Thermoelectric properties of Strontium related Perovskite \( \text{SrBO}_3 \) compounds

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Abstract

Thermoelectric materials are in great demand due to its conversion to thermal to electrical energy. So, researchers are continuously in study to investigate material with high figure of merit (ZT). The thermoelectric properties of different \( \text{SrBO}_3 \) compounds have studied here. Boltzmann transport phenomenon along with density functional theory are used for investigating thermoelectric properties. The thermoelectric properties i.e. Seebeck Coefficient, Thermal conductivity, Electrical conductivity and figure of merit have evaluated at different temperature from room temperature to about 800K. Strontium iridates (\( \text{SrIrO}_3 \)) have been examined using DFT with full potential- linearized augmented plane wave FP-LAPW as used in Wien2K and Strontium titanate (\( \text{SrTiO}_3 \)) have examined using DFT and plane wave pseudo potential formulation which is used in Quantum espresso coding. Calculations done by using Perdew Burke Ernzerhof (PBE) exchange correlation function with generalized gradient approximation (GGA).

Keywords: Perovskite compounds, PBE, GGA, SOC, DFT calculation, thermoelectric properties

1. Introduction

Transport properties of \( \text{SrBO}_3 \) (B=Ru, Ir, Ti) have been studied for understanding the trend between them. Thermoelectric properties of perovskites material are great in demand for its future application in industry. The performance of thermoelectric material depends on Seebeck Coefficient, electrical conductivity and thermal conductivity. The material with high Seebeck coefficient, high electrical conductivity and low thermal conductivity are best performer for conversion of thermal to electrical energy. These kinds of material retain heat at junction and heat transfer losses are very less. Figure of merit denoted by ZT; a dimensionless quantity determines the effectiveness of thermoelectric substances. Z can be expressed as

\[
Z = S^2 \sigma / \kappa \tag{1}
\]

where \( S \) is Seebeck coefficient, \( \kappa \) is thermal conductivity, \( \sigma \) is electrical conductivity and \( T \) is absolute temperature[1-2]. Thermal conductivity \( \kappa \) includes electronic as well as ionic thermal conductivity. For practical application ZT is to be more than or equal to 1. Equation 1 shows that Z is directly proportional to \( S^2 \sigma \), which is known as power factor and inversely proportional to thermal conductivity \( \kappa \). Also, \( \sigma = 1/\rho \), where \( \rho \) is electrical resistivity. For theoretical investigation, BoltzTrap code [9] which uses Boltzmann transport phenomenon is used for measuring transport properties of thermoelectric materials. Result are compared with experimental result.

Perovskite material are of \( \text{ABO}_3 \) type where \( \text{A} \) is large oxide ion present at the centre of the cubic lattice, \( \text{B} \) is the metal ion of smaller radius present at the 8 corners of the lattice and oxygen ions are at 12 edges of
cube. $A^{2+}$ ions present in the twelve-fold cavities in between the polyhedra. $[BO_6]^{2-}$ forming octahedral structure in which B is present at the octahedral voids[3]. It can be arranged in other way also in which A (Sr) large cation occupy the corner position of the cube and oxygen occupy the centre of the faces of the cube and B (Ti, Ir) smaller cation occupy centre of the cube. In both the form, Oxygen ions form octahedral hole which was occupied by $B^{4+}$ ion. Together $A^{2+}$ and $O^{2-}$ form a solid cubical lattice as shown in figure 1.

In this work we will study the thermoelectric properties of SrBO$_3$ perovskite material. In Section 2 we briefly discuss about the methodology used in calculating thermoelectric properties of SrBO$_3$(B= Ru, Ir, Ti) and in section 3 discusses about the results in detailed. We concluded finally in section 4.

![Perovskite material ABX3 representing two different forms](image)

**Figure 1**: Perovskite material ABX3 representing two different forms [13-14]

### 2. Methodology

Thermoelectric properties of SrRuO$_3$ is calculated experimentally in which Seebeck coefficient and electrical resistivity were calculated at temperature ranges from room temperature to 1000k [2].

For calculating thermoelectric properties of SrTiO$_3$ and SrIrO$_3$ authors [1,4] have used theoretical method. Semi classical Boltzmann transport theory was used for calculating thermoelectric properties of SrTiO$_3$ using a maxi-mally localized Wannier function (MLWF) [5]. These properties of SrTiO$_3$ were calculated at different-different temperatures ranging from 300 K to 800 K with chemical potential $\mu$ as a function [1]. The theoretical examination was done through Density functional theory with plane wave pseudopotential formalism as incorporated in Quantum expresso packages [6]. Calculation uses Perdew Burke Ernzerhof exchange correlation function [7].

