Supplemental Material

Effect of Bi^{3+}-doping on the electronic structure and thermoelectric properties of $(Sr_{0.889-x}La_{0.111}Bi_x)TiO_{2.963}$: First-principles calculations

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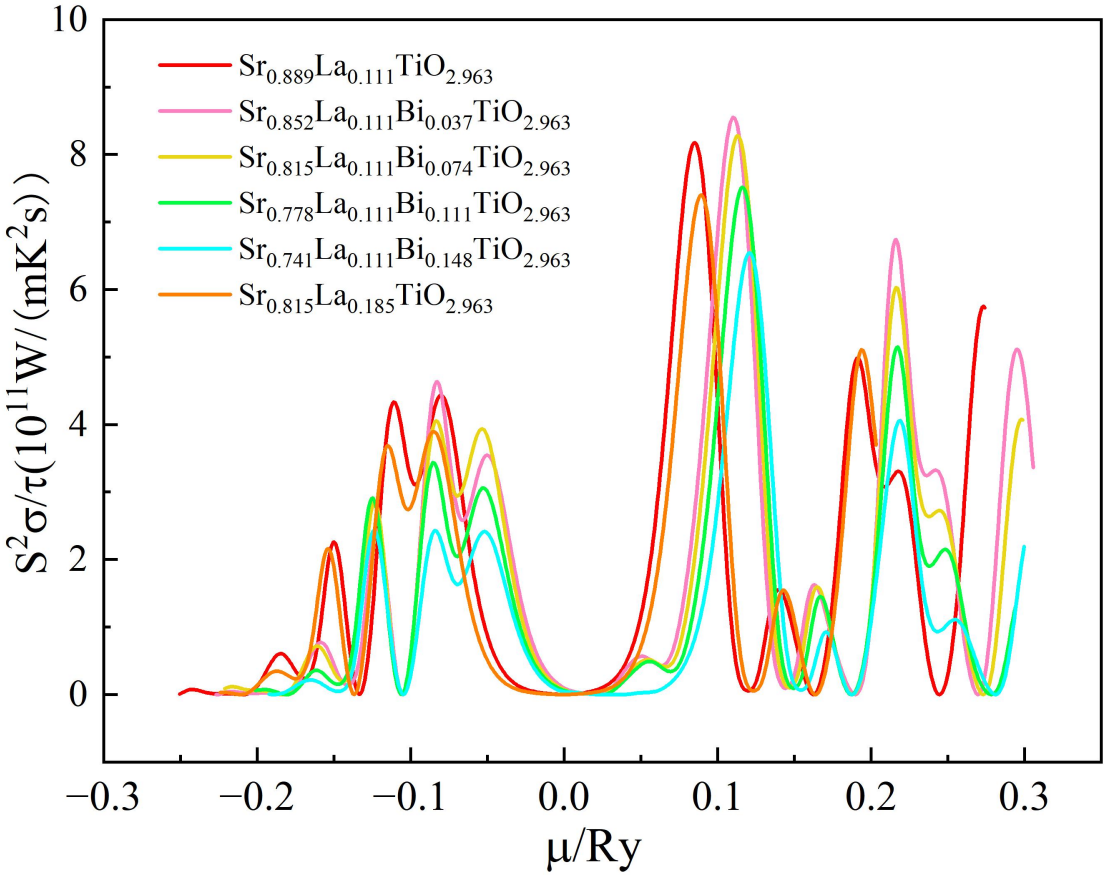

Figure S1. Chemical potential dependent of $S^2\sigma/\tau$ for $(Sr_{0.889-x}La_{0.111}Bi_x)TiO_{2.963}$ at 1200K

