First principles study on copper and iridium co-doped SrTiO_3 for shifting the optical absorption into visible region

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Abstract

Density functional theory (DFT) investigation is performed to observe the opto-electronic properties of iridium and copper co-doped structure of Pristine SrTiO_3 (Cubic Perovskite). Results suggest that copper and iridium co-doped structure of SrTiO_3 has significant absorption in visible region of the spectrum, which is a result of red shift phenomenon in the wavelength range 400–750 nm observed in this structure. However, in individual copper and iridium structures the optical absorption is mainly in ultraviolet (UV) region which limits its use in light-based devices and applications. The shift in absorption from UV to visible region in the co-doped structure extracts the maximum utilization of solar light and finds wide range of optical applications like solar cells. Refractive index and dielectric constants were also calculated and their peak values were found to be in correlation with the peaks in absorption spectrum.

Keywords Perovskite · Optical absorption · SrTiO_3 · Visible region · Co-doped structure · Photo catalysis

1 Introduction

The perovskite materials came to light as the most favorable and structured compound with minimal cost energy that finds extensive applications in opto-electronics as well as photonic devices [1, 2]. A general perovskite structure has general composition formula in the form of ABX_3 , where A and B serve as cations in which basically A is a Group I or Group II element, B can be a transition metal and X serves as anion, for example halides (like chlorine, bromine, iodine) or oxides [3]. The distinctive electronic properties of perovskite such as large absorption coefficient, high dielectric constant, less non-radiative emission made them interesting materials for photo voltaic cells [4–6], active photo catalysts [7] and Nano lasers. The ground work in perovskite compounds has attained an expeditious development such that the photo conversion efficiency based on perovskite compounds has progressed from 3.7% to 22% within a span of 5 years. The efficiency

in performance and stability of the photodevice [8, 9] can still be improved with proper conception of the perovskites. The key limitations for enhancing the performance are the building up of defect states formed by doping of transition metals replacing cations or anions. One of such limitations is formation of oxygen deficiency [10] resulting in high defect formation energy. However, the peculiar optical properties had set up their applications in prominent scale even with the existing limitations.

Strontium titanate (SrTiO_3) has a perovskite structure which is a mineral containing strontium, titanium and oxygen in the form of ternary oxide [11]. SrTiO_3 has wider energy gap of about 3.2 eV and hence classified under insulator type of compound. Due to this wide bandgap, absorption spectrum of SrTiO_3 has peaks mainly in UV region with wavelength less than 386 nm and almost negligible amount of absorption is present in the visible region [12]. The lower absorption in visible region results in wastage of available natural sunlight since it is absorbing

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less than 3% of available solar energy. The research issue with SrTiO_3 is to either enhance the absorption in visible region or shift its absorption spectrum from UV region to visible region for utilizing the abundantly available solar energy. Doping SrTiO_3 with other suitable materials have been suggested in [13–40] to tune the optical absorption and other electronic properties.

The photocatalytic capacities of SrTiO_3 are enhanced by depletion of anion (X) or by impurity doping [14, 15] at the cation sites (A or B) such as chromium, boron, nitrogen or iridium. These dopants are certain to change electronic properties which inevitably affect the optical properties which is the basic prerequisite for the accomplishment of photo voltaic devices or process of photo catalysis [16]. Investigations on SrTiO_3 doped with silver have shown that there are isolated traps in the energy band gap [17]. In lead doped SrTiO_3 [18, 19] the valence band switches to high energies that leads to lowering of the energy gap. It is revealed in recent times that chromium (Cr) [20–24] doping at the cation site makes the absorption peaks to lie in the visible region at around 440 nm, with negligible absorption in the higher wavelengths resulting in lesser power dissipation. In past, investigations on TiO_2 doped with nitrogen [25–27] have suggested better absorption efficiency in the desired region of light spectrum, and the efficiency was also seen to improve in direct proportion to the nitrogen doping percentage in the compound [28–30]. Recent studies demonstrated that co-doping sulphur and carbon [31–36] in SrTiO_3 improves photo catalysis in visible region.

