Investigations of structural, electronic and optical properties of TM-GaO$_3$ (TM = Sc, Ti, Ag) perovskite oxides for optoelectronic applications: a first principles study

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**Abstract**

We have examined structural, electronic and optical properties of TM-GaO$_3$ (TM = Sc, Ti, Ag) perovskite oxides by means of first Principles study based on density functional theory (DFT). TM represents transition metal elements. To investigate structural properties, exchange correlation potential was determined by employing Full Potential Linearly Augmented Plane Wave (FP-LAPW) technique along with Perdew-Burke-Ernzerhof – Generalized Gradient Approximation (PBE-GGA) functional. Moreover, Hubbard $U_{\text{eff}}$ parameter LDA + $U$ was used to overcome limitations of PBE-GGA functional. All compounds TM-GaO$_3$ (TM = Sc, Ti, Ag) seem semi-conductor in nature because indirect band gap in each case has been observed with energies 1.33 eV, 0.75 eV and 1.95 eV, respectively. Partial density of states (PDOS) analyses portrayed that 3$d$ orbitals of Sc & Ti, 4$d$ orbital of Ag, and 2$p$ orbital of anions contribute mainly to increase electronic conductivity of the studied compounds. Charge density contour plots depicted ionic nature of TM-cations, while, significant sharing of isolines between O and Ga atoms showed covalent character between them. These contours have also confirmed accumulation of charges around O atoms. Optical analysis revealed that the considered perovskite oxides show sharp increase in optical conductivity and absorptivity in higher energy range when energetic photons are incident upon. Remarkably, they displayed poor reflectivity. However, defect states introduced in the band gap region might be due to cations. These composites are suitable for photovoltaics and other optoelectronic applications.

1. **Introduction**

Energy crises [1] and pollution free environment are the main challenges to this era of Science & Technology. Optoelectronic based solar system is a cleaner system. It is environment friendly and miraculous invention towards energy crises. It is found innovative technology having ability to utilize free and inexhaustible light source to convert it into electrical energy. To find a suitable material for efficient solar applications has been a global challenge for the researchers. Perovskites are found abundantly on the mantle of our earth crust. Therefore, perovskite structured solids with fascinating characteristics have great attention in material science. These are relatively simple structures and viable to execute commercially. Nowadays, ternary perovskite oxides, with its generalized form ABO$_3$, have attained great attention globally [2].

During the last few decades not only theoretical investigations have been done but extensive experimental work also exists regarding feasibility of such material to boost up efficiency of the solar system. 33.5% efficiency of material used in photovoltaic has been reported theoretically by Owen et al [3]. Thus, it is dire need of the era
to dredge up a viable material for even more efficient absorption of the electromagnetic radiations. In the recent past, numerous experimental and theoretical work has been carried out to explore perovskite oxides RE–TM–O₃ [4–6]. In 2002, PbTiO₃, PbZrₓTi₁₋ₓO₃ and PbZrO₃ have been found suitable for optoelectronic applications [7] wherein lead carrying perovskites have been reported as toxic materials. Likewise, elastic and electronic properties of SrTiO₃, BaTiO₃, PbTiO₃ have been reported by Piskunov et al [8]. The first theoretical prediction of the elastic and optoelectronic properties of BaHFO₃ were made in 2008 using the pseudo-potential plane wave method wherein authors have declared it a potential candidate for optoelectronic applications [9]. Mahmood et al have explored physical properties of the cubic perovskite materials AgMO₃ (M = V, Nb, Ta) [10]. The electronic structure and elastic properties of ATiO₃ (A = Ba, Sr, Ca) have been reported by Sakhya et al [11]. Bouadjemi et al have observed structural, magnetic and optical properties of NdMnO₃ and found it a potential candidate for applications in spintronic and optoelectronic [12]. The electronics, magnetic, and thermoelectric properties of rare earth based PrYO₃ (Y = Cr, V) are reported by Sabir et al [13]. They unveiled that it is a suitable material for the applications in renewable energy and spin based devices. The electromagnetic [14], structural, magnetic and optical properties have extensively been discussed in SrRuO₃, XAlO₃ (X = Cs, Rb, K) [15]. Theoretical investigation on SrRhO₃, it revealed its ductile and metallic nature while SrZrO₃ has been reported as insulator and brittle in nature [16]. The structural, elastic and thermodynamic properties of SrTiO₃ are presented by Benyettou et al [17]. KTaO₃ has been reported as a superconductive compound by Wadehra et al [18]. Furthermore, BaTiO₃ like compound were found useful for manufacturing multilayer ceramic capacitors, electro-optic devices and sensors, etc [19] besides Thi et al have improved its polarization property [20]. It has been explored through previous studies that BaThO₃ is a suitable material for optoelectronic applications in the ultra-violet range of the electromagnetic radiations. The studies of BiBO₃ and BiAlO₃ have disclosed their potential candidacy for optoelectronic devices both in visible and lower UV range of the electromagnetic radiations [21]. In 2018, Sabir et al have discussed the optoelectronic, mechanical and thermoelectric behavior of CsMnO₃ (M = Ta, Nb) ternary perovskite oxides [22]. The similar studies have extensively been conducted to investigate physical properties of cubic perovskite oxides [23, 24].

