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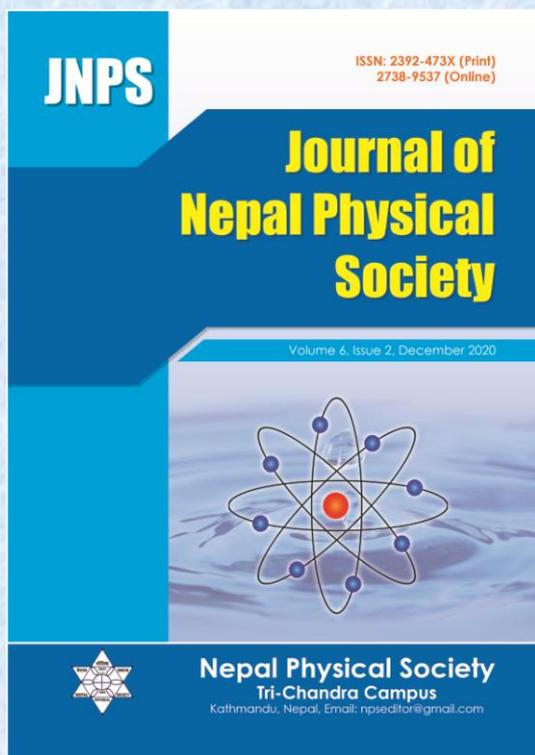
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# Electronic Structure and Transport Properties of Superlattices: $\text{La}_{(1-x)}\text{Sr}_x\text{TiO}_3$ ( $x = 0, 0.20, 0.80, 1$ )

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## Abstract

The conventional density functional theory (DFT) and dynamical mean field theory (DMFT) is used to study the structural, electronic and the Mott-Hubbard metal-insulator phase transition of the pristine and superstructures,  $\text{La}_{(1-x)}\text{Sr}_x\text{TiO}_3$  ( $x = 0, 0.20, 0.80, 1$ ). The electrical and thermal conductivities, Seebeck coefficient, Figure of merit are calculated using the BoltzTraP codes. The present study reveals that the direct band gap of 2.20 eV and indirect band gap  $\sim 2.0$  eV at the  $\Gamma$  point in the Brillouin zone of  $\text{SrTiO}_3$  is upgraded to 3.423eV by using modified Beck-Johnson (mBJ) interaction potential. The metal-insulator transition (MIT) of  $\text{LaTiO}_3$  and the superlattice  $\text{La}_{(1-x)}\text{Sr}_x\text{TiO}_3$  have been investigated by using conventional density functional theory (DFT) and dynamical mean field theory (DMFT). The Mott-Hubbard metal-insulator transitions for pristine  $\text{LaTiO}_3$  for a Coulombian parameter,  $U = 2.5$  eV and the thermodynamic parameter  $\beta = 6$  (eV)<sup>-1</sup> are consistent with the experimental results. A typical set of these correlation parameters for MIT  $\text{La}_{0.20}\text{Sr}_{0.80}\text{TiO}_3$  and  $\text{La}_{0.80}\text{Sr}_{0.20}\text{TiO}_3$  systems are found to be  $U = 3.5$  eV and  $\beta = 10$ (eV)<sup>-1</sup> and  $U = 3.2$  eV and  $\beta = 10$  (eV)<sup>-1</sup> respectively. The characteristic sharp quasi-particle peak for a sample of  $\text{La}_{0.80}\text{Sr}_{0.20}\text{TiO}_3$  superlattice systems is obtained correlation parameter  $U = 3.0$  eV and  $\beta = 6$ (eV)<sup>-1</sup>. A thermoelectric phase transition is observed for Seebeck Coefficient at temperature 300 K at near chemical potential,  $\mu = 1$ eV of  $\text{SrTiO}_3$ . The corresponding figure of merit (ZT) with chemical potential ( $\mu$ ) appears to be unity at near  $\mu = 1$ eV.

**Keywords:** DFT, DMFT, MIT, Superlattice, TMOs.

## 1. INTRODUCTION

The complex transition metal oxides (TMOs) are the promising smart materials for the scientific and technological innovations as well as theoretical investigation of material world. The TMOs are complex strongly correlated materials with various degrees of freedom (dof), such as charge, spin, orbital, valley and lattice interactions. The heterostructures and nanostructures of such compounds have exotic and novel properties highly useful for Mottronics applications [1, 2].

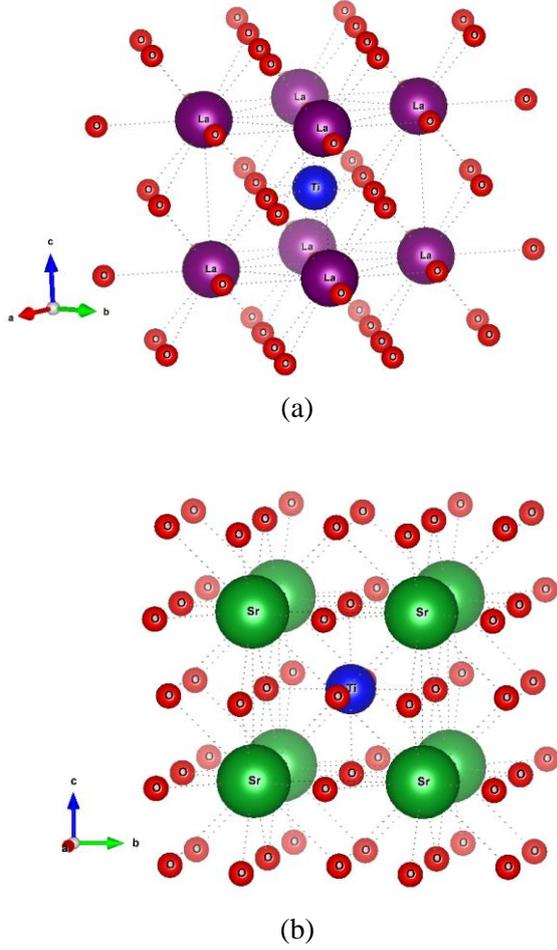
In general, these materials are found in a simple cubic perovskite  $\text{ABO}_3$  type structures, where the A and B cations are arranged on a simple cubic lattice, and the O anions lie on the face centers

nearest to the cations (B = transition metals) as shown in Fig. 1.

The cations (A = earlier transition metals or rare earths) are at the centers of the oxygen, O octahedral, while the A cations lie at the larger 12-fold coordinated sites [3-6]. The bonding between La and  $\text{TiO}_2$  is mainly ionic, and the  $\text{TiO}_2$  entity is bound covalently in the  $\text{LaTiO}_3$  system.

The density functional theory (DFT) along with the dynamical mean field theory (DMFT) is employed for figuring out the realistic electronic structure of strongly correlated system. The spectral density of distribution (spectral function) is obtained using the maximum entropy model for the La-atom substituted on Sr-site  $\text{La}_{(1-x)}\text{Sr}_x\text{TiO}_3$  supercell have

been studied using various impurity solvers including quantum Monte Carlo (QMC) [7].



**Fig. 1:** (color online) The crystal structures of cubic phase of pristine (a)  $\text{LaTiO}_3$  and (b)  $\text{SrTiO}_3$  systems.

The strong electron correlation and other anomalous electronic properties in the metallic phase transition (MIT) are of great interest. The Mott transition in  $\text{La}_{(1-x)}\text{Sr}_x\text{TiO}_3$  system is studied experimentally employing filling control method, through the appropriate doping of the holes or electrons to the system and band control method through the site substitution of Sr-ion with La-ion to the system [4,8-10].