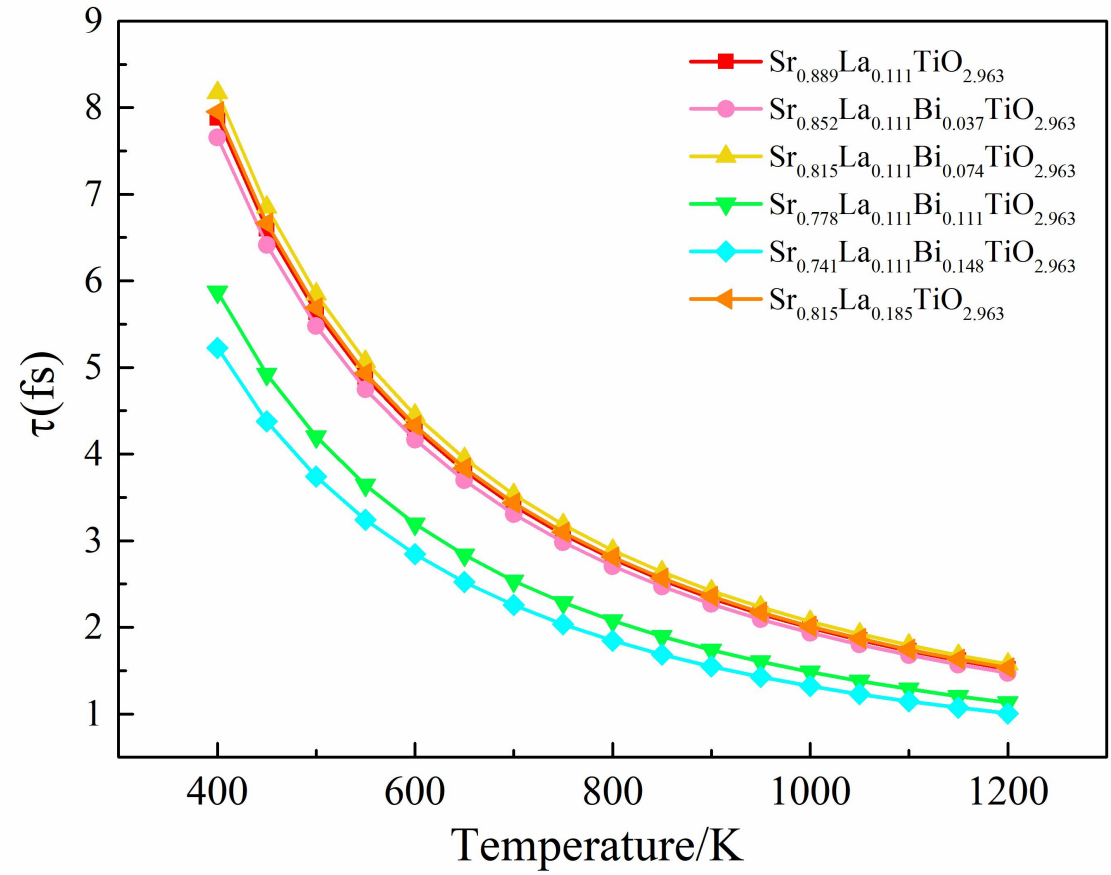

Figure S2. Temperature dependent of τ for $(Sr_{0.889-x}La_{0.111}Bi_x)TiO_{2.963}$

Table S1 Mechanical properties of $(Sr_{0.889-x}La_{0.111}Bi_x)TiO_{2.963}$

Crystals	Young's modulus E(GPa)	Poisson's ratio σ(m/s)	Debye temperature Θ_D
$Sr_{0.889}La_{0.111}TiO_{2.963}$	265.7	0.252	648.9
$Sr_{0.852}La_{0.111}Bi_{0.037}TiO_{2.963}$	288.2	0.218	674.8
$Sr_{0.815}La_{0.111}Bi_{0.074}TiO_{2.963}$	269.9	0.243	641.9
$Sr_{0.778}La_{0.111}Bi_{0.111}TiO_{2.963}$	258.7	0.245	620.7
$Sr_{0.741}La_{0.111}Bi_{0.148}TiO_{2.963}$	268.2	0.234	626.8
$Sr_{0.815}La_{0.185}TiO_{2.963}$	272.8	0.246	652.4