As per our knowledge, heretofore, ScGaO₃, TiGaO₃ and AgGaO₃ perovskite oxides have not attained much attention of the researchers for their feasibility in the optoelectronic applications. Neither experimental nor theoretical data exist for TM-GaO₃ compounds, this is why, we are motivated to consider these materials theoretically. A worldwide rise in demand for solar energy has opened new horizons for the researchers to explore and devise innovative and optoelectronic based devices that could absorb visible range of the electromagnetic radiations. To cope up such needs of the current era, considered perovskite oxides seem suitable because of their high optical conductivity and absorptivity.

In this manuscript, the structural, electronic and optical properties of TM-GaO₃ (TM = Sc, Ti, Ag) perovskite oxides are investigated using first Principles calculation scheme via FP-LAPW technique by employing PBE-GGA and LDA + U functional within the framework of the DFT. It is expected that such perovskites can find their applications in optoelectronic devices etc.

2. Computational approach

In the present study, FP-LAPW technique is used for the first Principles calculations based on DFT [25]. In our calculations, we have used PBE-GGA [26, 27] functional to determine exchange-correlation potential. As PBE-GGA does not consider the on-site coulomb and on-site exchange interactions of localized d state electrons. In order to address on-site self-interactions error [28–30] and overcome limitations of PBE-GGA, Hubbard U_{eff} parameter [31] LDA + U is used to calculate improved electronic band gap energy and optical properties because localized 3d states are entailed elongated the s-p states of TM-cations in the studied compounds. Hubbard corrections U of 2.0 eV, 2.5 eV, 2.0 eV are used for Sc-3d, Ti-3d and Ag-4d/5s states, respectively. The considered space was divided into spherical muffin-tin and interstitial regions between the muffin-tin. RMT reduction by 6.5% was selected so lattice parameters could be optimized finely. RMT was set as 2.47 a.u., 2.40 a.u., 2.50 for each Sc, Ti, Ag and 1.79 a.u., 1.6 a.u. for Ga and O, respectively. The cut-off energy, to separate core and valence states, equal to −9.0 Ry and 5000 k-points in full Brillouin zone were selected for seeking optimum results. Muffin-tin radius (R_{MT} × K_{max} = 8.0) and Gaussian parameter (G_{max} = 14 (a.u)^{-1/2}) were set for seeking optimized results, particularly, consistency in band gap energies were obtained both from band structure and T DOS. System stability was sought through self-consistency check using convergence energy 0.0001 Ry. Optical properties are investigated using Fermi energies, i.e., E_F (eV) = 0.4868, 0.8342, 0.2029 for ScGaO₃, TiGaO₃ and AgGaO₃, respectively, to seek their viability for technological applications.
3. Results and discussion