The transition metal oxides have narrow conduction bands due to weak orbital overlap, which leads to localized electrons with low carrier mobilities. Transition metal oxides have recently been considered as thermoelectric (TE) materials that can operate at high temperature and they have their transport properties with high Seebeck coefficients (S) and low thermal conductivity ( $K$ ). We have

computed the thermal conductivity  $K$ , electrical conductivity ( $\sigma/\tau$ ), Seebeck coefficients (S), and Figure of merit (ZT) etc. for the  $\text{SrTiO}_3$  and  $\text{LaTiO}_3$  [11, 12].

The Mottness (the resistive switching) behaviours of TMOs are highly applicable for designing novel devices, including sensing, signal conversion, non-volatile memory, artificial neurons and so on. Those oxides devices have far more better over the conventional semiconductor devices in terms of efficiency, durability, additional functionality and future downsizing to the nanoscale structures [13, 14].

## 2. METHODOLOGY AND COMPUTATIONAL DETAILS

### 2.1 Theoretical Backgrounds:

The electronic structure and transport properties of Mott-insulator  $\text{LaTiO}_3$  and band-insulator  $\text{SrTiO}_3$  and their superlattices systems have been investigated by using density functional theory (DFT) based quantum mechanical approach [15-17].

The optimized cubic phase of  $\text{SrTiO}_3$  and  $\text{LaTiO}_3$  are taken for the GGA, GGA+U+J, SOC and DOS calculations by solving self consistent Kohn-Sham equation for the many-body system as given by,

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + v_{\text{eff}}(\mathbf{r}) \right] \Psi_i = \epsilon_i \Psi_i \quad (1)$$

Where the effective Kohn-Sham potential is expressed as,

$$v_{\text{eff}}(\mathbf{r}) = v(\mathbf{r}) + \int \frac{[n_e(\mathbf{r}')]^2}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r}' + v_{\text{xc}}(\mathbf{r}) \quad (2)$$

And,  $v_{\text{xc}}(\mathbf{r}) = \frac{\delta E[n_e(\mathbf{r})]}{\delta n_e(\mathbf{r})}$  is the exchange

correlation potential with the probability density as,

$$n_e(\mathbf{r}) = \sum_{i=1}^N |\Psi_i(\mathbf{r})|^2$$

The electronic structure and other properties of these materials are also examined by using statistical method, such as the density of states (DOS) per unit energy range as given by

$$D_n(\epsilon) = \frac{2}{8\pi^2} \int \delta(E_F - \epsilon_n(\mathbf{k})) d\epsilon \quad (3)$$

with the allowed wavevector in the  $n^{\text{th}}$  band energy range,  $\varepsilon \leq \varepsilon_n(\mathbf{k}) \leq \varepsilon + d\varepsilon$  is just the volume of a  $\mathbf{k}$ -space primitive cell, divided by the volume per allowed wave vector,

$$\Delta k = 2\pi^3/V.$$

The transport coefficients of the TMOs are investigated for the optimized systems by using BoltzTraP code, a patching software of WIEN2k framework, which implements the linearized Boltzmann Transport Equation (BTE) [18] as given by,

$$\frac{\partial f_{\mu}(T, \mu)}{\partial t} = -v_{\alpha}(i, \mathbf{k}) \cdot \frac{\partial f_{\mu}(T, \mu)}{\partial \mathbf{r}} - \frac{e}{\hbar} \left( E - \frac{1}{c} v_{\alpha}(i, \mathbf{k}) \times H \right) \cdot \frac{\partial f_{\mu}(T, \mu)}{\partial k_{\alpha}} + \frac{\partial f_{\mu}(T, \mu)}{\partial t} \Big|_{\text{scattering}} \quad (4)$$

with  $f_{\mu}(T, \mu) = \frac{1}{\exp[(\mu - E_F)/k_B T] + 1}$  is the Fermi-Dirac distribution for electron and

$v_{\alpha}(i, \mathbf{k}) = \frac{1}{\hbar} \frac{\partial \varepsilon_{i, \mathbf{k}}}{\partial k_{\alpha}}$  is the group velocity of the carriers.

From the first-principle, the Seebeck coefficient (S) and figure of merit (ZT) are calculated as,

$$ZT = \frac{\sigma_{\alpha\beta} S_{\alpha\beta}^2}{\kappa_{\alpha\beta}} T \quad (5)$$

Where ,

$$\sigma_{\alpha\beta}(T, \mu) = \frac{1}{\Omega} \int \bar{\sigma}_{\alpha\beta}(\varepsilon) \left[ -\frac{\partial f_{\mu}(T, \mu)}{\partial \varepsilon} \right] d\varepsilon \quad (6)$$

is the electrical conductivity tensor,

$$\kappa_{\alpha\beta}(T, \mu) = \frac{1}{\Omega e^2 T} \int \bar{\sigma}_{\alpha\beta}(\varepsilon) (\varepsilon - \mu)^2 \left[ -\frac{\partial f_{\mu}(T, \mu)}{\partial \varepsilon} \right] d\varepsilon \quad (7)$$

is the thermal conductivity tensor,

$$S_{\alpha\beta}(T, \mu) = \frac{1}{\Omega e T \sigma_{\gamma\alpha}(T, \mu)} \int \bar{\sigma}_{\gamma\beta}(\varepsilon) (\varepsilon - \mu) \left[ -\frac{\partial f_{\mu}(T, \mu)}{\partial \varepsilon} \right] d\varepsilon \quad (8)$$

is the thermoelectric Seebeck coefficients,

And,

$$\bar{\sigma}_{\alpha\beta}(\varepsilon) = \frac{e^2}{N} \sum_{i, \mathbf{k}} \tau_{i, \mathbf{k}} v_{\alpha}(i, \mathbf{k}) v_{\beta}(i, \mathbf{k}) \delta(\varepsilon - \varepsilon_{i, \mathbf{k}}) \quad (9)$$

is the kernel of all transport coefficients, that is necessary for calculating the Figure of merit.

Where  $\alpha$  and  $\beta$  are tensor indices,  $\Omega$ ,  $\mu$  and  $N$  are the volume of the unit cell, chemical potential and number of  $\mathbf{K}$ -points implemented respectively.

Furthermore, the dynamical mean field theory (DMFT) can be applied for realistic picture of electronic system by using the Hubbard Hamiltonian for strongly correlated system as,

$$\hat{H} = \sum_{ijlm\sigma} t_{ijlm} \hat{c}_{il}^{\sigma\dagger} \hat{c}_{jm}^{\sigma} + \sum_{ilmno\sigma\sigma'} U_{ilmno} \hat{c}_{il}^{\sigma\dagger} \hat{c}_{im}^{\sigma\dagger} \hat{c}_{in}^{\sigma'} \hat{c}_{io}^{\sigma} \quad (10)$$

Where,  $\hat{c}_{il}^{\sigma\dagger} (\hat{c}_{il}^{\sigma})$  creates (annihilates) an electron with spin  $\sigma$  and orbital index  $l$  at lattice site  $i$ .

$t_{ijlm}$  is the hopping amplitude between lattice sites  $i$  and  $j$  and orbitals  $l$  and  $m$ .

$U_{ilmno}$  denotes a general local Coulomb interaction [19-21].

