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Ab initio investigation of the role of vanadium impurity states in SrTiO₃ for thermoelectricity

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Abstract

Despite their low cost, non-toxicity, thermal/chemical stability and relative abundance, oxides are not considered as promising materials for future thermoelectric devices. The main reason behind this lack of interest is their relatively high thermal conductivity. However, some oxides, such as n doped bulk SrTiO₃ exhibit a rather good power factor. Keeping in mind that alloying and nanostructuring are two efficient procedures to suppress the thermal conductivity, it is worth exploring pathways towards an enhancement of the thermopower. Here, we report that vanadium doping of SrTiO₃ gives rise to well defined resonant states allowing power factor of both n and p type over a relatively broad range of carrier concentrations. We investigate both the effects of a rigid band shift of the Fermi level and of realistic co-doping using DFT calculations.

Keywords: thermoelectricity, thermoelectric power factor, resonant states, Seebeck coefficient, oxides, SrTiO₃, *ab initio* electronic transport

1. Introduction

Global energy demand, due to the ceaseless increase in population and industrialization is one of the major worldwide concerns of the 21st century [1, 2]. The unanticipated depletion of natural fossil energy resources, combined with the negative environmental impacts of pollution and global warming, has boosted the search for efficient alternative and sustainable energy harvesting methods. Thermoelectric (TE) materials are expected to play a major role in managing global energy crisis because they enable direct conversion from thermal to electrical energy, and thus provide an alternative source of power generation [3, 4]. Thermoelectric generators are a convenient means of generating green energy by harnessing the waste heat, and their conversion efficiency is primarily governed by the TE figure-of-merit defined as $ZT = \frac{\sigma S^2}{\kappa} T$, where S is the Seebeck coefficient, σ the electronic conductivity and κ the total thermal conductivity (sum of electronic and lattice contributions). The current focus of TE research is directed toward the development of TE materials, which are non

toxic, earth-abundant, and chemically stable at the operating temperatures. As TE generators are solid-state devices with no moving parts, they are silent, reliable and scalable, making them ideal for small, distributed power generation.

Oxide TE materials fulfill these restrictive constraints and have also the advantage of being of low cost. However, compared to traditional TE materials, they exhibit only modest TE performances due to their high thermal conductivity. Numerous studies have been done to improve their TE response by doping (significant increase of electrical conductivity). The perovskite material SrTiO₃ (STO) is particularly interesting because it has already a relatively large power factor of the order of $39 \mu\text{W.cm}^{-1}.\text{K}^{-2}$ [5], that is comparable to that of the best known TE materials such as Bi₂Te₃ [6]. However, because of its relatively high thermal conductivity of $\kappa \approx 11 \text{ W.m}^{-1}.\text{K}^{-1}$, [7] STO exhibits a relatively modest ZT of only 0.1, unlike Bi₂Te₃ which has a κ around $1.6 \text{ W.m}^{-1}.\text{K}^{-1}$ and a $ZT \approx 0.96$ [8, 9].

In recent years, the idea of using nanotechnology to improve the figure of merit of conventional TE materials has triggered active research. Most of the reported ZT enhancements are based on dimensionality reduction (thin films and nanowires) that leads to significant thermal conductivity reduction [10–12].

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The second strategy that could improve the ZT consists in focusing on the power factor $\sigma.S^2$. Mahan and Sofo [13] suggested that the introduction of a sharp peak in the density of states could significantly boost the figure of merit. Similar arguments have also been proposed by Hicks and Dresselhaus [14, 15] by dimensionality reductions. Improving the power factor can be achieved by dopants that would create sharp hybridized impurity states (resonant states) inside the conduction/valence band of the host material. **The procedure has been attempted by many researchers with chalcogenide compounds, for instance: Tl doped PbTe [16, 17], Sb doped CdTe alloyed PbTe [18], Sn doped Bi₂Te₃ [19], In doped SnTe [20, 21], Mg-In [22] co-doped SnTe or In doped [23] GeTe.**

The physics of impurity/resonant levels may be also relevant in the case of superconductivity. For instance in heavily doped semiconductors such as B doped diamond [24], an insulator to metal transition occurs with a superconducting behavior [25] at low temperature. However, the conventional mechanism corresponds to a shift from an impurity band to a degenerate situation where the Fermi level is located in the valence band. This “resonant valence band” is then leading to a clear superconducting behavior.

