

## Supporting Information

### Layered $\text{Tl}_2\text{O}$ : A Model Thermoelectric Material

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Figure S1.

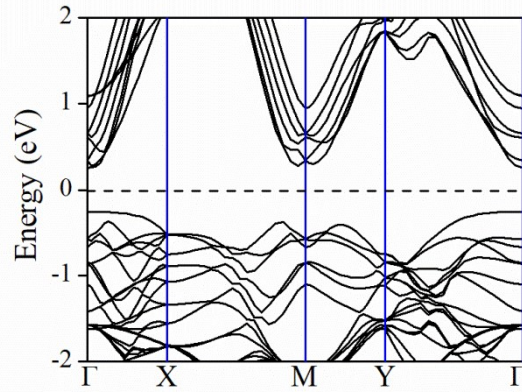


Fig.S1. Band structures of bulk  $Ti_2O$  at PBE level. The dash line denoted Fermi level.

Table S1. Effective masses along transport directions in bulk  $Ti_2O$  calculated by using PBE. The effective mass is in the unit of free electron ( $m_e$ )

	$(m^*)_x (\Gamma-X)$	$(m^*)_y (\Gamma-Y)$
<b>hole</b>	7.79	5.78
<b>electron</b>	0.11	0.31

Figure S2.

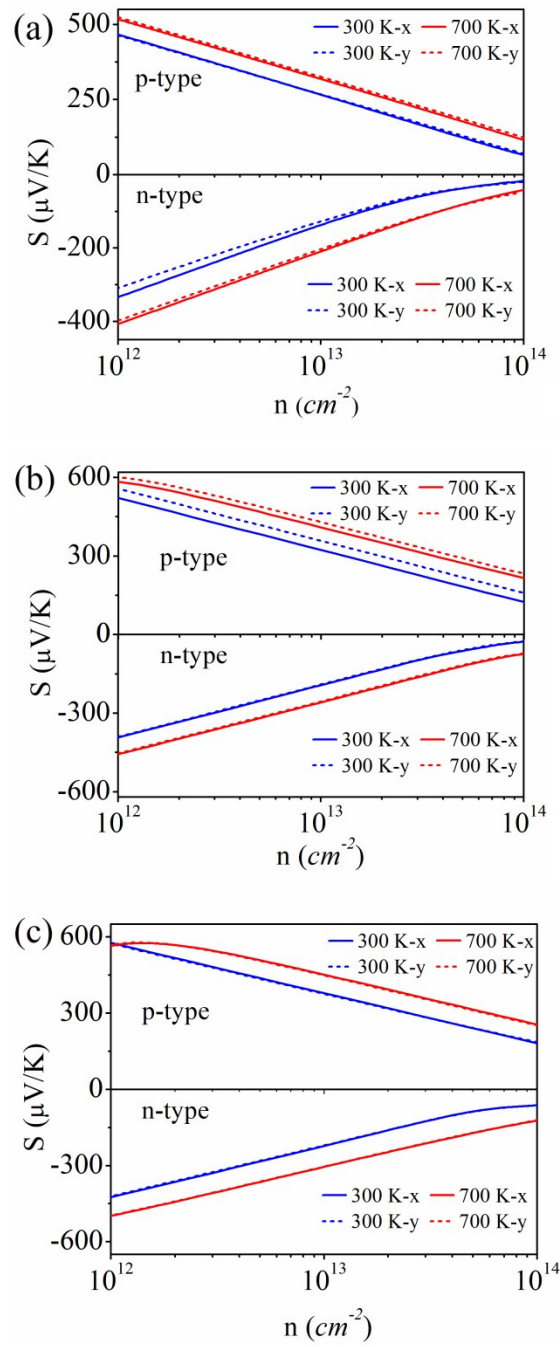


Fig.S2. Seebeck coefficient  $S$  as a function of carriers concentration at 300 K and 700 K along  $x$  and  $y$  directions for (a) SL, (b) BL and (c) TL  $\text{Tl}_2\text{O}$  with  $p$ -type and  $n$ -type.