Mapping onto the Anderson impurity model Hamiltonian for DMFT calculation as

$$\hat{H}_{AIM} = \sum_{kl\sigma} \varepsilon_l(k) \hat{a}_{kl}^{\sigma\dagger} \hat{a}_{kl}^{\sigma} + \sum_{kl\sigma} [V_{lm}(k) \hat{a}_{kl}^{\sigma\dagger} \hat{c}_m^{\sigma} + \text{h. c.}] + \sum_{ilmno\sigma\sigma'} U_{ilmno} \hat{c}_{il}^{\sigma\dagger} \hat{c}_{im}^{\sigma\dagger} \hat{c}_{in}^{\sigma'} \hat{c}_{io}^{\sigma} \quad (11)$$

Where  $\hat{a}_{kl}^{\sigma\dagger} (\hat{a}_{kl}^{\sigma})$  are creation and annihilation operators for non-interacting conduction electrons at wave vector  $\mathbf{k}$ , which have a dispersion  $\varepsilon_l(\mathbf{k})$  and hybridize with the localized interacting electrons  $\hat{c}_m^{\sigma\dagger}$  via  $V_{lm}(k)$ .

The equation with the modeled Hamiltonian (11) can be solved by various kinds of impurity solvers, such as CT-QMC, DMRG, NCA, IPT etc.

The interacting Green function and hence the self energy,  $\Sigma(\omega)$  can be calculated by using the Dyson equation as,

$$[G^0(\omega)]^{-1} = [G(\omega)]^{-1} + \Sigma(\omega) \quad (12)$$

The spectral function, which is associated with the imaginary part of Green function at a given momentum is a Dirac  $\delta$ -function [22-25] as,

$$A(\mathbf{k}, \omega) = -\frac{1}{\pi} \text{Im}[G(\mathbf{k}, \omega)] = \delta(\omega - \varepsilon_{\mathbf{k}}) \quad (13)$$

And, the total local spectral function coincides with the Bethe density of states (DOS).

Turning on correlations, the spectral function has a Lorentzian profile as,

$$A(\mathbf{k}, \omega) = -\frac{1}{\pi} \left[ \frac{\text{Im} \Sigma(\omega)}{(\omega + \mu - H_0(\mathbf{k}) - \text{Re}[\Sigma(\omega)])^2 + \text{Im}[\Sigma(\omega)]^2} \right] \quad (14)$$

The real part of the self-energy shows a shift of the non-interacting excitations, whereas the imaginary part of self-energy indicates the broadening of the quasiparticles excitations. Since, the self-energy strongly depends on the frequency and in the case of the Mott insulator, it will lead to a notable transfer of spectral weights.

The maximum likelihood of spectral function,  $A(\omega)$ , is obtained by maximizing the probability using Bayesian theorem[26] as,

$$P[A(\omega)|G(\omega)] = \frac{P[G(\omega)|A(\omega)]}{P[G(\omega)]} P[G(\omega)] \sim e^{\alpha S - \frac{1}{2} \chi^2} \quad (15)$$

The Green function,  $G(\omega)$  is data obtained from the DMFT calculation using CT-QMC-hybridization technique as the impurity solver. The reliable features of the spectral function, such as height and width of the central peak, and the overall weight and position of the Hubbard bands are obtained by using the maximum entropy method with the optimized value of adjustable parameter,  $\alpha$  that will have the required information of the system concerned. The algorithm first computes the solution to  $\min(\chi^2 - \alpha S)$  for a large range of  $\alpha$ . The location of the optimal value of  $\alpha$  can be found by plotting a graph between  $\log_{10}(\chi^2)$  as a function of  $\log_{10}(\alpha)$ , which gives the maximum likelihood of the required information lies somewhere in the portion of information fitting region of the logistic regression curve (sigmoid curve).

## 2.2 Computational Details and Experimental Information

The electronic structure, density of states (DOS), electronic charge density distribution and transport behaviours the cubical TMO systems are studied using the full potential-linearized augmented plane wave (FP-LAPW) with local orbitals (lo) based on DFT frameworks. The Kohn-Sham equations have been solved by the method of self-consistent total energy calculations within the generalized gradient approximation (GGA) developed by three scientists Perdew, Burke and Ernzerhof [26, 27] for

approximating the electronic exchange and correlation effects.

We have employed the various schemes, such as GGA+U, GGA+U+J, GGA+SOC, GGA+mBJ etc. for improving the underestimated electronic structure based on the conventional density functional theory [28,29].

Despite the whole story of DFT calculation, we have employed the dynamical mean field theory (DMFT) with the continuous time quantum Monte Carlo (CT-QMC) -hybridization technique as the impurity solver for computing the realistic picture of electronic structure of TMOs, so as to explore the Mott-Hubbard metal-insulator transition [30,31]. The statistical inferences are implemented by applying Maximum Entropy Model for obtaining the spectral density distribution from DMFT data [32, 33].

The Mott-Hubbard band splitting of strongly correlated system have been investigated by using dynamical mean field theory (DMFT)

The theoretical study of MIT is done using the density functional theory (DFT) and the dynamical mean field theory (DMFT) [34, 35]. A band controlled transition metal oxide system,  $\text{La}_{(1-x)}\text{Sr}_x\text{TiO}_3$ , which are reconstructed by site substitution of extended pristine superlattice of cubic perovskite,  $\text{SrTiO}_3$ . The MIT phase transition are investigated for the strongly correlated parameter,  $U$  and the thermodynamic parameter,  $\beta$  through DFT + DMFT [36, 37].

In the present study, we have used Monk-horst pack of  $7 \times 7 \times 7$  k-mesh grid for the pristine TMOs unit cell. The k-mesh grid of  $13 \times 13 \times 2$  for both of the superstructures is used for DFT calculation with the energy and charge convergence criteria for the entire systems are  $10^{-5}$  eV and  $10^{-3}$  e respectively. And the force convergence criterion is  $0.05$  eV/Å used for the entire calculation.

Furthermore, the BoltzTraP codes are used for computing the thermal conductivity, electrical conductivity, Seebeck coefficients and figure of merit (ZT) etc. of the  $\text{La}_{1-x}\text{Sr}_x\text{TiO}_3$  superlattices.

The transport properties of interfaces of  $\text{LaTiO}_3$  and  $\text{SrTiO}_3$  i.e. Mott and band insulators have shown high mobility of electron gas due to charge redistribution of substitutional dopant such as La or Sr, by charge transfer, crystal polarity etc. [38]. All the heterostructures are grown on  $\text{SrTiO}_3$  (100) substrates preannealed at  $900$  °C and  $\text{LaTiO}_3$  films were grown using pulsed laser deposition at a substrate temperature of  $500$  °C and an oxygen

background pressure of  $10^{-6}$  Torr. using polycrystalline  $\text{La}_2\text{Ti}_2\text{O}_7$  target. All of the heterostructures grown found to be metallic on measuring the transport and Hall measurement of the system upto 5 T of magnetic field [39].

### 3. RESULTS AND DISCUSSION

#### 3.1 Structural Stability and Optimization

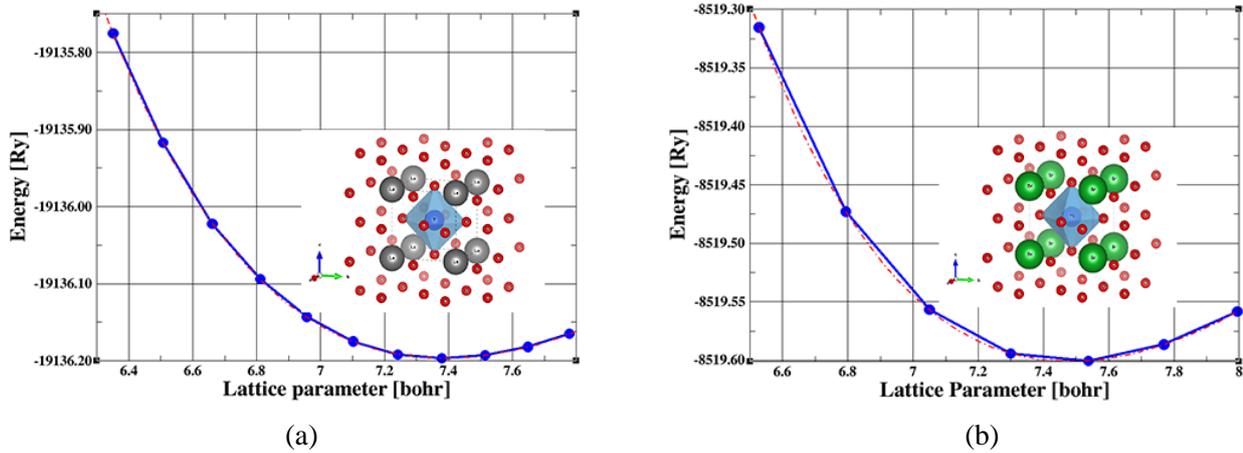
The optimized parameters for the given TMOs (systems) are obtained through energy minimization technique using first-principle method.