In contrast to this scenario, it has recently been proposed that impurity states actually suppress the conductivity although with a strong variations of the transport distribution function leading to a boost in the Seebeck coefficient which overcompensates the conductivity reduction [26]. Herein, we report on the theoretical basis of *ab initio* calculations the use of vanadium to dope STO which advantageously exhibits impurity states within the gap which promotes a boost of the Seebeck coefficient.

2. Theoretical background

In what follow, the TE properties are calculated using the Landauer formalism combined with *ab initio* calculations. In the linear response regime, the electrical conductance and the Seebeck coefficient can be written as:

$$G = -\frac{2e^2}{h}L_0, \quad S = -\frac{1}{k_B T}L_1/L_0, \quad (1)$$

$$\text{with, } L_n = \int_{-\infty}^{+\infty} (E - E_F)^n \tilde{T}(E) \left(\frac{\partial f}{\partial E} \right) dE,$$

where T is the temperature, e the magnitude of the electron charge, \hbar the Planck's constant, k_B the Boltzmann's constant, E_F the Fermi level, f the Fermi distribution and $\tilde{T}(E)$ the energy dependent transmission.

For a conductor of length l_z , the transmission can be recast as $\tilde{T}(E) = \frac{\lambda(E)}{l_z} M(E)$, where $\lambda(E)$ is the mean free path and $M(E)$ the density of modes (DOM) [27]. For this work, we have used a constant mean free path approximation [28] *i.e.* $\lambda(E) = \lambda_0$ with $\lambda_0 \simeq 20$ Å which reproduces the room-temperature resistivity measured in 10 % La-doped STO samples [5, 6, 29]. The DOM can be evaluated by a direct diagonalization of the Hamiltonian of the system using the eigenvalues (see for instance Ref.30). This DOM corresponds to a count of the bands intersecting the energy of interest. Finally, the electrical conductivity is defined as $\sigma = \frac{l_z}{l_x \times l_y} G$, where l_x and l_y are the dimensions of the system perpendicular to the transport direction.

The *ab initio* calculations are performed with the DFT package SIESTA [31]. This code is very well suited to study oxides as it is based on atomic like orbitals. We have used the Perdew, Burke & Ernzerhof [32] exchange-correlation functional corresponding to a generalized gradient approximation. A Troullier-Martin norm-conserving pseudopotentials [33] has been used. The basis corresponds to a double- ζ -polarized basis optimized with the simplex tool of the SIESTA package. All the atomic structures were optimized up to forces less than 0.01 eV/Å and to an hydrostatic pressure less than 0.1 kbar. Finally, a Monkhorst-pack of $6 \times 6 \times 6$ k-points has been used for the self consistent calculations ($80 \times 80 \times 80$ for the transport calculations) along with a mesh cutoff of 400 Ry.

3. Vanadium doping

In Fig. 1 is given the band structure along with the density of states (DOS) of pristine STO and vanadium doped STO. As pointed out in Ref. 29 the lowest conduction bands of pristine STO are mainly due to the *d*-type orbitals of Ti (namely, it corresponds to t_{2g} orbitals). When doped with vanadium (in substitution of a Ti atom), the main issue is the occurrence of impurity bands at the bottom of the conduction bands. As illustrated by the projected density of states, these bands are mainly due to the *d* orbitals of V and, as can be seen, they are acting as resonant states. Indeed, they are in close vicinity of the t_{2g} bands and this is leading to a large increase of the DOS and, as pointed hereafter, of the Seebeck coefficient. However, in order

to use these resonant states for TE application, the Fermi level must be in close vicinity of them. For the vanadium concentration used in Fig. 1, the Fermi level is definitely located far from the resonant region. This point raises the need to fill the conduction bands up to the resonant states either by means of a device based on a field effect or by using a co-dopant that would shift the Fermi level.

