on a larger scale on semiconductors [4-6]. The conventional semiconductor materials used in electronics are changing every single second. For example, the quantum dots are replacing the conventional narrow and wide band gap semiconductor materials whose range is recorded by many researchers and scientists in

between 1.8 to 4.0 eV [7,8]. Quantum dots are semiconductor particles having a few nanometer sizes. For example, SrTiO_3 , also known as strontium titanate, has less than 1.8 eV band gap and at room temperature and low electric field, a very large dielectric constant (300) [9,10]. Due to this a low band gap and a large dielectric constant value, it can store more charge, and that is why it has a wide range of uses, such as high-voltage capacitors, voltage-dependent resistors, optical instruments, jewelry stone, advanced ceramics, and substrates for superconductors [11,12].

However, the commercialization of DSSCs gets notably dragged due to the areal cost and bustling synthesis procedures of organic dyes and limited quantum efficiency. On the other hand, quantum dots (QDs) are considered excellent light harvesters to substitute organic dyes in these macroscopic solar cells due to their tunable band gaps, light-response ranges, scalable materials, and cost-effectiveness.

Narrow band gap semiconductors are a class of Quantum dots that have benefits like tunable band gaps due to the quantum confinement result [13], higher absorption coefficients than most organic dyes [14,15], and various exactions generation have more [16,17]. For macroscopic solar cells QDs have been analyzed to serve as light absorbers, such as CdS, CdSe, PbS, PbSe and integrated CdS/CdSe, CdS/PbS, CuInS₂/CdS, CuInS₂/In₂S₃, CdSe/CdTe, CdSe/GO, etc [18], inverter [5], Double Perovskites [19,20]. However, these materials are always restricted due to their intrinsic band gaps. Due to negligible toxicity, easy formulation, scalable materials, and performances, a class of lead-free perovskite-structured Quantum Dots has been highlighted nowadays [21,22]. The reduction of band gap using the doping process can make SrTiO₃ more efficient quantum dots, and this investigation is based on the same principle.

In this investigation, the band gap was determined using computational tools, which supports less time and cost than experiments and compares the calculated band gap to the experiment value for its validation [23-30]. Additionally, to develop and enhance its activity, Ag was doped on SrTiO₃ because Ag increases electron density, doping power, and decreases band gap by overlapping with the orbital of the materials and enhances quantum dots efficiency [24,31-34].

As quantum dots, there are not enormous studies on SrTi_{0.94}Ag_{0.06}O₃. For this view, the main goal of this study is to investigate the effect of Ag-doped replacing Ti atom on the SrTiO₃ compound, and its molecular formula becomes SrTi_{0.94}Ag_{0.06}O₃ after 6% Ag doping. As a result, these properties, which have been derived from simulation after doping, have significant intensive attention for potential applications. For using the SrTiO₃, this study supports to development of the theoretical concept using the first principle study and opens a new window for potential application by Ag doping in SrTiO₃.

Computational Methods

With instigating, before energy calculation, the geometrical optimization was acquired where the convergence criterion for the force between atoms was 3×10^{-6} eV/Å, and the maximum displacement, the total energy, and the maximal stress were at 1×10^{-3} Å, 1×10^{-5} eV/atom and 5×10^{-2} GPa, respectively. After geometrical stability of the configuration, using the GGA with PBE functional from CASTEP code of the material studio version 8.0, the electronic band structure, the total density of state (TDOS), and partial density of state (PDOS) were computed [35].

The main reason is the most viable and acceptable method for computing the electronic structure and optical properties [31-33, 36, 37]. Using this condition and keeping the cut off at 500 eV, and k point at $2 \times 2 \times 2$ with norm-conserving pseudopotentials, the band structure, density of state, and Generalized Gradient Approximation (GGA) with Perdew-Burke-Ernzerhof (PBE) [38] functional of SrTiO₃ and SrTi_{0.94}Ag_{0.06}O₃ for the comparative study of band gaps were calculated and after that the optical properties like refractive index, reflectivity, absorption, conductivity, and loss function, were similarly simulated for computation.