3.1. Structural and electronic properties

The figure 1 describes crystal structures of cubic perovskite oxides TM-GaO$_3$ (TM = Sc, Ti, Ag) with the Pm-3m space group (No. 221). While optimizing crystal structures, the following positions were occupied by the atoms in a cubic unit cell: transition metals (TM-cations) were located at (0, 0, 0), poor metal (Ga) small cation was positioned at (0.5, 0.5, 0.5), oxygen atoms (O) sit at face centered positions (0, 0.5, 0.5), (0.5, 0.5, 0), (0.5, 0.5, 0.5). As shown in figures 2(a)–(c), energy versus optimized volume graphs were plotted following the well-known Birch-Murnaghan equation of state \[ E_{tot}(V) = E_o(V) + \frac{B_o V}{B'_o(B'_o - 1)} \left[ B \left(1 - \frac{V_o}{V}\right) + \left(\frac{V_o}{V}\right)^{B'_o} - 1\right] \] (1)

Where $E_o$ represents ground state total energy per primitive cell. $B_o$ symbolizes bulk modulus and $V_o$ represents equilibrium volume at zero pressure. Very fabulous results obtained from the energy versus volume optimization graphs are summarized in table 1. An anomalous trend in lattice constants of the studied compounds is observed, i.e., $a_o$(ScGaO$_3$) > $a_o$(TiGaO$_3$) < $a_o$(AgGaO$_3$) due to similar anomaly in ionic radii of TM-cations. Bulk modulus ($B_o$) show their decreasing trend, i.e., ScGaO$_3$ > TiGaO$_3$ > AgGaO$_3$. This decrease in bulk modulus might be occurred due to the internal stresses of the system. Whatever, bulk modulus and volume at static equilibrium of studied compounds both justify the following relation [33]:

$$B_o = V_o^{-1}$$

Bulk modulus is a measure of crystal rigidity. An eminent French scientist R.A.F. de Réaumur introduced the term ‘hardness’ [34]. According to Vicker’s hardness any material having its bulk modulus greater than 40 GPa be considered a superhard [35, 36]. In all our cases, obtained values of $B_o$ are greater than 40 GPa which is utter evidence of their crystal rigidity. Amongst three composites, ScGaO$_3$ have greatest value of the bulk modulus. Thus it is harder than the other two, i.e., TiGaO$_3$ and AgGaO$_3$.

As per our knowledge, heretofore, neither experimental nor theoretical data is available to compare-with the data summarized in table 1. The equilibrium state of the systems has been achieved at lattice parameter 3.7852Å for ScGaO$_3$, 3.7669Å for TiGaO$_3$ and 3.8894Å for AgGaO$_3$ with ground state energy ($E_o$) −5868.53 Ry, −6047.47 Ry and −14974.10 Ry, respectively. The ground state energy is being decreased (AgGaO$_3$ < TiGaO$_3$ < ScGaO$_3$) due to increase in electronic shells, where, in case of AgGaO$_3$, furthest energetic valence electrons are loosely bounded and required less energy for its bond breaking as compared to ScGaO$_3$ and TiGaO$_3$.

It is obvious that crystal structure of any solid material can be determined through its electronic band gap energy and density of states [37, 38]. In figures 3(a)–(c) the Fermi level is set at zero eV energy to calculate band gap energies at zero pressure. In ScGaO$_3$ valence band maxima occurred at point R and conduction band minima at $\Gamma$ point of symmetry of the Brillouin zone with an indirect energy gap 1.33 eV. Whereas in cases of TiGaO$_3$ and AgGaO$_3$ electron hole pair recombination took place at M and $\Gamma$ symmetry points of the Brillouin zone with their indirect band gap energies, i.e., 0.75 eV and 1.95 eV, respectively. Defect states introduced in the
band gap region might be due to TM-cations. The significant reduction in band gap of TiGaO$_3$ might be occurred due to least ionic radius of Ti-cation among the TM-cations.

To visualize bonding character, total and partial density of states for three perovskite oxides are shown in figures 4(a)–(d) for energy ranging from $-6$ to $7$ eV. In figure 4(a), total density of states (TDOS) reveal that in all cases of TM-GaO$_3$ (TM = Sc, Ti, Ag), localized energy states have crossed the Fermi level which is set at zero eV energy.