In Fig 2 is represented the electrical conductivity σ , the Seebeck coefficient S and the power factor (PF) $\sigma \cdot S^2$ using a rigid band shift model for n-type doping. This model, which consists in moving rigidly the Fermi level, illustrates the equivalent effect of a field effect device. As a guide to the eyes, we have added at the top of the figure the corresponding equivalent doping of lanthanum in the hypothesis of a perfect electron reservoir. We have investigated the pristine case (undoped STO) and STO doped with vanadium for 2 different concentrations. It should be noted that the abscissa corresponds to the added carrier charge with respect to the neutral material. It is obtained by integrating the DOS from the Fermi level. For this reason, the conductivity for V doped STO at zero added carrier charge has a non-zero value. Conversely, for pristine STO the conductivity is exactly zero at zero added carrier charge.

For pristine STO the behavior is quite conventional. As a matter of fact, the conductivity increases with the added carrier charge and the Seebeck coefficient is negative and decreases with the added carrier. This is leading to the familiar behavior for the PF with a sharp peak

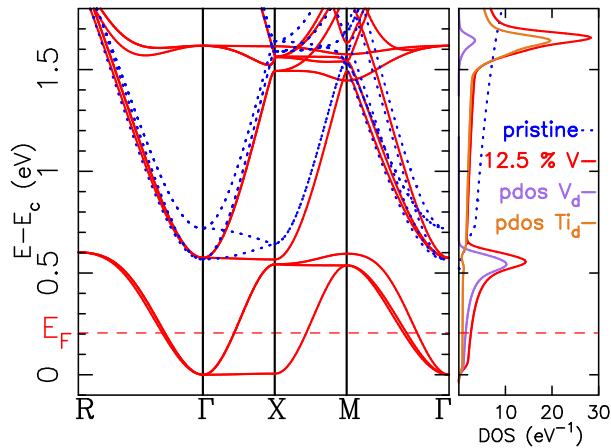


Figure 1: Band structure and density of states for pristine SrTiO_3 and $\text{SrTi}_{0.875}\text{V}_{0.125}\text{O}_3$ along with its projected density of states for the d orbitals of V and Ti as function of the energy (centered relatively to the bottom of the conduction band of $\text{SrTi}_{0.875}\text{V}_{0.125}\text{O}_3$ and denoted E_c).