Results and Discussions

Geometry of optimized structure

The lattice parameters value was computed for the crystals after the geometry optimization. Here, $a = 5.629$ Å, $b = 5.629$ Å and $c = 13.886$ Å while angles among them as $\alpha = 90.00^\circ$, $\beta = 90.00^\circ$, and $\gamma = 120.00^\circ$. It is a monoclinic SrTiO₃ crystal, and the space group is Hermann Mauguin P63/mmc [194], triclinic crystal system, point group 6/mmm, hall-P 6c 2c, density 4.80 g/cm³ shown in Figure 1a. The Ag atom doping in optimized structures are accounted for in Figure 1b.

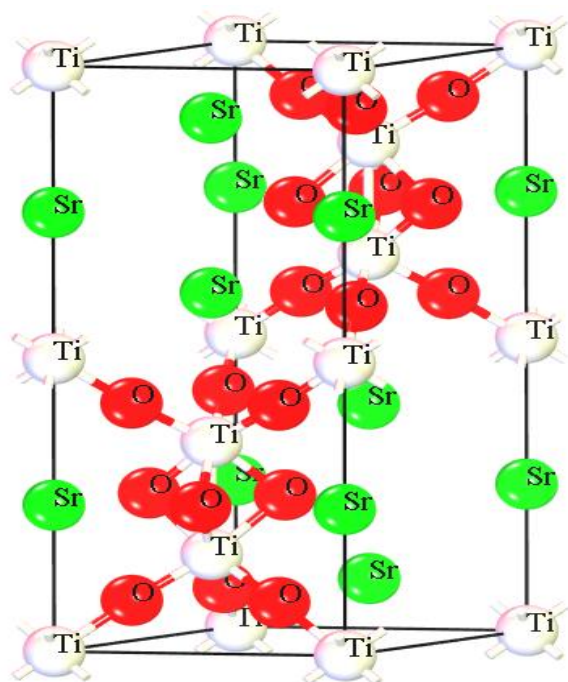


Figure 1a. Structure for SrTiO_3

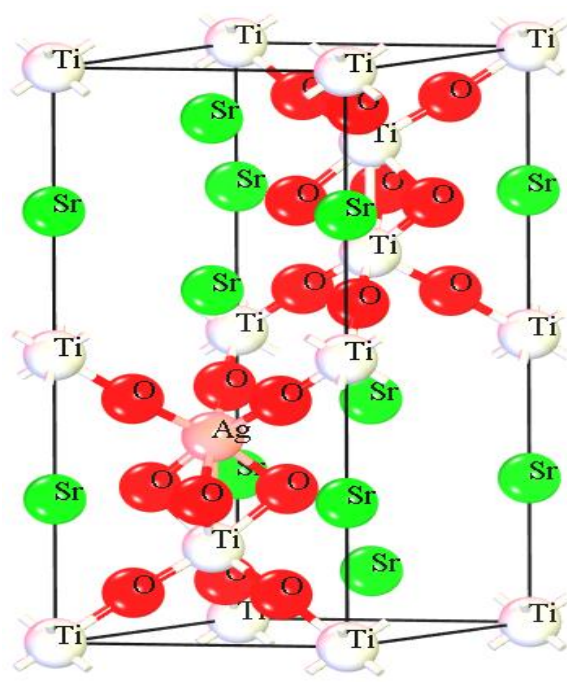


Figure 1b. Structure for $\text{SrTi}_{0.94}\text{Ag}_{0.06}\text{O}_3$

Electronic band structure

The Fermi energy level is situated at zero energy level to determine the electronic band structure of SrTiO_3 and $\text{SrTi}_{0.94}\text{Ag}_{0.06}\text{O}_3$. From Figure 2a for SrTiO_3 quantum dots, the minimum of conduction (MCB) is obtained at the G symmetry point, whereas the maximum of valance bands (MVB) is also found at G symmetry points. A direct band gap is calculated with a value of 1.77 eV. The main key point of this research was noted that the band gap of SrTiO_3