Figure S3.

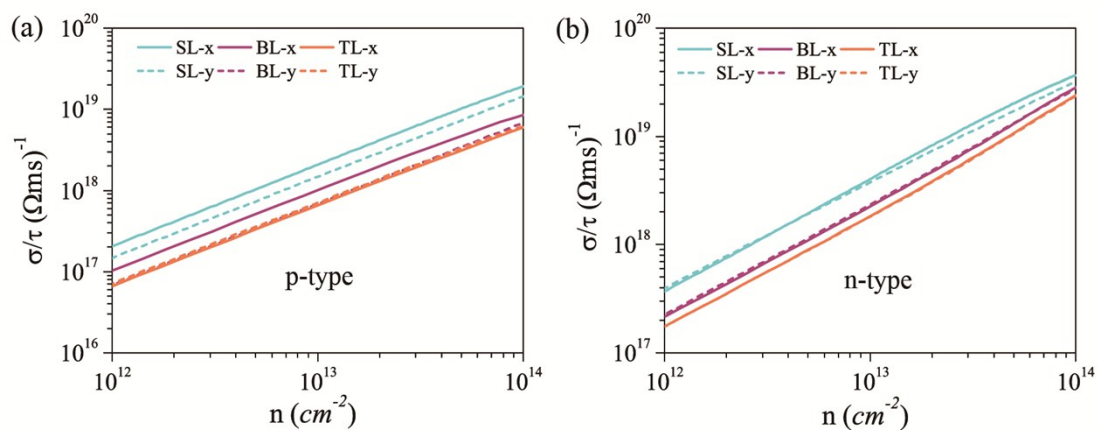


Fig.S3. Electrical conductivities with respect to scattering time  $\sigma/\tau$  at room temperature as a function of carriers concentration along  $x$  and  $y$  directions for SL, BL, TL and bulk  $\text{Ti}_2\text{O}$  with (a)  $p$ -type and (b)  $n$ -type.

Figure S4.