Partial density of states (PDOS) shown in figures 4(b)–(d) divulge that only Ag-4$d$ orbital amongst the TM-cations have shown its significant contribution in valence band formation. Whereas, 3$d$ orbitals of Scandium and Titanium are contributing chiefly in conduction band formation (beyond the Fermi level). It is worth notice that Ti-3$d$ states are found on the Fermi level and their shifting towards the conduction band is in line with those states which are seen on Fermi level of the band structure of TiGaO$_3$. Pseudo-states of Gallium atom didn’t show its sufficient contribution in the conduction band, however, these states have imparted adequately in valence band formation. While crossing the Fermi level, 2$p$-states of anions have shown their substantial contribution both in valence and conduction bands formation.

PDOS results highlight that in all cases, 3$d$ orbitals of Sc & Ti, 4$d$ orbital of Ag, and 2$p$ orbital of anions contribute mainly to increase electronic conductivity through shifting of localized energy states across the Fermi level.

| Parameters      | ScGaO$_3$ | TiGaO$_3$ | AgGaO$_3$ |
|-----------------|-----------|-----------|-----------|
| $a_0$ (Å)       | 3.7852    | 3.7669    | 3.8894    |
| $B_0$ (GPa)     | 187.30    | 185.71    | 133.82    |
| $\beta''$      | 4.55      | 4.33      | 5.04      |
| $E_g$ (eV)      | 1.33      | 0.75      | 1.95      |
| $E_o$ (Ry)      | $-5868.53$| $-6047.47$| $-14974.10$|
| $V_o$           | 366.24    | 360.88    | 397.08    |
In order to determine nature of the chemical bonding and charge transfer in TM-GaO$_3$ (TM = Sc, Ti, Ag) compounds, electronic charge density (in units of e/a.u.$^3$) in two dimensional is calculated in the crystallographic plane (0 ½ ½) as shown in figures 5(a)–(c). Spherical charge density contours around the TM-cations reflect their ionic nature. While the rate of isolines-compaction around the O-atoms and significant sharing of isolines among Ga atoms show covalent character between Ga—O atoms. It also confirms shifting of the charges from valence to conduction band indicating accumulation and depletion of charges around O and Ga atoms, respectively.
The decreasing trend (ScGaO$_3$ $>$ TiGaO$_3$ $>$ AgGaO$_3$) of the lowest rendered values (as obvious from thermo-scale) is replicating pattern of the ionic radii of TM-cations in order of symmetry. The highest rendered value (+0.3000, purple color) for all perovskites designate maximum charge accumulating site. The difference between highest and lowest rendered value for ScGaO$_3$ is +0.2892, for TiGaO$_3$ this difference is +0.2945 and for AgGaO$_3$ it is found +0.2993. This difference in isovalue indicates transfer of the charges. Thus, ScGaO$_3$ having smallest difference may transfer the most charges.

Figure 5. Iso-surface charge density plot for (a) ScGaO$_3$ (b) TiGaO$_3$ (c) AgGaO$_3$ ternary Perovskites and thermo-scales are shown beside each charge density contour.
For further insight, prescribed Pauling electronegativity of the constituent elements of the studied compounds is 3.5, 1.6, 1.4, 1.5, 1.9 for O, Ga, Sc, Ti and Ag atoms, respectively. Tendency to accumulate charges by any element is purely associated with its electronegativity. Thus, oxygen being more electronegative element has greatest tendency to accumulate charges. Obviously, Silver atom amongst the realm of TM-cations has highest electronegativity (1.9), thereby, accumulating more charges than Scandium and Titaniumatoms as shown in figure 5(c). It is seen that electronic calculations, i.e., band gap energy, total and partial charge densities and isosurface charge density plots have good coherence.

3.2. Optical properties
The veracity of how electromagnetic radiations interact with the materials can be visualized through detailed descriptions of optical properties. Thereby, we investigated complex dielectric function along with various other frequency dependent optical parameters, i.e., refractive index \( n(\omega) \) and extinction coefficient \( k(\omega) \), absorption coefficient \( \alpha(\omega) \) and energy loss function \( L(\omega) \), optical conductivity \( \sigma(\omega) \) and reflectivity \( R(\omega) \) of the studied compounds to determine its optoelectronic nature for various applications. In all cases, the black color line represents the behavior of ScGaO\(_3\), red color denotes the optical trend of TiGaO\(_3\) and blue color defines AgGaO\(_3\).