Doping of metal ions [37] is a method used to decrease the bandgap and makes SrTiO_3 respond to visible region. This reduction in bandgap is because of traps formed in the forbidden energy gap which acts like impurities and resonates with bottom of conduction band or top of valence band. Doping SrTiO_3 with Cu results in bandgap reduction and also the nature of bandgap changes from indirect to direct. Doping of carbon (C), fluorine (F), phosphorus (P), sulphur (S) and boron (B) at the titanium (Ti) site in SrTiO_3 results in reduction of the energy gap and aids photo catalysis. Doping with elements such as chromium (Cr), manganese (Mn), ruthenium (Ru), rhodium (Rh) and palladium (Pa) [38–42] enhances absorption in visible region but cannot act as effective catalyst in splitting polluted water. Hence, it is envisaged that photo catalysis and absorption in visible region can both be achieved together by co-doping of elements like C, F, P, S and B that provide stability in photo catalysis and elements like Cr, Mn, Ru, Rh, Pa that enhance the photo catalysis efficiency.

It is therefore, of interest to investigate the tuning/shifting of absorption spectrum of SrTiO_3 into the visible region by co-doping it with impurities that can provide stability in photocatalysis and that can also enhance the photo

catalysis efficiency. In this study, the shifting and enhancement of absorption in SrTiO_3 is investigated by co-doping it with transition metal elements like Ir and Cu. The results of this study are based on First principle calculations using density functional theory (DFT) formulations for extracting the band structure and optical properties of SrTiO_3 .

2 Computational details

Atomistix tool kit which relies on DFT is used for carrying out the band structure and optical simulations. Generalized gradient approximation (GGA) [43–46] with Perdew–Burke–Ernzerhofer is used in the calculation of band structure to represent the exchange correlation energy. This method of computation using DFT [47–52] will determine the wave functions and energy states allowed using the time dependent Schrodinger wave equation.

The co-doping should be such that the defect formation energy is small and does not affect the stability of SrTiO_3 . For example, when an oxygen atom is replaced with any type of dopant there will be oxygen deficiency and would result in high defect formation energy because of difference in bond lengths with the doped atom and oxygen atom. This difference in bond lengths is because of difference in atomic sizes of oxygen and dopant.

Copper doping at the strontium site in the SrTiO_3 structure results in smaller defect formation energy in comparison to doping at Ti or O site [53]. Ir doping at the titanium site aids in H_2 evolution which improves the efficiency as catalyst in the decomposition of polluted water [54]. Doped structures of SrTiO_3 are optimized using LBFGS algorithm for relaxing the atomic structure to the extent where forces on each atom are not more than $0.005 \text{ eV}/\text{\AA}$. Monkhorst-Pack scheme is involved for Brillouin zone k-point sampling of $7 \times 7 \times 7$ grid in all three directions with the mesh cut-off energy maintained at 150 Ry. SrTiO_3 is invoked in the form of cubic structure that comes under the space group of Pm-3m [55]. In the cubic structure, strontium atoms are at the corners of the cube, titanium atoms are located at the body center and three oxygen atoms at the face centers.

In this study, cubic structure of SrTiO_3 with lattice constant of ideal value $a=b=c=0.3905 \text{ nm}$ is considered [56]. For our calculations we considered a $2 \times 2 \times 2$ super cell to avoid boundary effects with total 40 number of atoms in the supercell. For obtaining a copper doped SrTiO_3 structure a Sr atom of the supercell is substituted with Cu atom and the structure is then relaxed. Since the difference in atomic radius of Cu (0.128 nm) with Sr (0.113 nm) [55] is smaller in comparison with Ti and O, this would result in reduced defect formations for doping copper at Sr site than doping at Ti or O site. Similarly, Ir doping at Ti site is more effective.

The co-doped structures of SrTiO₃ with Cu and Ir are thus obtained by replacing Sr and Ti atoms, respectively.

