Supplementary information

Low lattice thermal conductivity and promising thermoelectric figure of merit of Zintl type $TlInTe_2$

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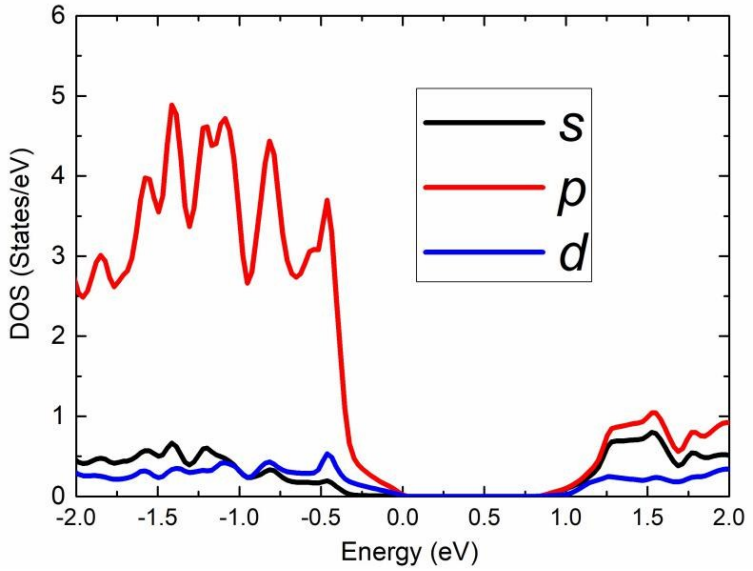

Fig. S1. Contribution of different atomic state to the density of states in $TlInTe_2$.

Table S1. Calculated elastic constant C, carrier effective mass m^*, deformation potential (DP) constant E, and relaxation time τ of $TlInTe_2$ at room temperature.

Carriers	C (eV/Å^3)	m^* (m_e)	E (eV)	τ (10^{-14} s)
Hole	3.45	0.2	-34.05	18
Electron	3.45	0.47	-26.78	9.8

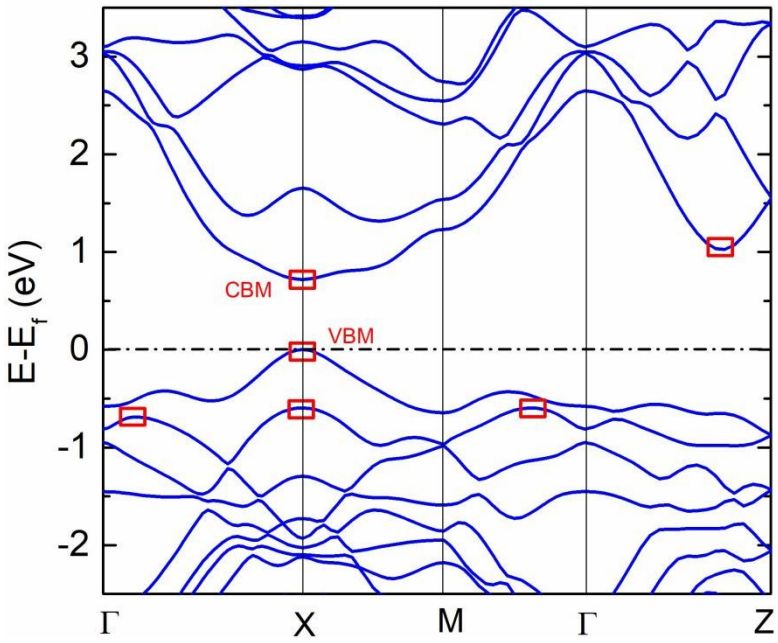

Fig. S2. Calculated band structure of $TlGaTe_2$.

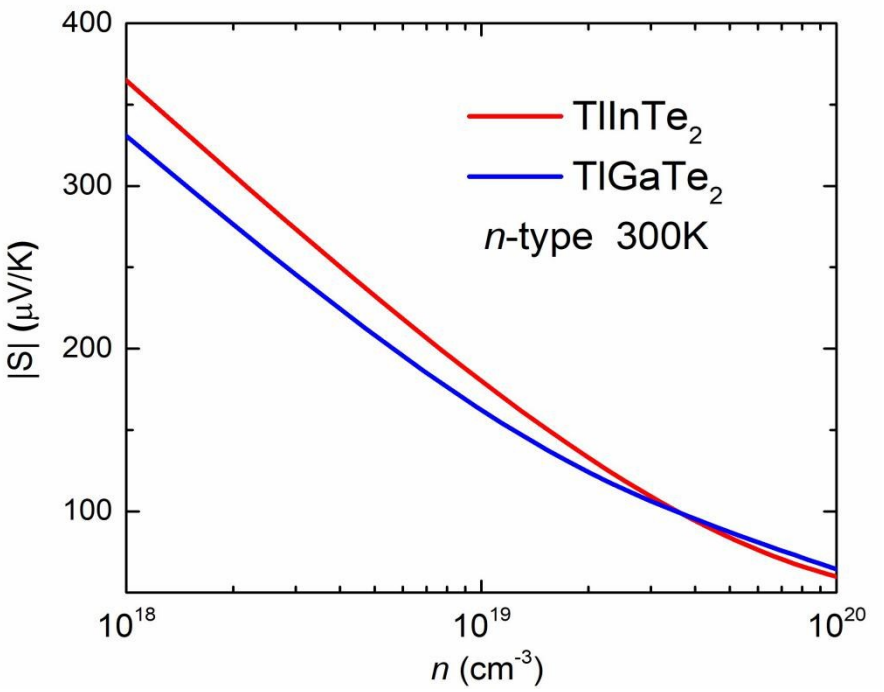

Fig. S3. Comparison of *n*-type Seebeck coefficient between $TlInTe_2$ and $TlGaTe_2$ at

300K.