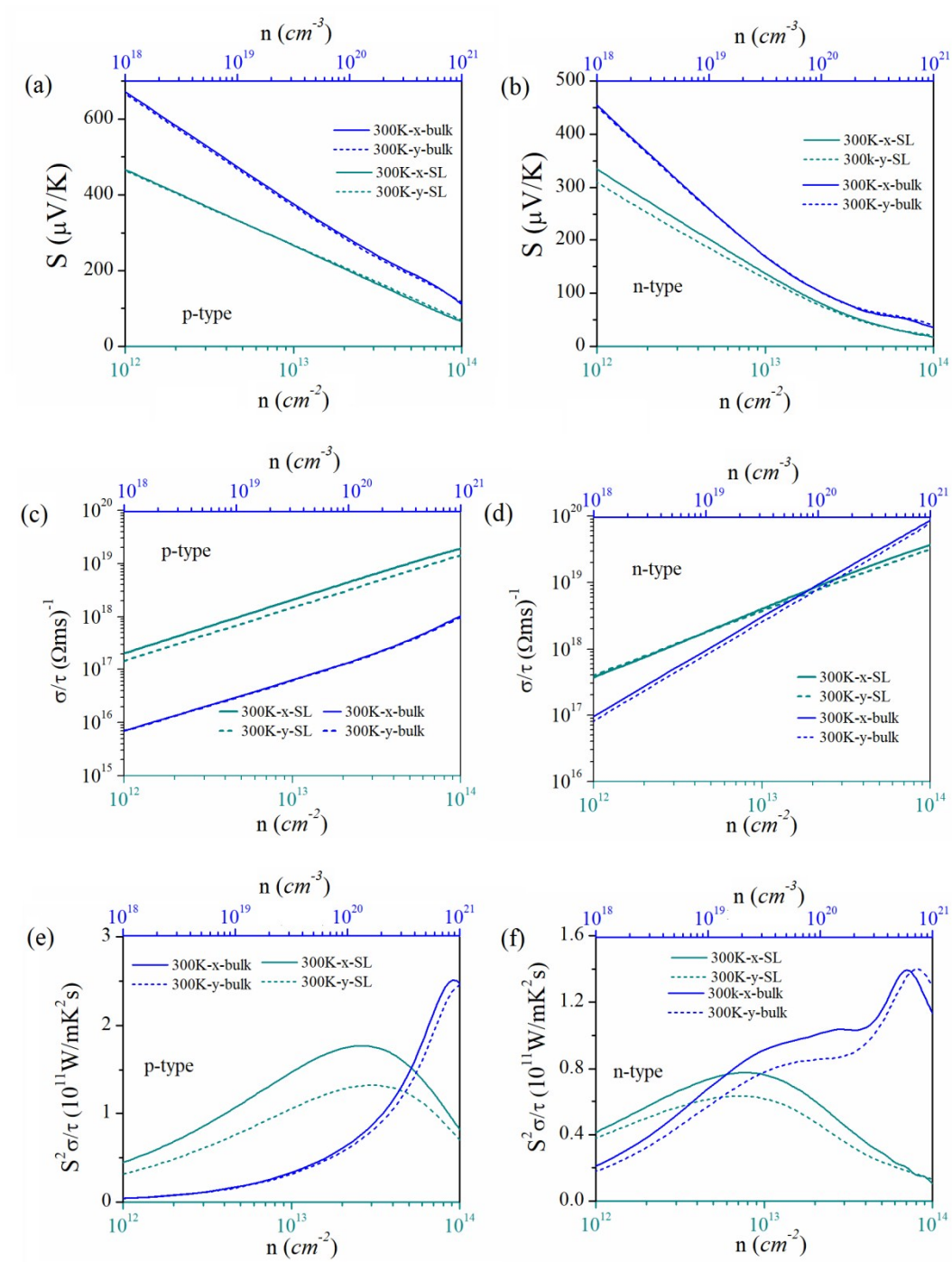


Fig.S4. Seebeck coefficient  $S$ , electronic conductivity with respect to scattering time  $\tau$  ( $\sigma/\tau$ ) and reduced power factor ( $S^2\sigma/\tau$ ) at room temperature as a function of carriers concentration along  $x$  and  $y$  directions for SL and bulk  $\text{Ti}_2\text{O}$  with (a, c, e) p-type, (b, d, f) n-type, respectively.

Figure S5.