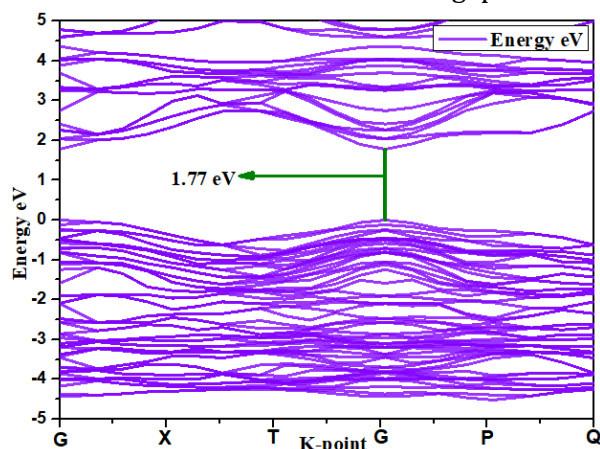


Figure 2a. Electronic structure for SrTiO_3

has been reduced, and it becomes more effective quantum dots when the Ag has doped by 6%. The reason is that Ag atom can enhance the electron density in both areas of valance band and conduction band besides d and p orbitals of Ag atom have quickly overlapped with the p and d orbitals with Sr and Ti metals for quickly transferring the hole electrons. That is why the minimum portion of Ag by 6% was doped in SrTiO_3 and illustrated the effect on the band structure. The band gap was recorded at the G sy-

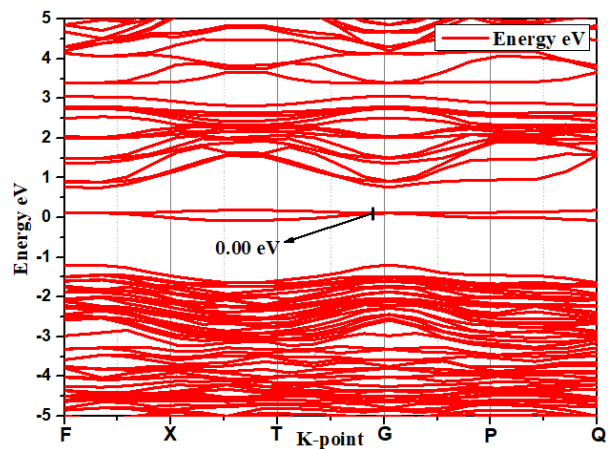


Figure 2b. Electronic structure for $\text{SrTi}_{0.94}\text{Ag}_{0.06}\text{O}_3$

-mmetry point for both MCB and MVB after doping, showing a direct band gap by 0.00 eV, which stands for that Ag atom has a high capacity on SrTiO_3 to reduce the band gap and make it more efficient quantum dots.

The Density of states (DOS) and Partial density of state (PDOS)

The splitting of an orbital and the position of the electronic band structures are designated by a parameter known as the DOS. For calculating the

DOS of Sr, Ti, Ag, and O atoms for SrTiO_3 and $\text{SrTi}_{0.94}\text{Ag}_{0.06}\text{O}_3$ crystals, the GGA with PBE method was executed. From the Figure 3b to 3c, the sum of DOS for SrTiO_3 and $\text{SrTi}_{0.94}\text{Ag}_{0.06}\text{O}_3$ crystals consists of 5s, 4p, and 3d orbitals for a Sr atom, 4s, 3p and 3d orbitals for Ti atom, and 5s, 4p, and 4d orbitals for Ag atom and 2s and 2p orbitals for O atom. Figure 3d to Figure 3f demonstrated that comparison s, p and d orbitals for SrTiO_3 and $\text{SrTi}_{0.94}\text{Ag}_{0.06}\text{O}_3$ and the comparison study focus that s, p, and d orbital of $\text{SrTi}_{0.94}\text{Ag}_{0.06}\text{O}_3$ higher than SrTiO_3 .