The cubic phase of  $\text{SrTiO}_3$ , which belongs to the space group  $\text{pm-3m}$  is known to be a band insulating material. The cubic unit cell contains one molecule with the Sr-atom sitting at the origin (0.0, 0.0, 0.0)a, the Ti-atom at the body center (0.5, 0.5, 0.5)a and the three O-atoms at the three face centers (0.5, 0.5, 0.0)a, (0.0, 0.5, 0.5)a, and (0.5, 0.0, 0.5)a; the lattice constant is  $a = 7.297$  bohr. Similarly, the cubic phase unit cell of  $\text{LaTiO}_3$  contains one molecule with the La-atom sitting at the origin (0.0, 0.0, 0.0)a, the Ti-atom at the body center (0.5, 0.5, 0.5)a and the three O-atoms at the three face centers (0.5, 0.5, 0.0)a, (0.0, 0.5, 0.5)a, and (0.5, 0.0, 0.5)a; the lattice constant is  $a = 7.100$  bohr (1 bohr = 0.529 Å) [40,41].

In this study the convergence parameters, such as K-points, rKmax and Gmax values for  $\text{SrTiO}_3$  are obtained as 500, 7.0 and 17.0 respectively along with RMT-values 2.50 for Sr-atom, 1.87 for Ti-atom and 1.69 for O-atoms respectively. Similarly, the convergence parameters, such as K-points, rKmax and Gmax values for  $\text{LaTiO}_3$  are obtained as 500, 7.5 and 18.0 respectively along with RMT-values 2.50 for Sr-atom, 1.82 for Ti-atom and 1.65 for O-atoms respectively.

The crystal structure of  $\text{SrTiO}_3$  and  $\text{LaTiO}_3$  (inset) with their lattice parameters optimization curves is shown in Fig. 2.

The optimized unitcell of  $\text{LaTiO}_3$  is promoted to  $1 \times 1 \times 5$  supercell, so as to study the effect of the site substitution of Sr-atom on  $\text{LaTiO}_3$  supercell on the electronic structure and transport properties of  $\text{La}_{(1-x)}\text{Sr}_x\text{TiO}_3$  superlattice system[42-44]. The superlattice,  $\text{La}_{0.80}\text{Sr}_{0.20}\text{TiO}_3$  system of space group  $\text{p4/mm}$  with lattice parameters,  $a = b = 3.592$  Å and  $c = 18.126$  Å with RMT values for La-, Sr-, Ti-, O- are found to be 2.50, 2.36, 1.65 and 1.49 respectively. For superlattice,  $\text{La}_{0.20}\text{Sr}_{0.80}\text{TiO}_3$  system of space group  $\text{p4/mm}$  with lattice parameters,  $a = b = 3.853$  Å and  $c = 19.445$  Å with RMT values for La-, Sr-, Ti-, O- are found to be 2.50, 2.50, 1.77 and 1.60 respectively.



**Fig. 2:** (color online) The lattice parameter optimization curves of the cubic phases of (a)  $\text{LaTiO}_3$  and (b)  $\text{SrTiO}_3$  systems (crystal structures in inset).

#### 3.2 Electronic band structure and Density of States (DOS)

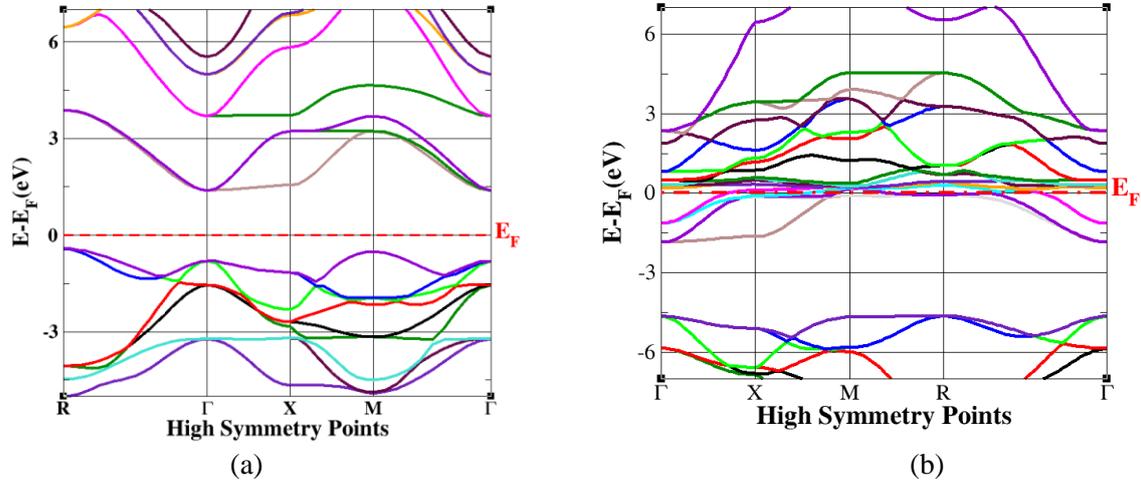
The optimized pristine  $\text{SrTiO}_3$  and  $\text{LaTiO}_3$  systems have been taken through self-consistent calculation for investigating their electronic structure and transport properties [45-47]. The ground state

calculation was performed through the energy minimization technique for the given system. The calculated energy band structure for cubic phases  $\text{SrTiO}_3$  is shown in Fig. 3(a).

In the case of  $\text{LaTiO}_3$  system Fig. 3(b), it is observed that the band at around the Fermi-level is

mostly contributed by  $e_g$  and  $t_{2g}$  orbitals of transition metals (Ti). The crystal field and the electrostatic interaction between the V-cation and

the non-bonding O-2p electrons that produces the splitting of d-orbitals [48].