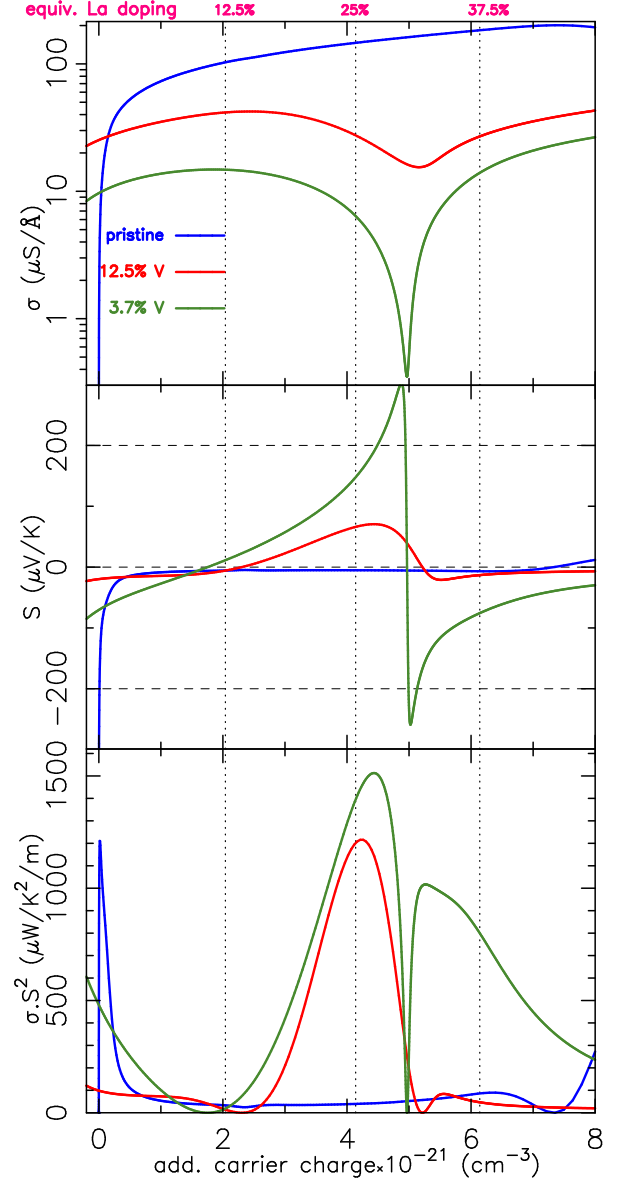


Figure 2: From top to bottom, electrical conductivity, Seebeck coefficient and power factor obtained with a rigid band shift model for pristine and V doped STO as function of the added carrier charge to the neutral material. On top is given the theoretical equivalent La co-doping required to achieve the corresponding added carrier charge.

linked with the two opposite trends of S and σ .

For doped STO, the behavior is completely different. The major effect occurs for the Seebeck coefficient which exhibits a sign inversion close to the resonant states. This point, as we have already pointed out in a previous work [26], is opening new perspectives for obtaining both n and p-type TE materials using the same dopant. Moreover, for a concentration of

3.7%, the amplitude of the Seebeck coefficient (at the maximum of the PF) is of the same amplitude that pristine STO. One can argue that the increase of the Seebeck comes with a decrease of the conductivity, but as the PF depends on the square of the Seebeck coefficient, the resulting PF is as large as that of the pristine material. Finally, it should be noted that the range of the carrier charge, for which these large values of the PF are observed with V doped STO, is much greater than the pristine case.

4. Co-doping

Another way to fill the conduction band up to the resonant state could come from a second dopant which would act as an electron reservoir for STO *i.e.* which would lead to a significant charge transfer without modifying the band structure. Actually, La in substitution to Sr appears to be a very good candidate for electron doping in STO [29]. For instance, this reservoir behavior is also observed with yttrium and niobium doping [34, 35]. The whole strategy is thus to use vanadium to create resonant states and to use a co-dopant as an electron reservoir in order to fill the conduction band up to these resonant states. However, it is definitely not obvious that for STO doped with both vanadium and a co-dopant the particular behavior pointed out previously will be preserved.

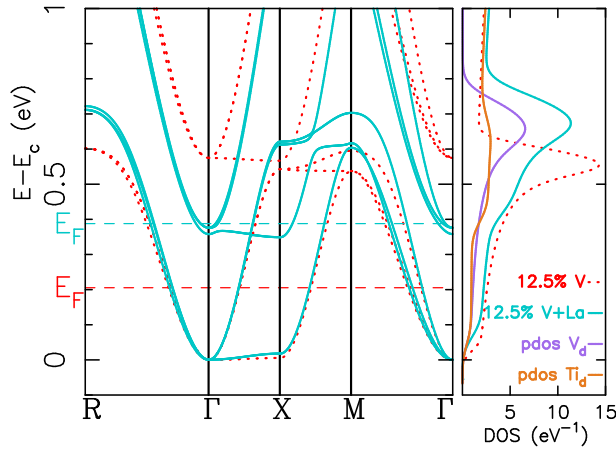


Figure 3: Band structure and density of states (DOS) for $\text{SrTi}_{0.875}\text{V}_{0.125}\text{O}_3$ and $\text{Sr}_{0.875}\text{La}_{0.125}\text{Ti}_{0.875}\text{V}_{0.125}\text{O}_3$ along with its projected density of states for the d orbitals of V and Ti as function of the energy (centered relatively to the bottom of the conduction band).