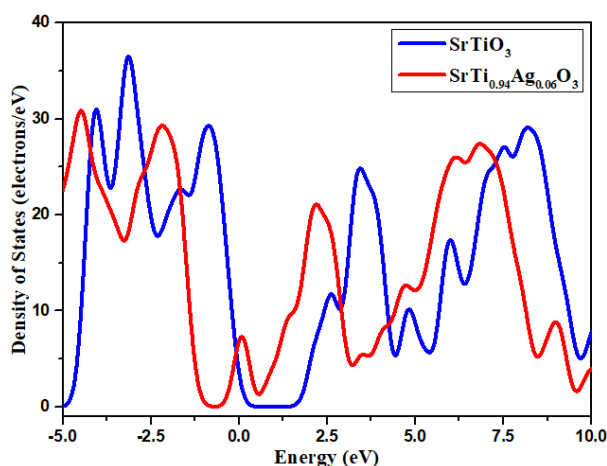


Figure 3a. Total density of states for SrTiO_3 and $\text{SrTi}_{0.94}\text{Ag}_{0.06}\text{O}_3$

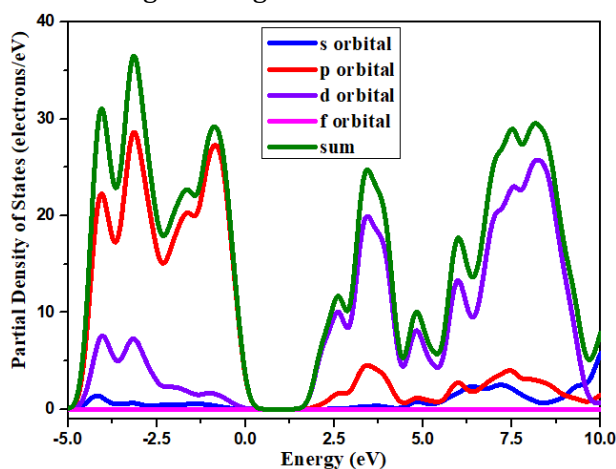


Figure 3b. Partial Total density of states for SrTiO_3

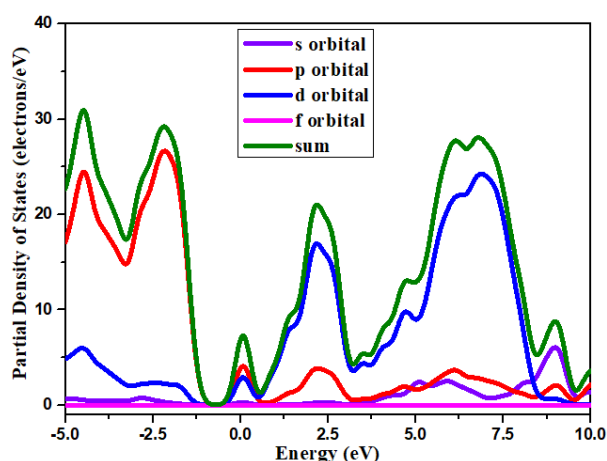


Figure 3c. Partial Total density of states for $\text{SrTi}_{0.94}\text{Ag}_{0.06}\text{O}_3$

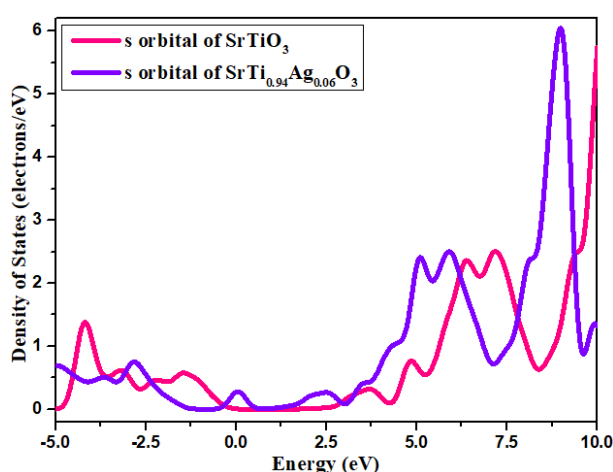


Figure 3d. Comparison s orbital for SrTiO_3 and $\text{SrTi}_{0.94}\text{Ag}_{0.06}\text{O}_3$