Optical properties are calculated using MGGA with a k-point sampling of 3 × 3 × 3 in Brillouin zone grid. Broadening is set to 0.1 eV and stress tolerance to 0.1 GPa.

The refractive index (η) relation with relative dielectric constant, real and imaginary parts (ϵ_1 and ϵ_2) is shown in the below equations

$$\eta + i\kappa = \sqrt{\epsilon_r} \quad (1)$$

where κ is the extinction coefficient.

Susceptibility using the Kubo-Greenwood formula is given by:

$$\chi_{ij}(\omega) = -\frac{e^2 \hbar^4}{\epsilon_0 m^2 \omega^2 V} \sum_{nm} \frac{f(E_m) - f(E_n)}{E_{nm} - \hbar\omega - i\Gamma} \pi_{nm}^i \pi_{mn}^j \quad (2)$$

where π_{nm}^i is the i th component of dipole matrix element between state n and m , V is the volume, Γ the broadening and f is the fermi function.

Optical properties like relative dielectric constant ' ϵ_r ', polarizability ' α ', and optical conductivity ' σ ', are related to susceptibility as below [57]:

$$\epsilon_r = (1 + \chi(\omega))$$

$$\alpha(\omega) = V\epsilon_0\chi(\omega)$$

$$\sigma(\omega) = -img(\omega\epsilon_0\chi(\omega))$$

$$\eta = \sqrt{\frac{\sqrt{\epsilon_1^2 + \epsilon_2^2} + \epsilon_1}{2}} \quad \kappa = \sqrt{\frac{\sqrt{\epsilon_1^2 + \epsilon_2^2} - \epsilon_1}{2}} \quad (3)$$

Optical absorption coefficient is extracted from extinction coefficient by [58, 59]

$$\alpha_a = 2\frac{\omega}{c}\kappa \quad (4)$$

3 Results and discussion

3.1 Geometric structure

Pristine SrTiO₃ in its cubic form has bond length between Sr–O as 2.755 Å and Ti–O as 1.945 Å. Geometry optimizations are performed on doped structures of SrTiO₃ for accuracy in calculations. The optimized structures are shown in Fig. 1.

At first, pure SrTiO₃ structure is optimized and it is observed that the lattice constant of cubic structure does not deviate much from the ideal value of 0.3905 nm [55]. Similar process is applied to doped structures which obviously deviate from their pristine form because of the difference in electronegativity [60]. The formation energy (E_f) provides the information about how easy dopants Cu and Ir immerse into the host. The special crystal structure in Fig. 1c seems more distorted than conventional perovskite structure as two of its atoms are replaced and volume of the structure also increases

Fig. 1 Optimized structures of (a) copper doped SrTiO₃, (b) iridium doped SrTiO₃, and (c) copper and iridium co-doped SrTiO₃

slightly, and hence Vander wall forces will be disturbed. Geometry optimizations were performed on all the three structures so as to minimize forces on each atom to be lesser than $0.005 \text{ eV/\AA}$. However, because of the Cu and Ir doping, volume of the structure increases slightly as the radius of dopants copper and iridium is a bit larger than the host strontium and titanium atoms, which indirectly changes the bond lengths. If the impurity ions can be embedded into the system with less effort, proportionally less will be the defect formation energy.

3.2 Electronic structure

The band structure gives the information about the possible filled states that electrons can occupy and energy gap can be computed by taking the difference of maxima of valence band (VB) and minima of conduction band (CB). For Pristine SrTiO_3 the results agree with the indirect band gap nature as the valence band maximum lie at R point and conduction band minimum lie at the Γ point in the band structure with the band gap value of 1.807 eV and with direct bandgap of 2.167 eV at the gamma (Γ). These theoretically calculated values of bandgaps are in confirmation with [51]. However, the experimental value of bandgap of $\sim 3.12 \text{ eV}$ [15] is comparatively larger than the calculated theoretical value, which is due to the well know p-d repulsion between cation and anion within the GGA approximation. This dominance of indirect nature results in wastage of the incident photon energy as the electrons jumping from VB to CB will result in loss of energy with dissipation of heat.