In Fig. 3 is given the band structure along with the DOS of co-doped STO with V and La. We have also

represented the band structure of STO doped only with V (same as in Fig. 1) for comparison purposes. It can be noticed that La has not a neutral role when combined with V. The impurity bands induced by vanadium are still observed, but these bands are shifted at higher energy and are actually overlapping with the t_{2g} bands. Indeed, at the top of the impurity bands, we have now a clear mix with the intrinsic bands of STO. This behavior is very specific to the co-doping and for a doping with La alone, we have verified that the band structure of pristine STO is preserved *i.e.* that La is an electron reservoir. This mixing (or pinning) of the impurity bands with the t_{2g} ones has an influence on the resonant state as can be seen on the DOS. First, the resonant states are now shifted at higher energy and second, the amplitude of the DOS is reduced compared to the case where V is used alone. As presented hereafter, the amplitude of the Seebeck coefficient at the resonant states is affected too by this phenomenon.

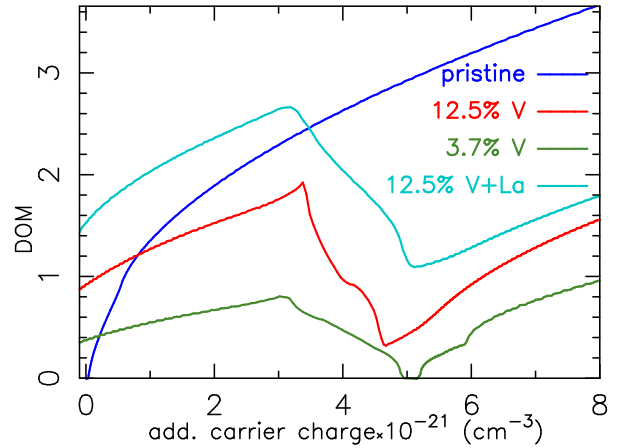


Figure 4: Density of modes (DOM) for pristine SrTiO_3 , $\text{SrTi}_{1-x}\text{V}_x\text{O}_3$ ($x = 12.5\%$ and 3.7%) and $\text{Sr}_{0.875}\text{La}_{0.125}\text{Ti}_{0.875}\text{V}_{0.125}\text{O}_3$ as function of the added carrier charge to the materials.

In order to have some insights on the effects associated with the co-doping, the DOM for pristine STO, V doped STO and co-doped STO with V and La are presented in Fig. 4. First of all, the sign inversion of the Seebeck coefficient pointed out previously (see Fig. 2) for V doped STO is actually directly linked with the slope inversion of the DOM. For pristine STO, the slope is strictly positive and thus the sign of the Seebeck coefficient remains constant. Conversely, for V doped STO this slope exhibits an inversion which is fully related to the resonant states induced by the vanadium. This phenomenon is observed for all doping concentrations and also when a co-dopant

is introduced. however, a close examination of the expression of the Seebeck (see eq. 1) leads us to the conclusion that, in order to obtain a large Seebeck coefficient, we both need a negative slope for the DOM and a slope transition which tends as close as possible to zero. This situation is achieved for STO solely doped with V when the dopant concentration is small enough. For co-doped STO we obtain a negative slope almost equivalent but, due to the pinning of the impurity bands with the t_{2g} bands, the DOM does not tend to zero. For this reason, and as presented hereafter, the amplitude of the Seebeck coefficient for co-doped STO is smaller than that of STO doped with V only.