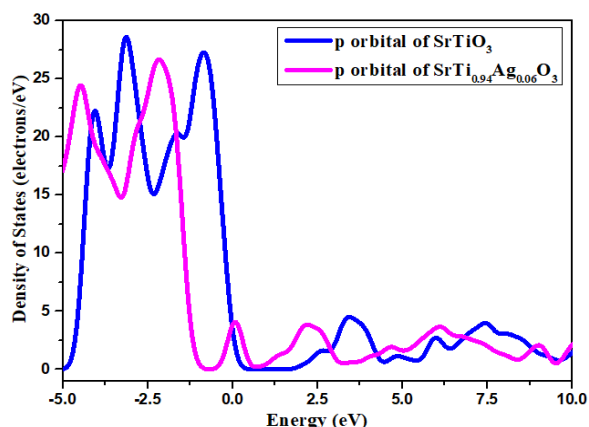


Figure 3e. Comparison p orbital for SrTiO_3 and $\text{SrTi}_{0.94}\text{Ag}_{0.06}\text{O}_3$

Secondly, the DOS of $\text{SrTi}_{0.94}\text{Ag}_{0.06}\text{O}_3$ in the conduction band is almost more significant than the DOS of SrTiO_3 at 0.2 eV to 2.5 eV. The DOS of the valance band is found at -0.1 to -5.0 electron/eV, while the DOS of the conduction band is recorded at about 30 electron/eV. To compare the s, p, and d orbitals for both doping and undoped, the orbitals for $\text{SrTi}_{0.94}\text{Ag}_{0.06}\text{O}_3$ are much higher than SrTiO_3 , and it can be said that the Ag doping on SrTiO_3 has increased the DOS of any crystal showing in figures 3a, 3b, 3c, 3d, 3e, and 3f.

Optical Properties

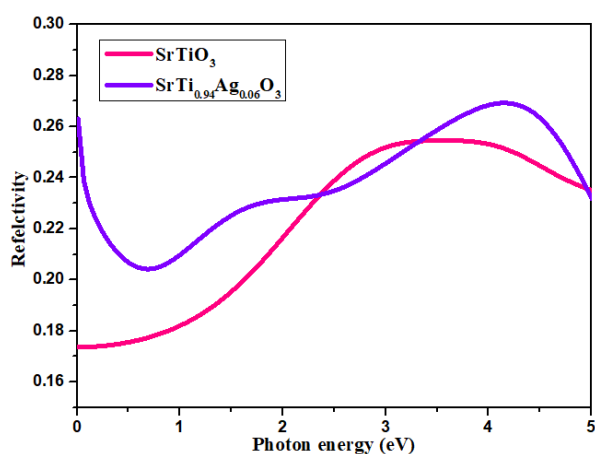


Figure 4. Reflectivity

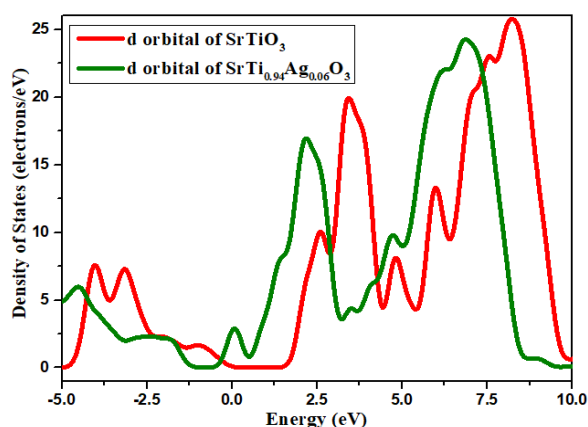


Figure 3f. Comparison d orbital for SrTiO_3 and $\text{SrTi}_{0.94}\text{Ag}_{0.06}\text{O}_3$