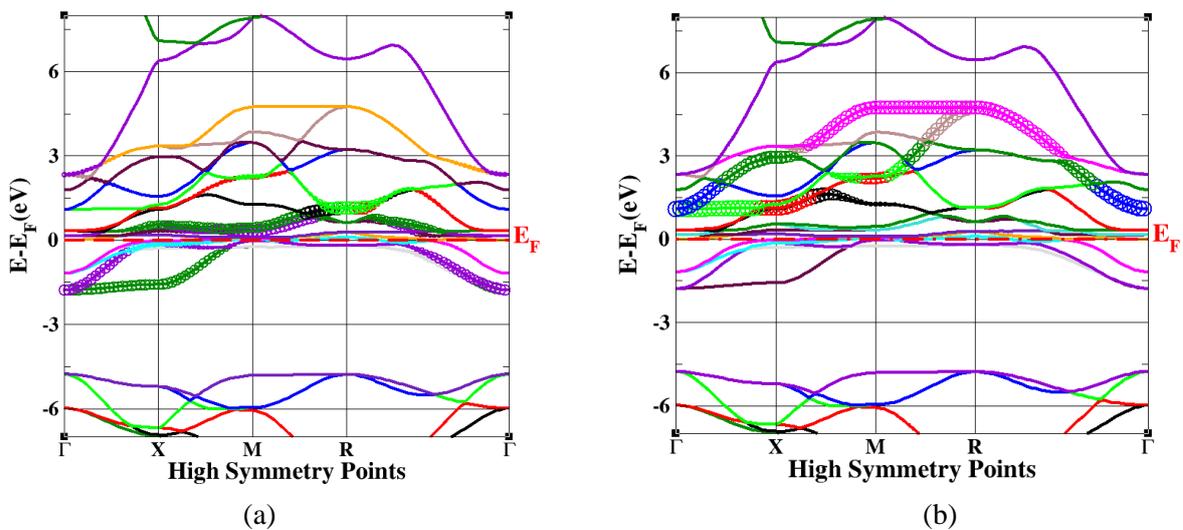
**Fig. 3:** (color online) The band structure plotted between the total energy versus the various symmetry points for  $\text{SrTiO}_3$  (left) and  $\text{LaTiO}_3$  (right) unit cell.

There are three doubly degenerate valence bands are derived mainly from the oxygen 2p orbital which are separated by a direct gap of 2.20 eV (at the  $\Gamma$  point) from the transition-metal d-derived (Ti) conduction band. This band gap is corrected to 3.423 eV by applying the modified Beck-Johnson interaction potential. It is somewhat lower than the experimental band gap of 3.75 eV for  $\text{SrTiO}_3$  [49, 50].

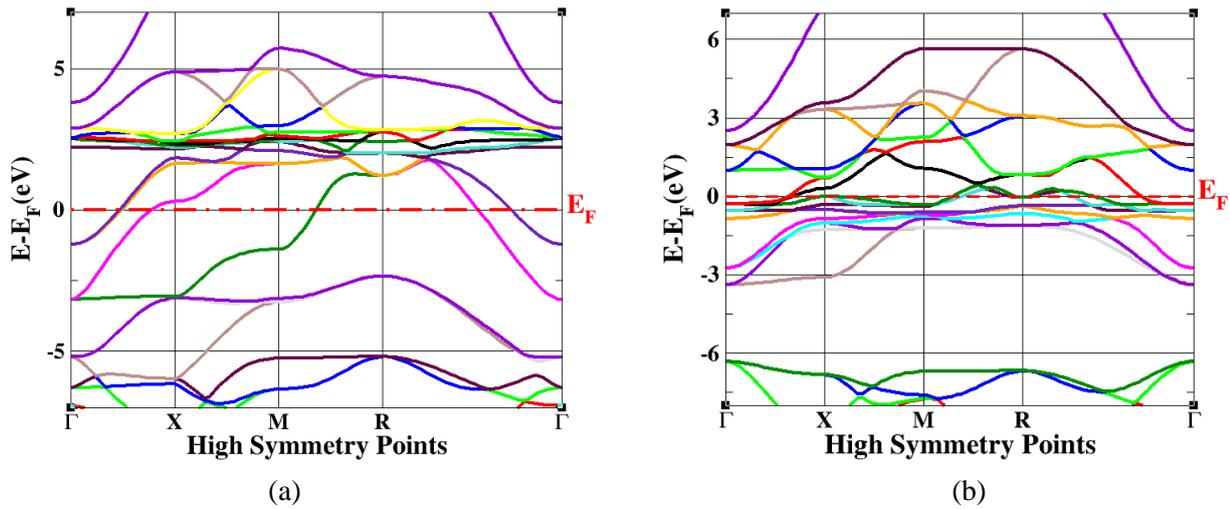
The fatbandstructures of the Ti-atom of  $\text{LaTiO}_3$  system is shown in Fig. 4.

The bandstructure of  $\text{LaTiO}_3$  is shifted by introducing the Coulomb interaction  $U$  and it is shifted further with higher value of  $U$  and Hund's exchange interactions,  $J$  and along with spin-orbit coupling, (SOC) as in Fig. 5 (a),(b).

It has been revealed that the introduction of modified Beck-Johnson interaction potential with GGA calculation for the strongly correlated system,  $\text{SrTiO}_3$  increases the band gap [49- 51].



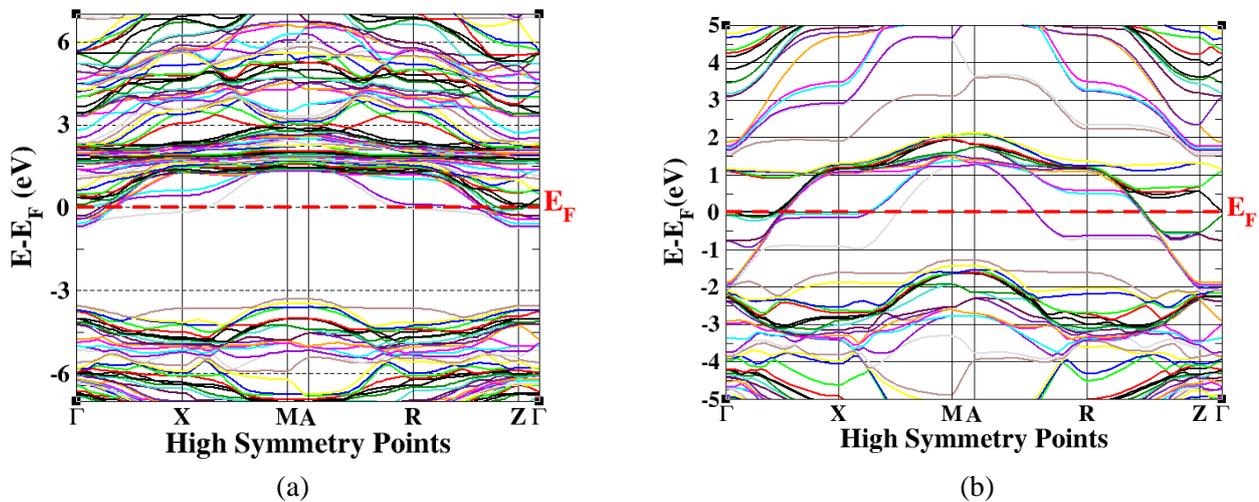
**Fig. 4:** (color online) Fatbandstructures of (a) Ti- $t_{2g}$ -orbitals on (left) and (b) Ti- $e_g$ -orbitals on (right) of  $\text{LaTiO}_3$



**Fig. 5:** (a) (color online) The shifting of band of  $LaTiO_3$  with,  $U=2.11\text{eV}$  and  $J=0.20\text{eV}$  (b) The effect of spin-orbit coupling (SOC) in  $LaTiO_3$  system.

The electronic bandstructure of superlattice,  $La_{0.80}Sr_{0.20}TiO_3$  reveals that the system is metallic and the introduction of Coulombian interaction,  $U$  and exchange interaction,  $J$  along with spin-orbit

coupling (SOC) seems to be the important parameters for determining the electronic structures of the materials as shown in Fig. 6.



**Fig. 6:** (a) (color online) Bandstructure of the  $La_{0.80}Sr_{0.20}TiO_3$  system without  $U$  and  $J$  (b) Bandstructure of same system with  $U=2.11\text{eV}$ ,  $J=0.25\text{eV}$  and SOC.