3.3. Dielectric function
Although the dielectric function is a complex function, it is considered an important parameter in the optical world. It has been splitted in two components through well-known expression \( \varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) \) which describes an optical response of the material to the incident photons [39]. Its real part \( \varepsilon_1(\omega) \) tells about dispersion and polarization of electromagnetic radiations while its imaginary component \( \varepsilon_2(\omega) \) discuss about absorptive nature of the material. \( \varepsilon_1(\omega) \) and \( \varepsilon_2(\omega) \)are interlinked with the Kramers-Kronig relation [40]. Here, optical parameters are investigated using optical energy range 0–15 eV as shown in figures 6–9. From figure 6(a) values of the static real dielectric constants \( \varepsilon_1(0) \) are calculated as 221.1, 75.0 and 175.0 for ScGaO\(_3\), TiGaO\(_3\) and AgGaO\(_3\), respectively. The \( \varepsilon_1(\omega) \) decreases sharply in lower energy range upto 0.82 eV wherein AgGaO\(_3\) and ScGaO\(_3\) gain negative values of dielectric constants, i.e., \(-18.59\) at 0.40 eV and \(-18.27\) at 0.8 eV, respectively. Its negative part is responsible for occurrence of the energy losses and poor transmission of light through the material with significant reflection [41]. However, in higher energy range, \( \varepsilon_1(\omega) \) raises its flight toward positive region. The slight variations in real dielectric seen above the Fermi level are happened due to the different transition rate of photons. Beyond 3 eV energy, \( \varepsilon_1(\omega) \) in all cases becomes almost equals and extending parallel to the x-axis which is clear signature of minimal dispersion and polarization of electromagnetic radiations.

The imaginary component of the dielectric function \( \varepsilon_2(\omega) \) is an important optical parameter and its comprehensive study is mandatory. The variation of \( \varepsilon_2(\omega) \) with incident photons energy in range 0–15 eV for considered compounds is displayed in figure 6(b). In all cases, imaginary zero frequency limit \( \varepsilon_2(0) \) within the inter-band transition is calculated as 53.0, 35 and 90.7 for ScGaO\(_3\), TiGaO\(_3\) and AgGaO\(_3\), respectively. In the present study, intra-band transition is not taken into account because it has dominant impact only if the electronic transitions indicating the metallic nature of the material [15]. The value of \( \varepsilon_2(\omega) \) decreases drastically in the lower energy range which shows that incident photons are not interacting with the material’s surface.

Figure 6. Calculated plot of (a) real dielectric constant (b) imaginary dielectric constant for TMGaO\(_3\) (TM = Sc, Ti, Ag) ternary Perovskites.
Figure 7. Graphs show (a) refractive index (b) extinction coefficient for TM-GaO$_3$ ($TM = Sc, Ti, Ag$) ternary Perovskites.

Figure 8. (a) Absorption coefficient (b) energy loss function for TMGaO$_3$ ($TM = Sc, Ti, Ag$) ternary Perovskites.

Figure 9. Calculated plots for (a) optical conductivity (b) Reflectivity for TMGaO$_3$ ($TM = Sc, Ti, Ag$) ternary Perovskites.
However, in higher energy range, $\varepsilon_2(\omega)$ increases and noticeable peaks are found situated at different values of the energy, i.e., 3.44 eV, 2.22 eV and 1.7 eV due to inner-band transitions of the valence electrons.

### 3.4. Refractive index and extinction coefficient

Once the real and imaginary components of dielectric function have been investigated, the refractive index $n(\omega)$ and extinction coefficient $k(\omega)$ are calculated to forecast transparency of the material and absorption of incident photons. Refractive index $n(\omega)$ shown in figure 7(a) follow similar trend as that of the imaginary part of the dielectric function. Its critical values $n(0)$ calculated for TM-GaO$_3$ (TM = Sc, Ti, Ag) are 2.50, 9.0 and 13.70, respectively with sharp decreasing edges in two cases (Ti and Ag cations) while $n(\omega)$ remains linear upto 0.9 eV. The maximum peak situated at 2.79 eV photons energy above the threshold frequency carries refractive index 3.63 for ScGaO$_3$. It is observed that the refractive index fluctuates between 0.8–1.5 beyond ~ 4.0 eV photo-energy wherein slight fluctuations occurred due to various inner-band transitions. Comparatively ScGaO$_3$ has high refractive index which shows that during transmission of light, incident photons interact with more valence electrons, causing polarization and reduction in speed of light.