Reflectivity

Reflectivity is the measurement of reflected light from the surface area of the material relative to the amount of light incident on the material. In this investigation, the reflectivity of SrTiO_3 and $\text{SrTi}_{0.94}\text{Ag}_{0.06}\text{O}_3$ is demonstrated in Figure 04. The initial reflectivity of SrTiO_3 was recorded at 0.17, and with the increase of energy, it increases. Less reflectivity means more efficient quantum dots. After doping Ag, the initial reflectivity was recorded at 0.27, which decreased with the increase of energy and proved $\text{SrTi}_{0.94}\text{Ag}_{0.06}\text{O}_3$ more efficient quantum dots.

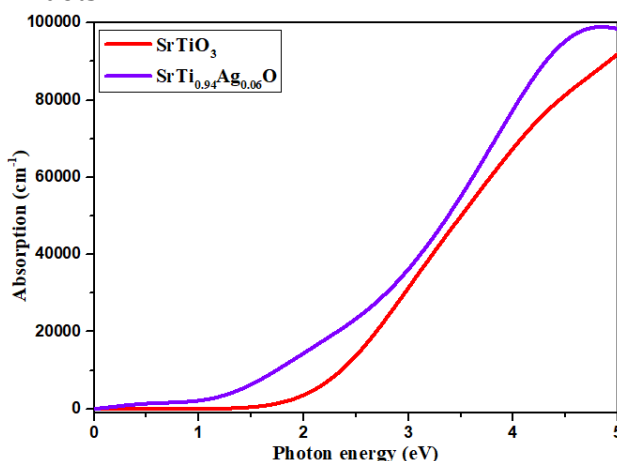


Figure 5. Absorption

Absorption

The absorption spectrum of a material depends on the nature of the energy band gap, which pursues the indirect band gap usually absorbs more temperature than the direct band gap semiconductor. The absorption spectrum of $\text{SrTi}_{0.94}\text{Ag}_{0.06}\text{O}_3$ is less than SrTiO_3 . With the increase of energy, the absorption of both materials SrTiO_3 and $\text{SrTi}_{0.94}\text{Ag}_{0.06}\text{O}_3$ increases. However, the $\text{SrTi}_{0.94}\text{Ag}_{0.06}\text{O}_3$ revealed a better value of absorption than SrTiO_3 , as demonstrated in Figure 5.

Refractive Index

The optical and electronic properties of a material depend on physical parameters like

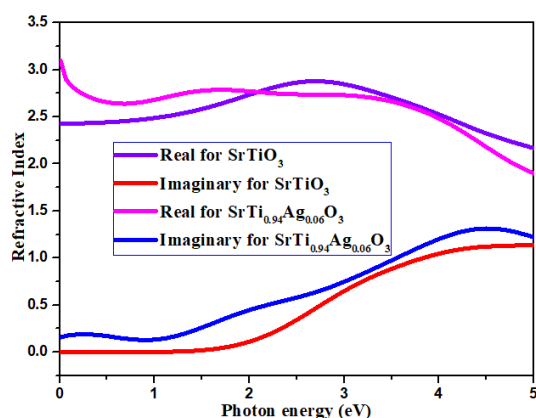


Figure 6. Refractive Index

Dielectric Function

The dielectric functions are calculated in the linear optical response regime within the electric dipole approximation. The required momentum matrix elements are obtained by using the calculated wave functions from our empirical pseudo potentials. Dielectric functions that describe the materials at the Nanoscale are needed, opening the way to interpret experimental data and design of the composites to obtain desired optical behavior. Despite the great interest in the research on NPs, there is

refractive index and energy band gap. These properties describe the nature of the applications of semiconductors, electronic, optical, and optoelectronic devices. The band gap engineered structures for continuous and optimal absorption of broad band spectral sources are also dependent on these properties. The real part and imaginary part of the refractive index of the SrTiO_3 and $\text{SrTi}_{0.94}\text{Ag}_{0.06}\text{O}_3$ are shown in Figure 6, which is an inverse pattern.