In case of Cu doped SrTiO_3 both the VB maximum and CB minimum lie at the Γ point and valence band is shifted upward resulting in direct bandgap (see Fig. 2b). This upward shift in the VB results in reducing bandgap, which leads to red-shift of the absorption peak (see Fig. 4d). The direct bandgap results in enhanced optical activity and photocatalysis process as the radiative recombination of electron and hole results in desired energy output rather than dissipating heat. Ir doped SrTiO_3 results in formation of impurity levels in the wide energy bandgap of pristine SrTiO_3 resulting in lowering of bandgap which is approximately 0.954 eV as shown in Fig. 2c. The co-doped structures of SrTiO_3 with Cu and Ir that has combined effect of both materials result in further lowering of bandgap with the absorption peak shifting entirely into the visible region (see Fig. 4h) and thus making efficient utilization of solar energy. This co-doping results in a direct bandgap of 0.181 eV (see Fig. 2d) with high optical conductivity that makes the co-doped structure more efficient for optical devices and photocatalytic applications.

Fig. 2 Band structures of (a) pristine SrTiO_3 , (b) copper doped SrTiO_3 , (c) iridium doped SrTiO_3 , and (d) copper and iridium co-doped SrTiO_3

3.3 Optical properties

Optical properties namely dielectric function, refractive index (η) and absorption coefficient with respect to energy and wavelength have been calculated for all the structures. These optical properties describe the mechanism with which light interacts with the system. The optical properties of pristine SrTiO_3 and its doped structures are calculated and compared to see the changes in the absorption in the visible region. Dielectric function which is complex in nature can provide information about the remaining parameters like absorption, refractive index and extinction coefficient (see Eqs. 1 and 2) [54, 55]. Real part of dielectric function signifies the amount of polarization and imaginary part corresponds to energy absorption within the structure.

Dielectric functions (both real and imaginary parts) with respect to energy along xx, yy and zz tensors are shown in the Fig. 3. Since energy dissipation within system (indirectly absorption) is of interest in the photonic applications, we emphasize only on the imaginary part (ϵ_2) of the dielectric function as the absorption coefficient has a major contribution from imaginary component with insignificant contribution from the real component of dielectric function (see Eqs. 1 and 2).

For pristine SrTiO_3 there is almost negligible dissipation (absorption) in the energy range $0\text{--}3.5 \text{ eV}$, which also signifies the existence of bandgap (see Fig. 4a). The absorption is seen to increase significantly in the energy range

Fig. 3 Complex dielectric function with real and imaginary parts with respect to energy for **(a, b)** pristine SrTiO₃, **(c, d)** copper doped SrTiO₃, **(e, f)** iridium doped SrTiO₃, **(g, h)** copper and iridium co-doped SrTiO₃ along xx, yy and zz tensors, respectively

3.5–5 eV and the absorption spectrum completely lies in the UV region with wavelength $\lambda < 380$ nm (see Fig. 4b). In case of Cu doped structure that has a smaller bandgap than pristine structure, absorption is seen to increase a little earlier at 3 eV in the energy range 3–5 eV (see Fig. 4c) and the absorption peaks have shifted a little into the visible region (see Fig. 4d). Iridium doped structure that has further smaller bandgap than pristine and Cu doped structure, absorption is seen to start much earlier at 1.8 eV (see Fig. 4e) in the energy range (1.8–5 eV), also shifting

Fig. 4 Absorption coefficient in response to energy and wavelength for **(a, b)** pristine SrTiO₃, **(c, d)** copper doped SrTiO₃, **(e, f)** iridium doped SrTiO₃, **(g, h)** copper and iridium doped SrTiO₃ along xx, yy and zz tensors, respectively

in absorption peak towards visible region with new peaks originating in the visible region can also be observed (see Fig. 4f). In Cu and Ir co-doped structure where further reduction in bandgap to insignificant values was observed, absorption is seen to be significant in the entire energy range (see Fig. 4g). Strong red-shift is observed in the co-doped structure with absorption peaks shifted majorly into visible region (see Fig. 4h). For the co-doped structure, peaks lie in the visible region which is the desired outcome