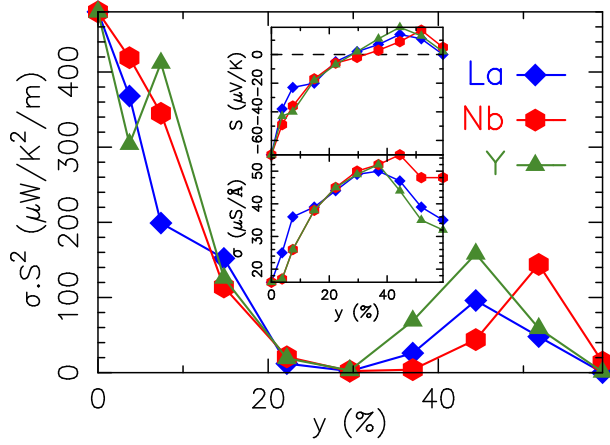


Figure 5: Power factor for $\text{Sr}_{1-y}\text{La}_y\text{Ti}_{1-x}\text{V}_x\text{O}_3$, $\text{Sr}_{1-y}\text{Y}_y\text{Ti}_{1-x}\text{V}_x\text{O}_3$ and $\text{SrTi}_{1-x-y}\text{V}_x\text{Nb}_y\text{O}_3$ with $x = 3.7\%$ as function of the co-dopant concentration. The Seebeck coefficient and the conductivity are given in inset.

In Fig. 5 is given the PF (the Seebeck and the conductivity are in inset) for co-doped STO. It corresponds to a vanadium concentration of 3.7% which has been observed to be the best choice to take benefit of the resonant states. The concentration of the co-dopant is ranging from 0 to almost 60%. We have considered three different co-dopants (La, Nb and Y) which all have been observed experimentally to be electron dopants for STO [34, 35]. However, as can be seen in this figure, all of them are leading to a very similar behavior.

The Seebeck coefficient is behaving in a rather close way to what we have already observed in Fig. 2, that is to say a sign which can be either positive or negative depending on the co-dopant concentration. For small co-dopant concentration, we have a negative sign for the Seebeck (as conventionally observed for electron doping) but for large concentration the Seebeck coefficient tends to zero and becomes positive. This behavior has a

direct impact on the PF.

For low co-dopant concentration, the PF decreases when the co-dopant concentration increases. It goes to zero when the Seebeck coefficient sign reverses and finally increases and reaches a second maximum but now with a positive Seebeck coefficient for large co-dopant concentration. This observation opens the perspective to obtain both n and p type TE materials doped with exactly the same dopants. In this paradigm, the n or p nature would be chosen by modifying only the co-dopant concentration. However, due to the pinning effect mentioned previously, conventional dopants such as La, Nb or Y do not allow to obtain a significant PF and further investigations are required in order to improve the amplitude of the Seebeck coefficient and thus of the PF.

5. Conclusion

In the present work, the mechanism for SrTiO_3 doped with vanadium based on resonant states to boost the power factor has been investigated. This mechanism, conversely to the accepted picture of a boost of the density of states, is linked with a reduction of the conductivity together with a boost of the Seebeck coefficient against all odds. This result may open the perspective to use only a single dopant to obtain both n and p type semiconductor for thermoelectricity thanks to the sign inversion of the Seebeck coefficient observed in the vicinity of the resonant peak. Moreover, by using co-dopant such as La, Nb or Y, an actual sign inversion of the Seebeck coefficient is observed by modifying the co-dopant concentration of the compound. However, the power factor amplitude is actually less significant than that observed within a rigid band shift which indicates that these co-dopants are no more simple electron reservoirs in V doped SrTiO_3 .

This demonstrates the possible use of the same compound (same dopant and co-dopant) to obtain both n and p type thermoelectric materials by tuning the co-dopant concentration, which can be a true benefit for building thermoelectric devices. However, the co-doping by conventional dopants such as La, Nb or Y is not satisfactory in terms of PF amplitude. Finally, nanostructuring could be an efficient way to both tune the position of the resonant peak and eventually further enhance the n(p)-type power factor.

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