The refractive index is higher for a real part at the primary point of photon energy at that time, the imaginary part showed a value almost close to 1 eV. Afterwards, they follow a constant pattern with slightly different refractive index values. It is the same for both undoped and doped.

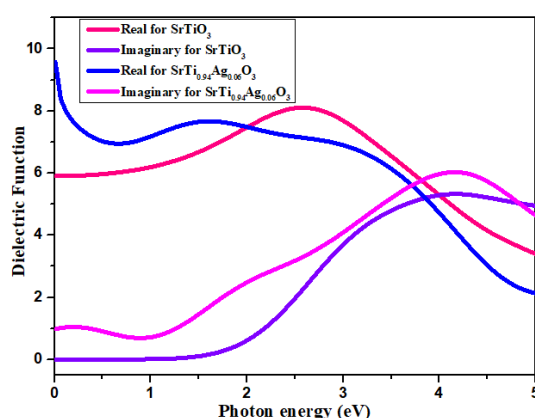


Figure 7. Dielectric Function

presently no available information about the dielectric functions of nano-sized semiconductors that could be readily used for macroscopic modeling applications. The dielectric function is an essential tool to investigate their optical properties, which is related to adsorption properties as the following equation for solid.

$$\varepsilon = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$$

Here, $\varepsilon_1(\omega)$, and $\varepsilon_2(\omega)$ denotes the dielectric constant (real part) and the dielectric loss factor (imaginary part). The probability of photon

absorption for the band structure of any material is closely related to the imaginary portion of the dielectric function. The real part of the dielectric constant maintained the energy storage potential in the electric field, while the imaginary segment indicates the opposite even for electric potential energy. From Figure 7, the actual portion is always higher than the imaginary part within the energy at 1.0 eV to 1.8 eV, but the energy range from 2 eV to 4 eV. The imaginary part shows a higher value than real portion for SrTiO_3 and $\text{SrTi}_{0.94}\text{Ag}_{0.06}\text{O}_3$.

Conductivity

The conductivity can be explained in terms of band gap. The electronic conduction is nothing but putting an electron in the conduction band by giving enough energy to electron and shining the material with light. This process can be accomplished. In a solid-state language, by

creating a hole in the valence band the electron can go to conduction band with the help of photon energy. After that, an electrical conduction will occur due to free electrons and holes.

Figure 8 depicts the comparative study of the conductivity value of SrTiO_3 and $\text{SrTi}_{0.94}\text{Ag}_{0.06}\text{O}_3$ crystals. The conductivity values of both real and imaginary parts start from almost zero at 0.0 eV. The real part of conductivity increased with a similar trend for SrTiO_3 and $\text{SrTi}_{0.94}\text{Ag}_{0.06}\text{O}_3$ in the energy range from 0 eV to 5 eV and reached conductivity real peaked value 2.8 and 3.0. However, the conductivity value of $\text{SrTi}_{0.94}\text{Ag}_{0.06}\text{O}_3$ within energy range 1 to 3 eV is higher than SrTiO_3 . On the other hand, the imaginary part values of SrTiO_3 and $\text{SrTi}_{0.94}\text{Ag}_{0.06}\text{O}_3$ declined gradually after Fermi energy in the energy range from 3 eV and reached conductivity imaginary peaked values-2.1 and -2.5.