Fig. 5 Refractive index with respect to energy for (a) pristine SrTiO_3 , (b) copper doped SrTiO_3 , (c) iridium doped SrTiO_3 , and (d) copper and iridium doped SrTiO_3 along xx, yy and zz tensors, respectively

that can find optical applications in the broad spectrum. It is also evident from the results that co doping has resulted in the broadening of peaks instead of sharp peaks as a result of mixed transitions.

Furthermore, refractive index of pristine and doped SrTiO_3 are also investigated for understanding the absorption peaks. The real part (ϵ_1) of dielectric function is directly related to the refractive index (n) and is in good agreement with its plot in Figs. 3 and 5. Refractive index specifies the amount of time the system is able to retain light, which means that a high refractive index would result in more absorption. However, this is true only in the case when real part (ϵ_1) of the dielectric constant is smaller than its imaginary part (ϵ_2), otherwise absorption can be small even when refractive index is large (see Eqs. 1 and 2). For example, in Cu and Ir co-doped structure, negligible absorption is seen at 0 eV (see Fig. 4d) even when refractive index is at its peak value ~ 4.9 (see Fig. 5d) which is due to the real part (ϵ_1) of the dielectric constant being larger than its imaginary part (ϵ_2). Similarly, at ~ 2 eV the absorption in co-doped structure is high ~ 190 units (see Fig. 4d) even when refractive index is negligibly small (see Fig. 5d), which is due to the real part (ϵ_1) of the dielectric constant being smaller than its imaginary part (ϵ_2). The absorption results for other energies can be understood in a similar way. A good amount of absorption is seen in the desired visible region of spectrum in co-doped structure in comparison to pristine and Cu or Ir doped SrTiO_3 structures

(see Fig. 4). Co-doping Cu and Ir has resulted into red-shift where absorption peaks are shifted from UV to desired region of the spectrum. For copper doped SrTiO_3 perovskite, results of this study agree with the results of DFT study on electronic and optical properties in [53]. Iridium doping in SrTiO_3 has been suggested for use in photocatalysis applications in [54] which is also confirmed in this study by the presence high absorption in visible region. The results can be further compared with [34, 36] for similarities in structural electronic and optical properties. The co-doped structure shows better absorption in visible region as an effect of bandgap reduction when compared with individual copper doped structure. The co-doped structure shows a better absorption in visible region as an effect of further band gap lowering when compared to individual copper doped structure. This is due to mixed transitions of orbitals which make energy states to lie near the valence band maxima and conduction band minima, resulting in higher absorption. The dielectric function's real and imaginary part are also in good agreement with the refractive index and optical absorption. The results suggest that SrTiO_3 material can find many applications such as in optoelectronic devices, photocatalysis and solar cells.

4 Conclusions

The effect of co-doping SrTiO_3 with Cu and Ir is investigated using the first principal calculations based on DFT. The results suggest that optical properties like absorption of the material can be tuned or shifted to the desired visible range of the spectrum, so that the material can be utilized in applications such as photocatalysts and solar cells. It is found that absorption shifts towards red end of the spectrum (well-known red-shift phenomenon) when co-doped with Cu and Ir in comparison to pristine and individual Cu or Ir doped SrTiO_3 structure. Furthermore, it is also observed that absorption follows trends in refractive index and dielectric constant. However, lower absorption values are observed when the real part of dielectric constant is larger than its imaginary part, even when refractive index is high. It is envisaged that the co-doped structure shall be useful in exploiting the abundantly available solar energy and can find use in broad range of optoelectronic applications.

Compliance with ethical standards

Conflict of interest On behalf of all authors the corresponding author states that there is no conflict of interest.

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