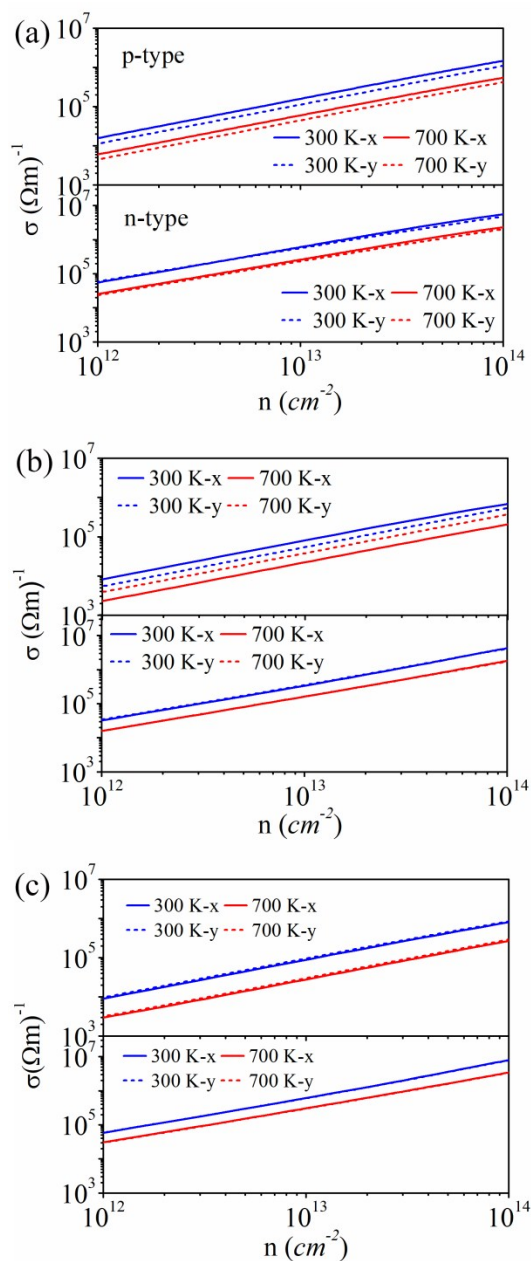


Fig.S5. Electrical conductivities as a function of carriers concentration along  $x$  and  $y$  directions at 300 K and 700 K for (a) single-layer, (b) bilayer and (c) trilayer  $\text{TI}_2\text{O}$  with  $p$ -type and  $n$ -type.

Figure S6.

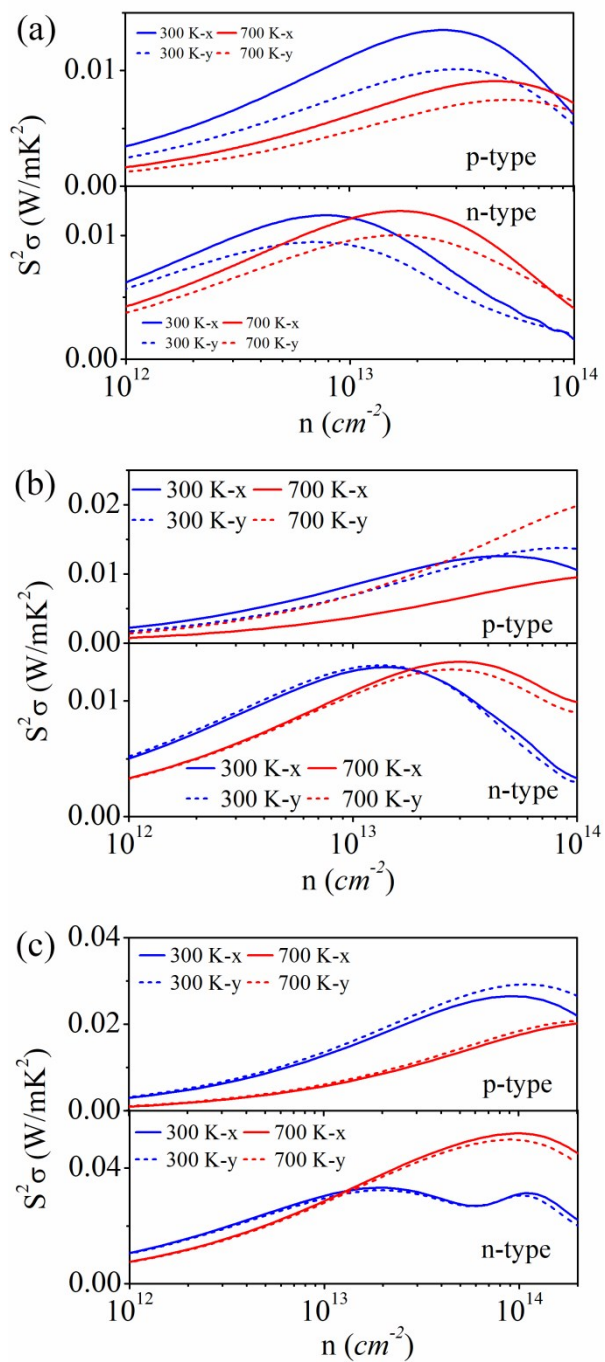


Fig.S6. Power factor  $S^2\sigma$  of (a) single-layer, (b) bilayer and (c) trilayer as a function of carriers concentration at 300 K and 700 K along  $x$  and  $y$  directions.