The extinction coefficient versus photon energy plot is shown in figure 7(b). Zero frequency limit $K(0)$ observed for TiGaO$_3$ and AgGaO$_3$ are 1.88 and 3.33 while the extinction coefficient for ScGaO$_3$ remains zero at the light frequency equal to the band gap energy. The initial drastic increase in $k(\omega)$ upto 4.0 (TiGaO$_3$) and 7.27 (AgGaO$_3$) follows steeper downfall below its critical value at 1.4 eV. Thereafter, in all cases, extinction coefficient rises to its maximum limit, i.e., 2.19 for ScGaO$_3$ above the threshold frequency. In higher energy upto 13.56 eV, their values fluctuate between 0.5 and 2.19. Only ScGaO$_3$ could attain 2.19 extinction coefficient at 13.56 eV due to its efficient interaction with incident photons emitting from the visible source of electromagnetic radiations. Thus, it is considered a good absorptive material and a potential candidate for a photovoltaics and other allied devices. The dielectric functions, $n(\omega)$ and $k(\omega)$ are interrelated with the following relations:

$$\alpha(\omega) = n^2 - k^2$$

and

$$\varepsilon_2(\omega) = 2nk$$

### 3.5. Absorption coefficient and Energy loss function

Absorption coefficient $\alpha(\omega)$ describes how the substance interacts with incident photons having energy $E = h\omega$ and its ability to absorb energy packets. Reportedly, it is correlated with the dielectric function through the relation [39] expressed as:

$$\alpha(\omega) = \frac{2\omega}{c} \left( -\text{Re}(\varepsilon(\omega)) + |\varepsilon(\omega)| \right)^{1/2}$$

Absorption coefficient versus photon energy plot is shown in figure 8(a). It is seen in all cases that absorption of incident photons (inner–band transitions) occurred as the photon’s energy becomes equal to the band gap of the particular material. The rate of absorption increases abruptly, particularly in the case of ScGaO$_3$, with increasing frequency of the incident photons. An unexpected decrease in absorptivity of incident photons in between 6.0 eV to 9.2 eV energy for ScGaO$_3$ and TiGaO$_3$ might be due to the internal stresses of the systems. However, in AgGaO$_3$, absorptivity increases linearly following the square trend of energy. Nevertheless, beyond the 9.2 eV photons energy, absorption rate shouuts interestingly upto 13.56 eV. Thus, maximum absorptivity was calculated for ScGaO$_3$, TiGaO$_3$ and AgGaO$_3$ is $215.15 \times 10^4$ cm$^{-1}$ at 13.56eV photo-energy.

As regard energy loss function, it describes energy lost during transition of high-speed electrons [42]. The energy lost during interaction of photoelectrons and other electrons in the material is recognized as plasmon losses. In inner–band transitions, the probability of scattering is directly proportional to the energy loss function. As shown in figure 8(b) energy loss function increases from origin to $L(\omega) = 1.1$ in lower energy range below threshold frequency with the dispense in the absorption on the material’s surface. Energy losses increase beyond 1.60eV incident photons energy. The peaks of maximum energy loss $L(\omega)$ = 0.56, 0.79 and 0.65 are found located at 7.79 eV, 7.10 eV and 2.79 eV respectively for TM-GaO$_3$ (TM = Sc, Ti, Ag), respectively. In the energy range beyond 7.10 eV, $L(\omega)$ alleviates sharply and fluctuates in all cases due to inner–band transitions. ScGaO$_3$ having least energy losses seems a potential candidate for absorption of the electromagnetic radiations.