Slack derived the quantitative expression of intrinsic lattice thermal conductivity[1]:

$$k_{\text{Slack}} = A\frac{M\Theta_D{}^3\delta}{\gamma^2 n^{2/3}T} \quad (1)$$

where A is constant, $A = 3.04 \times 10^7$ W·mol/kg/m^2 /K^3, M is the average atomic mass, n is the number of atoms in primitive cell, the δ^3 is average atomic volume, γ is Gruneisen parameters, which can be calculated by poisson's ratio σ[2], Θ_D is the Debye temperature. Poisson's ratio σ and Θ_D can be calculated by the elastic properties of first principles. The detailed data can be seen in Table S1. Parameters of the calculated Slack model are shown in Table S2.

Due to the scattering of acoustic phonons with the increase of temperature, the relationship between thermal conductivity and temperature in the experiment is often as follows: $\kappa = A/T + L\ \sigma T$, where A/T and $L\ \sigma T$ are respectively the lattice thermal conductivity and the electronic thermal conductivity[3].

At present, researchers have conducted a lot of research on the lattice thermal conductivity of La^{3+} doped $SrTiO_3$ materials in the experiment[4-11]. In the experiment, the lattice thermal conductivity of $Sr_{0.9}La_{0.1}TiO_3$ at 1073K is within the trend range of 2.0-2.6W/m·K. The relationship between the lattice thermal conductivity and temperature of $Sr_{0.9}La_{0.1}TiO_3$ fitted by the experiment is obtained as: $\kappa_l = 2860.0/T$. Since the material in the experiment often have oxygen vacancies, we used the $(Sr_{1-x}La_x)TiO_{2.963}$ cell model to fit the experimental data. In this paper, the relation between the lattice thermal conductivity of $(Sr_{1-x}La_x)TiO_{2.963}$ and temperature calculated by Slack model is $\kappa_l = 9475.4/T$, as shown in Table S2. The fitting parameter n=3.31 is obtained by dividing these two relationships. Then the lattice thermal conductivity models of $Sr_{0.852}La_{0.111}Bi_{0.037}TiO_{2.963}$, $Sr_{0.815}La_{0.111}Bi_{0.074}TiO_{2.963}$, $Sr_{0.778}La_{0.111}Bi_{0.111}TiO_{2.963}$, $Sr_{0.741}La_{0.111}Bi_{0.148}TiO_{2.963}$, $Sr_{0.889}La_{0.111}TiO_{2.963}$, $Sr_{0.815}La_{0.185}TiO_{2.963}$ calculated according to Slack model are divided by n. Finally, the lattice thermal conductivity changes with temperature is shown in Figure 8(e).

Table S2 Thermal properties of $(Sr_{0.889-x}La_{0.111}Bi_x)TiO_{2.963}$

Crystals	$\bar{M}$(g/mol)	δ^3 (Å^3)	δ (Å)	γ	κ_{Slack}	κ_{Slack}/n
$Sr_{0.889}La_{0.111}TiO_{2.963}$	37.999	8.385	2.032	1.510	9475.4/T	2860.0/T
$Sr_{0.852}La_{0.111}Bi_{0.037}TiO_{2.963}$	38.905	8.367	2.030	1.357	13763.3/T	4159.7/T
$Sr_{0.815}La_{0.111}Bi_{0.074}TiO_{2.963}$	39.811	8.350	2.029	1.471	10301.4/T	3112.2/T
$Sr_{0.778}La_{0.111}Bi_{0.111}TiO_{2.963}$	40.716	8.333	2.027	1.476	9466.1/T	2859.8/T
$Sr_{0.741}La_{0.111}Bi_{0.148}TiO_{2.963}$	41.622	8.315	2.026	1.426	10669.2/T	3223.3/T
$Sr_{0.815}La_{0.185}TiO_{2.963}$	38.764	8.351	2.029	1.481	9992.4/T	3018.9/T

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