Figure S7.

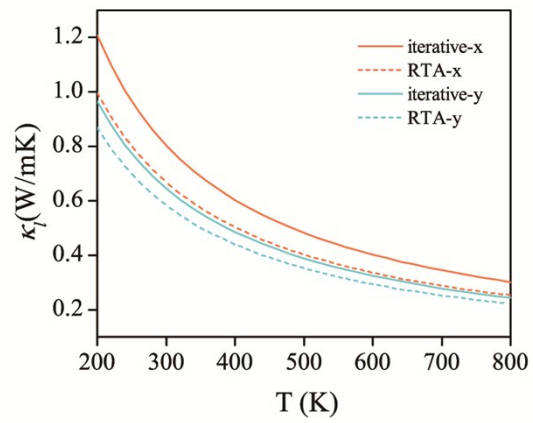


Fig.S7. Calculated  $\kappa_l$  of single-layer  $Ti_2O$  with relaxation time approximation (RTA) (dash line) and from the iterative solution (solid line) of BTE.



Figure S8.

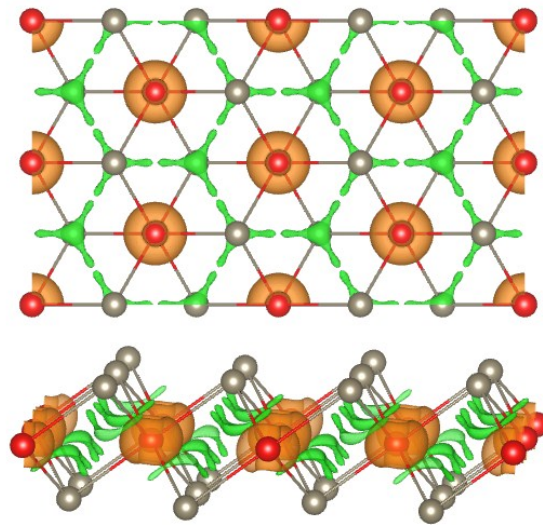


Fig.S8. Charge density difference of SL  $\text{Tl}_2\text{O}$ . Orange represents charge accumulation and green represents charge depletion. Red atom denotes O and grey atom denotes Tl.

Figure S9.

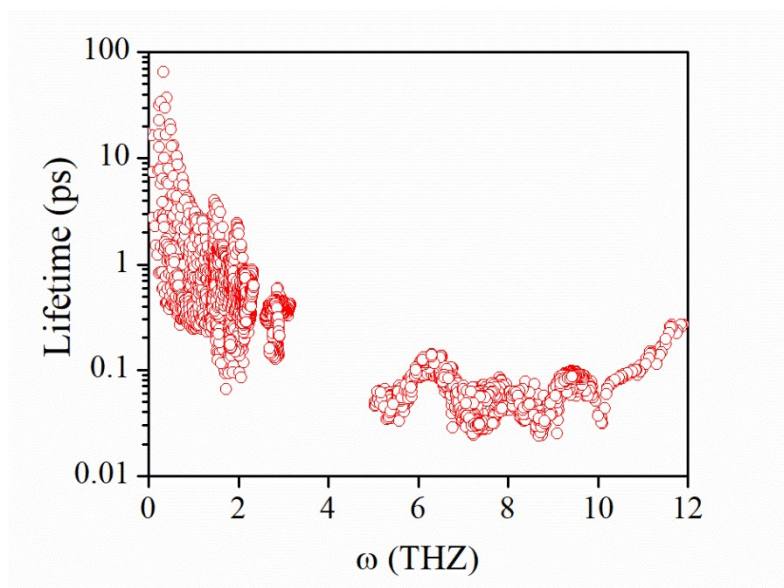


Fig.S9. Calculated phonon lifetime at 300K of SL  $\text{Tl}_2\text{O}$ .