The density of states (DOS) is essentially the number of different states at a particular energy level that electrons are allowed to occupy i.e the number of electronic states per unit volume per unit energy is a useful computational tools to find the electronic structures of materials in the ground states [14,15]. In order to find the constituent atomic contribution in the electronic structure and magnetic behaviors of the system, the partial

density of states (PDOS) have been employed with consideration of the spin polarization, so as to calculate the contribution on electronic structure of individual atom. The DOS in the vicinity of the Fermi level within the band structure of  $LaTiO_3$  were attributed mostly to these octahedral hybrid orbitals. In Fig. 7 (a) The DOS of  $SrTiO_3$  with mBJ interaction is consistent with the experimental result [49-51].

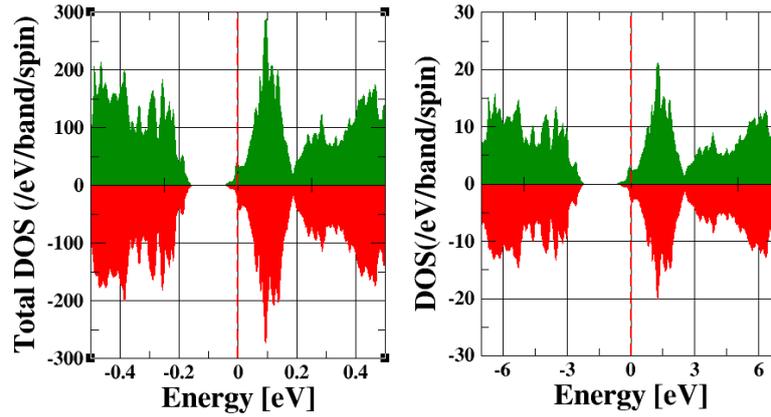


Fig. 7: (color online) The DOS of  $\text{La}_{0.20}\text{Sr}_{0.80}\text{TiO}_3$  system for both up and down spin channels.

The symmetrical distribution of DOS for both channels of the superstructures indicate that these systems are non-magnetic or paramagnetic in behaviour.

### 3.3 Charge Density Distribution and Fermi Surface of the system

The charge density 3D plot with 2D contour plot (in inset) of  $\text{LaTiO}_3$  are illustrated Fig. 8(a), and 8(b) respectively.

The strong covalent bondings between Ti- and O-atoms have been observed due to the overlap (hybridization) of O-2p and Ti-3d orbitals, which is in good agreement with the previously published papers of perovskites compounds [52,53]. The 2D-contour plot shows that the chemical bonding is mainly takes place nearest neighboring atoms.

The 3D-electron density distribution map for  $\text{LaTiO}_3$  as shown in Fig. 8(a), with the planes (011)

confirms that the electron density distribution is mainly localized near the ionic cores as expected, the high peaks of 3D plots shows the contribution of Ti-atoms, which is symmetric about the core of the atoms.

The study of Fermi surface of the system also supports the results obtained through band structure and DOS structure of the system. The Fermi surfaces around the various atomic lattice sites, constituted by several electron and hole orbits are demonstrated for the  $\text{LaTiO}_3$  systems as shown in Fig. 8(b). The Fermi surfaces constituted by 20-40 band levels are shown (inset-1) and the actual Fermi surfaces of 30-51 band levels with the tentacles, called monster is shown (inset-2). Furthermore, the Fermi level,  $E_f$  crossing through the energy bands of 30-40 band levels of the system is demonstrated in Fig. 8(b) [54, 55].

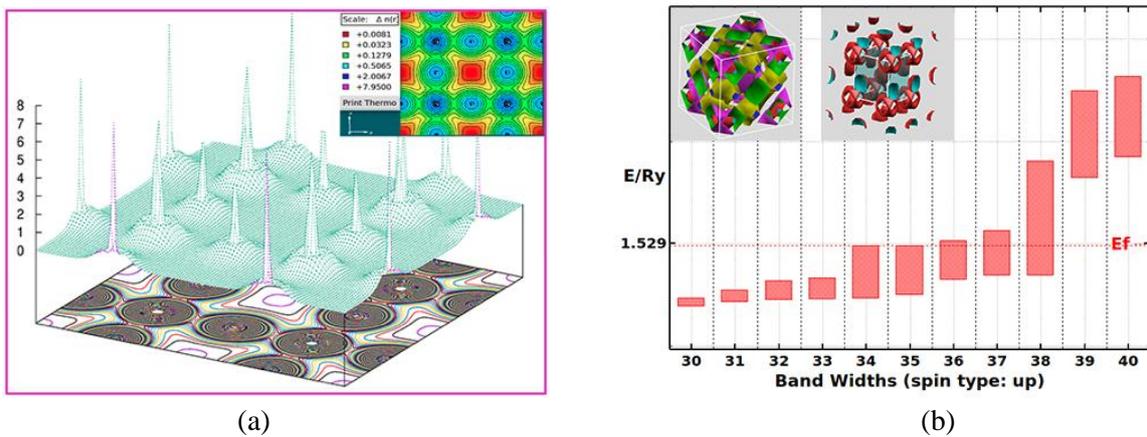


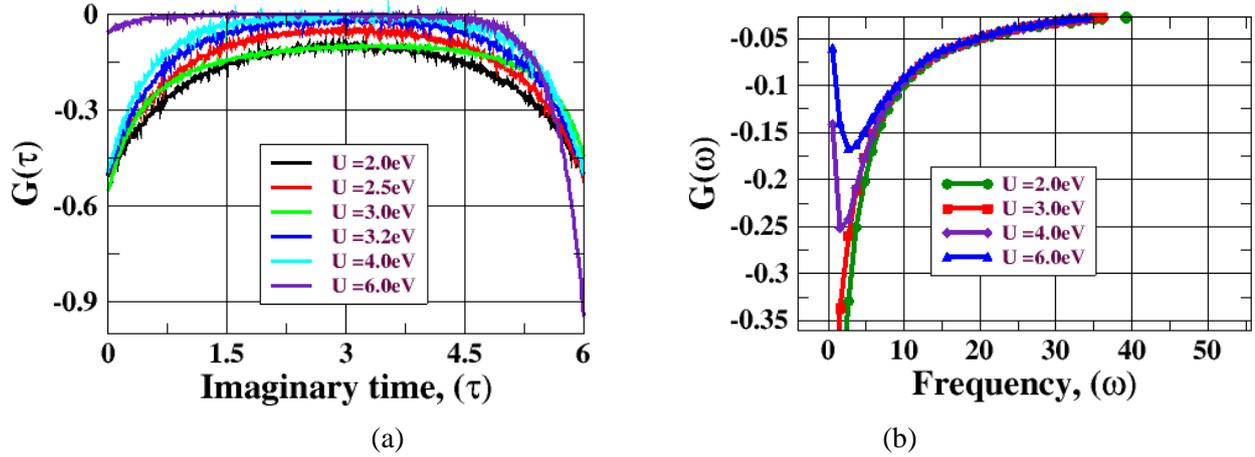
Fig. 8: (color online) (a) The 3D charge density plot along with the 2D contour plot (inset) of  $\text{LaTiO}_3$  in (011) plane (b) The Fermi level crossing through energy bands of 30-40 band levels of the  $\text{LaTiO}_3$  system with its Fermi surface and the actual Fermi surfaces of 30-51 band levels with the tentacles (inset).

### 3.4 Electronic Structure by DMFT

The conventional DFT calculation is not able to predict the realistic picture of electronic structure for strongly correlated materials, so we have employed the dynamical mean field theory (DMFT) with continuous time quantum Monte Carlo (CT-QMC) hybridization technique as the impurity solver for finding the electronic structure of the

transition metal oxides [56-59].