Thermoelectric properties of SrIrO$_3$ i.e. figure of merit ZT, Seebeck coefficient $S$, power factor $S^2\sigma$, thermal conductivity $\kappa$ are calculated with chemical potential with or without spin orbital coupling(SOC) [4]. Boltzmann transport theory which was used in BoltzTrap code [9] used for calculation of its transport properties. FP-LAPW method of DFT as included in the WIEN2k code [10] was used for calculations.
3. Result

SrRuO$_3$ is an orthorhombic structure with lattice parameter $a$, $b$, $c$ are 0.5569 nm, 0.5553 nm, and 0.7875 nm respectively.

![Figure 2: Temperature dependence of the a) Seebeck coefficient of SrRuO$_3$[2] b) thermal conductivity of SrRuO$_3$[2]](image)

Figure 2 (a) represent the effect of temperature on seebeck coefficient of SrRuO$_3$ perovskite. The graph shows the value of seebeck coefficient is around 30-40µVK$^{-1}$. Figure 2 (b) represents the effect of temperature on thermal conductivity. Thermal conductivity increases linearly with temperature. It is around 6Wm$^{-1}$K$^{-1}$. Result are compared with data of other compound data[11-12].

Boltzmann transport theory used for calculating transport properties of SrTiO$_3$ with approximate value of relaxation time to be equal to 10fs.

![Figure 3: Effect of chemical potential on Seebeck Coefficient and electrical conductivity of SrTiO$_3$ for different temperature ranges[1].](image)

Figure 3 shows the behavior of Seebeck coefficient and electrical conductivity on varying chemical potential for temperature range 300K, 400K,500K, 600K, 700K, 800K. The result shows that on increasing the temperature value of Seebeck coefficient decreases with respect to chemical potential. Electrical conductivity graph shows that chemical potential 11eV and 12.4eV are threshold value where electrical conductivity is minimum i.e. minimum conduction occur within these two values of chemical potential.
Figure 4: Effect of chemical potential on a) thermal conductivity b) figure of merit of SrTiO$_3$ with variation of temperature [1].

Figure 4 a) represents the effect of chemical potential $\mu$ on thermal conductivity of SrTiO$_3$ for different temperature ranges varying from 300K to 800 K. Figure 4 b) represents the graph between $\mu$ and ZT, figure of merit (300-800K). We interpreted from the graph that the thermal conductivity is minimum between 11-12.4 eV. Since figure of merit is inversely proportional to thermal conductivity that is, we should get maximum value of figure of merit between these values. The same result we are getting from the graph. Thermal conductivity has more effect of temperature beyond the threshold values. Higher the value of temperature lower is its thermal conductivity.

The thermoelectric properties of perovskite SrIrO$_3$ have been studied using Boltzmann transport theory at room temperature with chemical potential. Figure 5 shows the thermoelectric properties graph i.e. plot of seebeck coefficient ($S$), thermal conductivity ($\kappa$), electrical conductivity ($\sigma$) and figure of merit ($ZT$) versus chemical potential ($\mu$) at room temperature. Generalized gradient approximation and PBEsol is used along with or without spin orbital coupling. Range of chemical potential used is -2eV to 2eV. Negative values of seebeck coefficient are due to n type region and positive values are due to p type region. The high value of seebeck coefficient is in the range 0.38eV to 1.30 eV. The maximum value is around 900$\mu$V/K and minimum at -1200$\mu$V/K. Electrical and thermal conductivity has minimum value between 0.38-1.30eV. Minimum conduction occurs between these values. Figure of merit shows its highest value within these two values.
Figure 5: Thermoelectric properties versus chemical potential i.e. $S$, $\kappa$, $\sigma$ and $ZT$ are calculated with GGA-PBEsol (red dot) & GGA-PBEsol + SOC (black line) of SrIrO$_3$ compound [4].

4. CONCLUSION

In this review, the thermoelectric properties of Strontium related perovskite material were studied through different methods and trying to establish some trend. The thermoelectric property of SrRuO$_3$ is studied experimentally while the properties of SrTiO$_3$ and SrIrO$_3$ perovskite were studied theoretically using Boltzmann transport theory used in BoltzTraP coding with Quantum espresso and wien2k. SrRuO$_3$ shows positive temperature dependence it shows metallic behavior. Results shows that maximum value for seebeck coefficient for SrTiO$_3$ and SrIrO$_3$ are 11.7eV and 0.6eV. The minimum electrical and thermal conductivity for SrTiO$_3$ is between 11-12.4eV and for SrIrO$_3$ is between 0.38 to 1.30 eV. Beyond the threshold values thermal and electrical conductivity has maximum value. For better thermoelectric material their figure of merit is to be $\geq$ 1. Both SrTiO$_3$ and SrIrO$_3$ shows value $\geq$1. It proofs that they would have good thermoelectric character.

REFERENCES