### 3.6. Optical conductivity and reflectivity

The conduction mechanism of the photoelectrons which are emitted during the photoelectric effect has been examined through the optical conductivity [43] where $\sigma(\omega) = \frac{\text{Im} \sigma}{3\pi\varepsilon_0}$. The optical conductivity describes exactly how bonds break once energetic electromagnetic radiations fall upon the material’s surface. Plot of the optical conductivity versus incident photons energy is presented in figure 9(a). Optical conductivity follows an identical pattern as that of the absorption coefficient shown in figure 8(a). Initially the $\sigma(\omega)$ raised (1st peak) to the values of 1551.53 $\Omega^{-1}$cm$^{-1}$ (TiGaO$_3$) and 3138.86 $\Omega^{-1}$cm$^{-1}$ (AgGaO$_3$), however, it falls down to their minimum values in the lower energy range, i.e., 1.35 eV (TiGaO$_3$) and 0.91 eV (AgGaO$_3$) due to considerably
inactive and lethargic photons striking on the material’s surface. However, ScGaO₃ follows such a unique trend which is quite obvious for semiconductors that $\sigma(\omega)$ should be approaching zero at the light frequency equal to the band gap. After attaining the threshold frequency, all studied compounds show their fascinating trend that sharp growth of 2nd peak of the optical conductivity, i.e., $5333.59 \, (\text{fcm})^{-1}$, $3176.56 \, (\text{fcm})^{-1}$ and $1946.00 \, (\text{fcm})^{-1}$ was found situated at various photo-energies, i.e., $3.17 \, eV$, $2.52 \, eV$ and $1.81 \, eV$ for ScGaO₃, TiGaO₃ and AgGaO₃, respectively. Subsequently, conductivity fluctuates in between the photon energies $4.34$ to $7.30 \, eV$ due to a different rate of inner transitions. Nevertheless, conductivity increases significantly and approaches to $5378.63 \, (\text{fcm})^{-1}$, $5304.90 \, (\text{fcm})^{-1}$ and $4926.11 \, (\text{fcm})^{-1}$ in the high energy range $8.8 \, eV$–$11.60 \, eV$ for TM-GaO$_3$ (TM = Sc, Ti, Ag), respectively. Beyond this energy limit, optical conductivity decreases since the electromagnetic radiations fall in UV region. The optical analysis unveils that all compounds have shown good optical conductivity if sufficient energy photons (energy $\geq$ work function) fall upon the material’s surface. However, ScGaO₃ exhibited the highest conductivity, thus, it is considered a suitable material for potential applications in photovoltaics and other optoelectronic devices.

Reflectivity determines the portion of the electromagnetic radiations bounce back from the surface of the material. From figure 9(b) the static values of reflectivity R(0) are calculated as $0.19$, $0.65$ and $0.76$ for ScGaO₃, TiGaO₃ and AgGaO₃, respectively. To some extent, it follows an identical pattern as that of the extinction coefficient in figure 7(b). Reflectivity go on decreasing to attain its minimum $\leq 0.10$ till $10.24 \, eV$. In higher energy region, relatively ScGaO₃ showed the lowest reflection from its surface. Conversely, the absorption rate increases in this range. Away from $10.24 \, eV$, increasing trend of the reflectivity has been observed in all cases. Comparatively reflectivity range ($0$ to $1.0$) is much negligible than absorptivity ($0$ to $250 \times 10^4 \, \text{cm}^{-2}$).

4. Conclusions

In this manuscript, the structural, electronic and optical properties of cubic perovskites TM-GaO₃ (TM = Sc, Ti, Ag) are investigated. Lattice constants are found $a_0$(ScGaO₃) > $a_0$(TiGaO₃) < $a_0$(AgGaO₃) due to similar anomaly in ionic radii of TM-cations. The considered compounds TM-GaO₃ (TM = Sc, Ti, Ag) are semiconductor in nature because indirect band gap in each case was observed with energies, i.e., $1.33 \, eV$, $0.75 \, eV$ and $1.95 \, eV$, respectively. TDOS and PDOS results established chief contribution of $3d$-orbital from anion sites which have displayed plentiful improvement in electronic conductivity of the studied compounds. Charge density contour plots portrayed ionic nature of TM-cations, while, covalent character between Ga–O atoms. Sharp increase in optical conductivity and absorptivity in higher energy range is noted through optical analysis. It is anticipated that this theoretical investigations will encourage to synthesis ScGaO₃, TiGaO₃ and AgGaO₃ perovskite oxides experimentally, which are extensively useful for technological applications in photovoltaics and other allied devices.

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