The characteristic variation of Green function of imaginary time, ( $\tau = it$ ) with the variation of Coulombian interaction ( $U$ ) for the thermodynamic parameter,  $\beta=6(\text{eV})^{-1}$  is shown in Fig. 9(a) and the corresponding Fourier transform of  $G(\omega)$  for the DMFT data showing the MIT with kinks at near minimum frequency as shown in Fig.9(b).

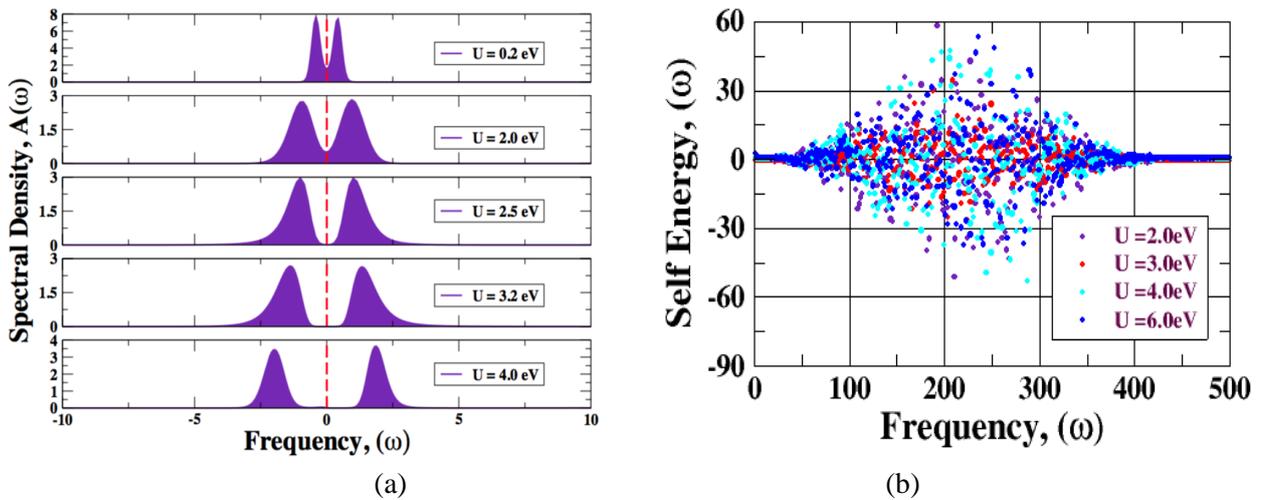


**Fig. 9:** (color online) (a) The variation of Green function vs. imaginary time with various values of  $U$  (b) the corresponding spectral density vs. frequency showing the Mott-Hubbard splitting with  $U = 4.0$  eV.

The complete metal-insulating phase transition is observed for  $U = 2.5$  eV and  $\beta = 6(\text{eV})^{-1}$  for  $LaTiO_3$  as shown in Fig. 10(a).

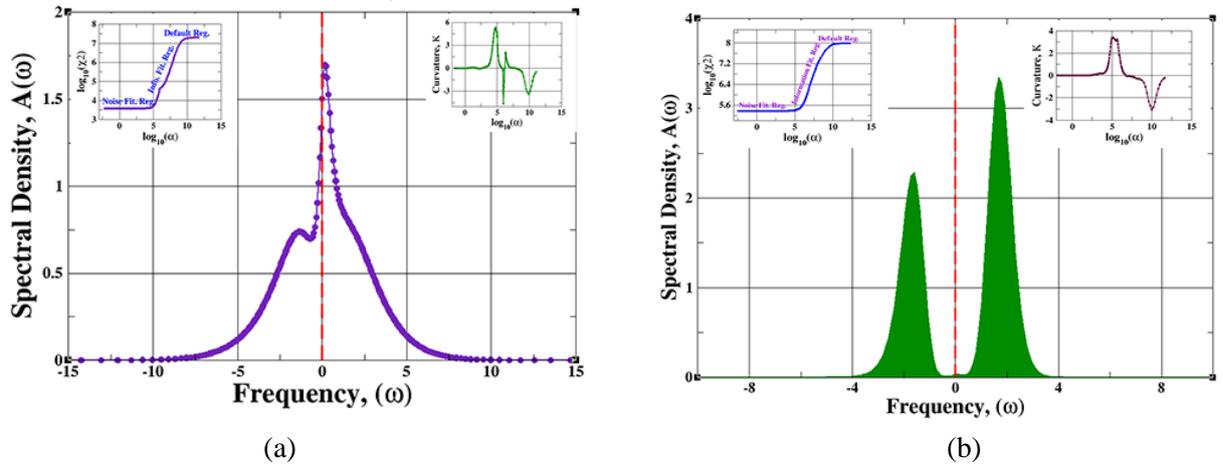
Similarly, the characteristic variation of the Green function of frequency, clearly supports the metallic and insulating phases of the materials as shown in

Fig. 10(a). The oscillation of self energy,  $\Sigma(\omega)$  oscillation with frequency is shown in Fig. 10(b) showing that there is no change in self energy,  $\Sigma(\omega)$  with the variation of the Coulombian parameter,  $U$ .



**Fig. 10:** (color online) (a) The variation of spectral density,  $A(\omega)$  vs. frequency for various  $U$  values (b) The self-energy vs. frequency.

Furthermore, the spectral density,  $A(\omega)$ , which is obtained from the Green function,  $G(\tau)$  of superlattice,  $\text{La}_{0.80}\text{Sr}_{0.20}\text{TiO}_3$  system using the Maximum Entropy model of data analysis algorithm. The metallic phase with quasi-particle peak for the superlattice,  $\text{La}_{0.80}\text{Sr}_{0.20}\text{TiO}_3$  is obtained for  $U = 3.0\text{eV}$  and  $\beta = 6(\text{eV})^{-1}$  as shown in Fig.11(a). Furthermore, on increasing the Coulombian parameter,  $U$  for a constant  $\beta = 10 (\text{eV})^{-1}$ , the system undergoes metal-insulator transition as shown in Fig. 11(b).



**Fig. 11:** (color online) (a) Green function of frequency vs. frequency showing the quasi-particle peak for  $\text{La}_{0.80}\text{Sr}_{0.20}\text{TiO}_3$ . The logistic regression curve or sigmoid curve (inset), which is the cross validation error analysis of calculation. (b) The metal insulator phase transition for  $U = 3.5 \text{ eV}$  and  $\beta = 10 \text{ eV}^{-1}$  for superlattice,  $\text{La}_{0.20}\text{Sr}_{0.80}\text{TiO}_3$  and the logistic regression curve along with the curvature of it (inset).