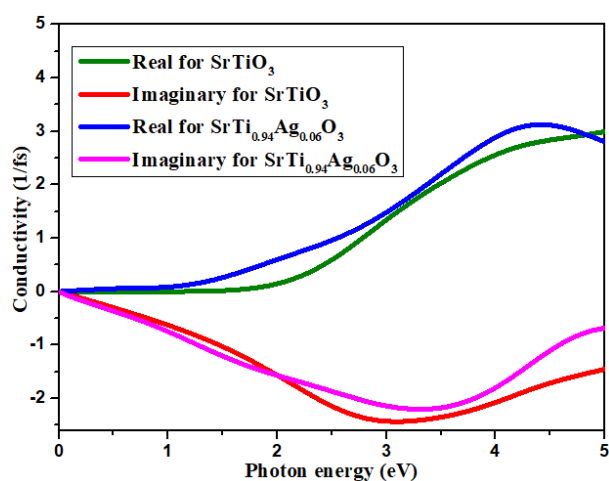


Figure 8. Conductivity

Loss function

The loss function is a crucial part of optical properties, which is composed of two regions of photon energy parts such as the lower photon energy part and higher photon energy part for crystal materials. The energy loss function is closely related to the dielectric function of the

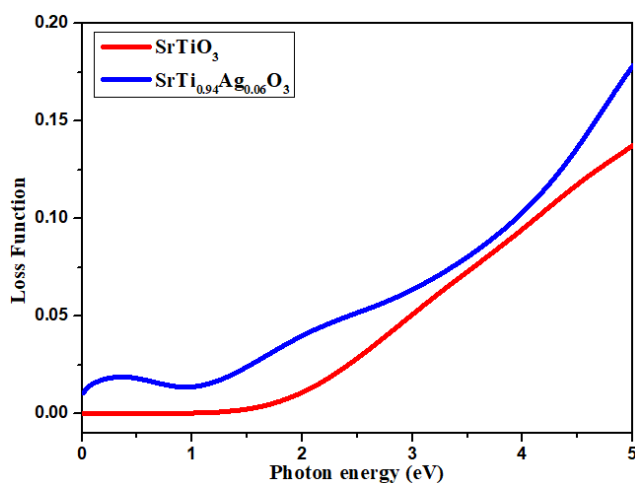


Figure 9. Loss Function

photocatalyst materials within the range of the dielectric theory validation. In the energy loss, function dielectric function reflects the response of a semiconductor to an external electromagnetic perturbation. The calculated exploration of loss function values for SrTiO_3 and $\text{SrTi}_{0.94}\text{Ag}_{0.06}\text{O}_3$ illustrates in figure 9. It can be

seen that the loss function of $\text{SrTi}_{0.94}\text{Ag}_{0.06}\text{O}_3$ is higher than $\text{SrTi}_{0.94}\text{Ag}_{0.06}\text{O}_3$.

Conclusion

To sum up, the electronic, structural, and optical properties of hexagonal SrTiO_3 and $\text{SrTi}_{0.94}\text{Ag}_{0.06}\text{O}_3$ quantum dots based semiconductor was studied for the first time using the Density functional theory (DFT) by the first principle approach. First of all, the band gap of SrTiO_3 has been recorded by 1.77 eV as supporting a semiconductor that has been filled up the lack of literacy about band gap and electronic structure for SrTiO_3 of a theoretical result. The superior outcome of this study was obtained by Ag atom doping effect on electronic structure, especially band gap, DOS, PDOS, and optical properties. After Ag doping by 6% in SrTiO_3 , the band gap has shifted to 0.00 eV, acting as no resistance materials for optoelectronic devices, which has justified the PDOS and DOS diagram for delocalization of electrons. Secondly, the optical properties due to Ag doping have changed. The optical absorption, reflectivity, loss function, and conductivity of doped SrTiO_3 are greater than undoped SrTiO_3 , but the real part of the dielectric function is lower than undoped. Finally, it can be said that the 6% Ag doping in SrTiO_3 is almost acted as a superconductor for a wide band gap QDs materials.

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Disclosure statement

No potential conflict of interest was reported by the authors.

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