### 3.5 Transport properties of $\text{SrTiO}_3$ and $\text{LaTiO}_3$

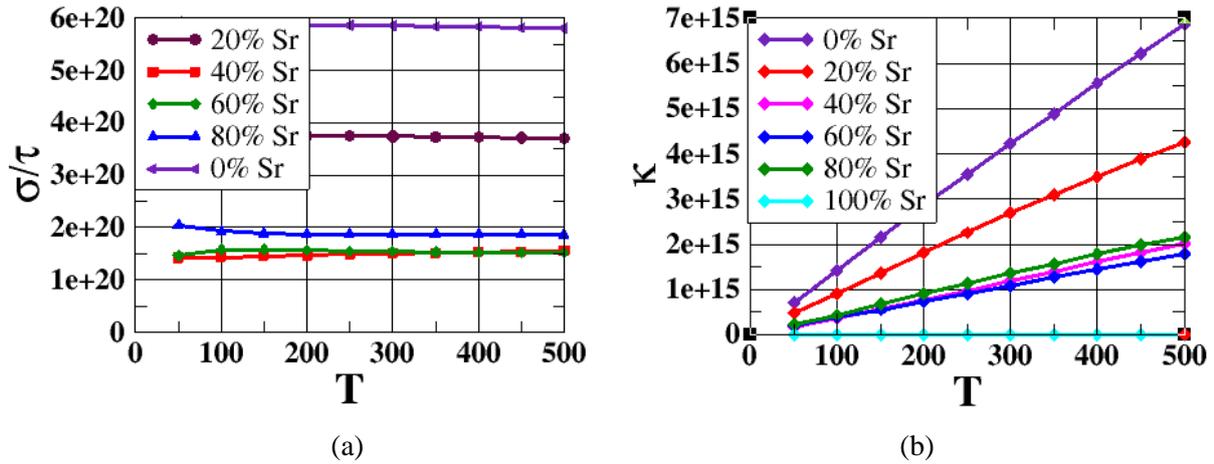
The various properties of materials, such as the transport properties are also associated with the electrons and lattice interactions. Here, the density functional theory (DFT) have employed for investigating electrical, thermal, and thermoelectric behaviours of TMOs based on the BoltzTrap module [11,61]. The ever-increasing computing power has made the first principles calculation more and more accurate and straightforward. As the transport properties of the materials are electronic bandstructure dependent quantities, the BoltzTrap codes, which implements the linearized Boltzmann transport equation is applicable to compute various transport coefficients including intermetallic compounds, high  $T_C$  superconductor and thermoelectric materials etc.

The study of transport properties are highly useful to predict and design a new materials for diverse fields, such as the superconductors, transparent

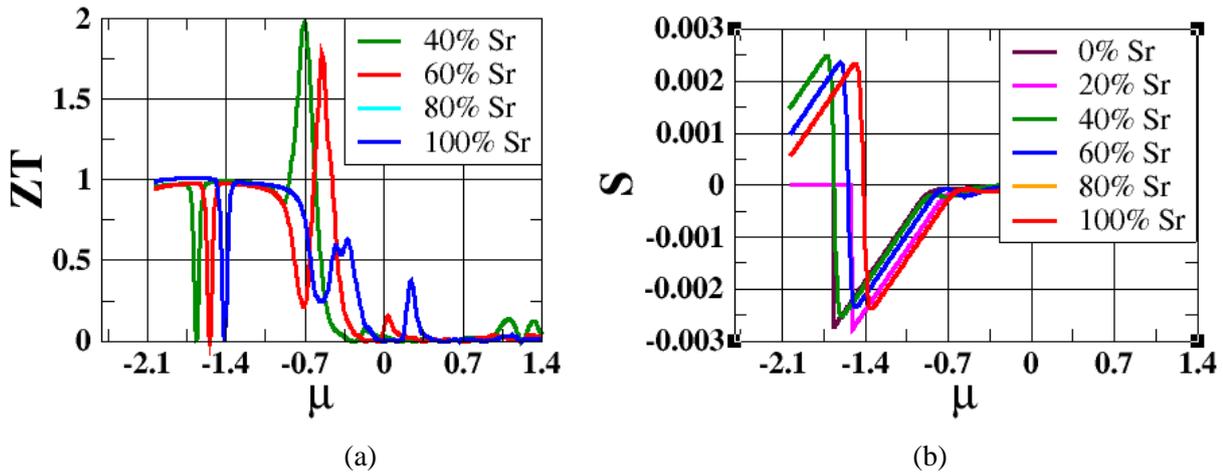
conductors, transparent insulators, inter-metallic phases as well as the efficient thermometric materials [18, 61].

The significant variation of electrical conductivity,  $(\sigma/\tau)$  and thermal conductivity,  $(\kappa)$  with temperature are observed for the different proportion of Sr-atom in the supercells for a constant chemical potential,  $\mu = 0.821 \text{ eV}$ . But, the change of electrical conductivity varies slowly (not significantly) with temperature whereas the thermal conductivity varies significantly with temperature along with the various proportions of Sr-atoms on the supercells.

The comparison of Figure of merit (ZT) vs. chemical potential ( $\mu$ ) at room temperature shows that the  $ZT \sim 1.78$  for a system with 40% of Sr-ions at around  $\mu = -0.7 \text{ eV}$ . A remarkable thermoelectric phase transitions are observed for Seebeck Coefficient at temperature, 300 K for the systems with higher proportion of Sr-ions.



**Fig. 12:** (color online) (a) The variation of electrical conductivity with temperature (b) The variation thermal conductivity with temperature for different proportion of Sr-ions having the same chemical potential,  $\mu = 0.821$  eV.



**Fig. 13:** (color online) (a) The comparison of Figure of merit ( $ZT$ ) with chemical potential ( $\mu$ ) at room temperature for various proportion of Sr-ions (b) The thermoelectric phase transition are observed for Seebeck Coefficient vs. chemical potential ( $\mu$ ) at temperature, 300 K.

The ultimate study of finding these transport properties is to investigate the possibility of promising thermoelectric materials by knowing the Figure of merit (transport coefficient) as shown in Fig.13. The higher the value of  $ZT$  confirms that the better the potential materials for thermoelectric application for recycling the wastage of heat energy [62,63].

#### 4. CONCLUSIONS

The electronic structure and transport properties of pristine  $LaTiO_3$  and  $SrTiO_3$  along with their superlattice system have been studied using conventional DFT and DMFT.

The shifts in the energy bands of TMOs are clearly observed by introducing the Coulombian interaction ( $U$ ), Hund's exchange ( $J$ ) and spin-orbit couplings (SOC). The calculated band gap for  $SrTiO_3$  is found to be 3.423 eV with mBJ interaction potential, which is close enough to the experimental information.

The dynamical mean field theory (DMFT) with CT-QMC-hybridization as impurity solver have employed to investigate metal-insulator (MIT) phase transition of pristine  $LaTiO_3$  and the superlattice of  $La_{(1-x)}Sr_xTiO_3$  system. The correlation parameters for the pristine  $LaTiO_3$  for a distinct metal-insulator transition (MIT) are

obtained for  $U = 2.5$  eV,  $\beta = 6(\text{eV})^{-1}$  and  $J = 0.60$  eV. Whereas these parameters are found to be  $U = 3.2$  eV,  $\beta = 10 (\text{eV})^{-1}$  and  $J = 0.60$  eV for the  $\text{La}_{0.80}\text{Sr}_{0.20}\text{TiO}_3$  system and  $U = 3.5$  eV,  $\beta = 10 (\text{eV})^{-1}$  and  $J = 0.60$  eV for the  $\text{La}_{0.20}\text{Sr}_{0.80}\text{TiO}_3$  system respectively. The spike of the quasiparticles at around the Fermi level of  $\text{La}_{0.80}\text{Sr}_{0.20}\text{TiO}_3$  system is observed for  $U = 3.0$  eV,  $\beta = 6(\text{eV})^{-1}$ ,  $J = 0.60$  eV.

The thermal conductivity varies significantly with the temperature but the electrical conductivity is observed to be remains same with temperature for a system. The higher value of Figure of merit,  $ZT \sim 1.75$  and  $1.99$  are calculated for the systems with 40% and 60% of the Sr-ions. The thermoelectric phase transition with chemical potential,  $\mu$  are observed at around  $\mu \sim -1.4$  eV for system with higher proportion of Sr-ions. Thus, the  $\text{La}_{(1-x)}\text{Sr}_x\text{TiO}_3$  systems are the potential candidates for the thermoelectric application at higher temperature.

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