

Novel room-temperature Full-Heusler Thermoelectric material Li_2TlSb [†]

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1 Supplementary Tables

Table S1: The calculated elastic constants C_{ij} (GPa), bulk modulus B (GPa), Young's modulus E (GPa), shear modulus G (GPa), Poisson's ratio ν , Pugh's Ratio (B/G) for Li_2TlSb .

Semiconductor	C_{11}	C_{12}	C_{44}	B	E	G	ν	B/G
Li_2TlSb	78.88	9.31	18.15	32.5	57.05	23.62	0.207	1.376

Table S2: The calculated static dielectric constant ϵ_s , Born effective charges Z^* , high-frequency dielectric constant ϵ_∞ , effective polar optical phonon frequency ω_{po} (THz), and Debey temperature Θ_D (K) for Li_2TlSb .

Semiconductor	ϵ_s	Z^* (Li)	Z^* (Tl)	Z^* (Sb)	ϵ_∞	ω_{po}	Θ_D
Li_2TlSb	125.59	1.46	3.49	-6.42	51.86	3.55	225.7

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Table S3: Calculated temperature-dependent phonon frequency of lowest phonon modes at X and K point using the self-consistent phonon method (loop diagram) compared with that further including the bubble diagram, respectively.

		100K	200K	300K	400K	500K	600K	700K
X	Loop	50.25	50.67	51.07	51.44	51.79	52.12	52.43
	Loop+Bubble	49.2	49.4	50	50.4	50.89	51.29	51.66
K	Loop	47.72	48.42	49.08	49.7	50.28	50.81	51.32
	Loop+Bubble	45.8	46.7	47.6	48.3	49.07	49.7	50.3

2 Supplementary Figures

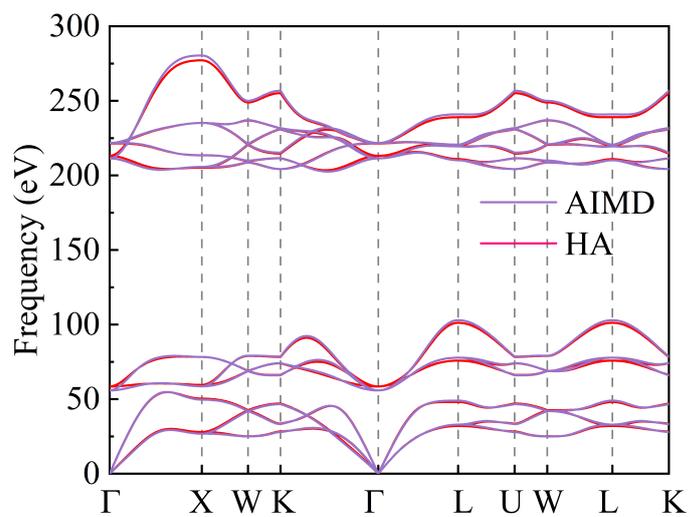


Figure S1: The comparison of phonon spectra is obtained from the phonon spectrum obtained from 60 snapshots and the phonon spectrum obtained from the harmonic force constant using the phonopy software.

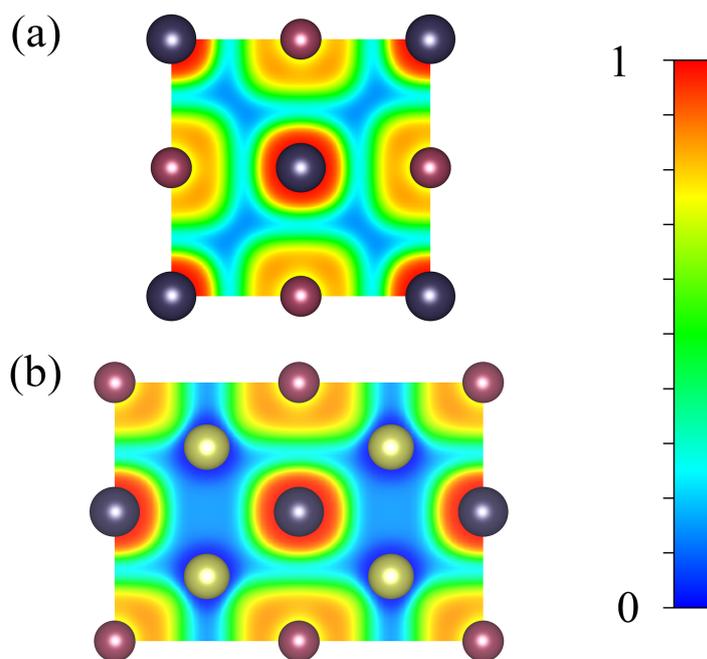


Figure S2: The calculated electronic local functions (ELF) of Li_2TlSb on (a) 100 and (b) 110 plane, respectively.

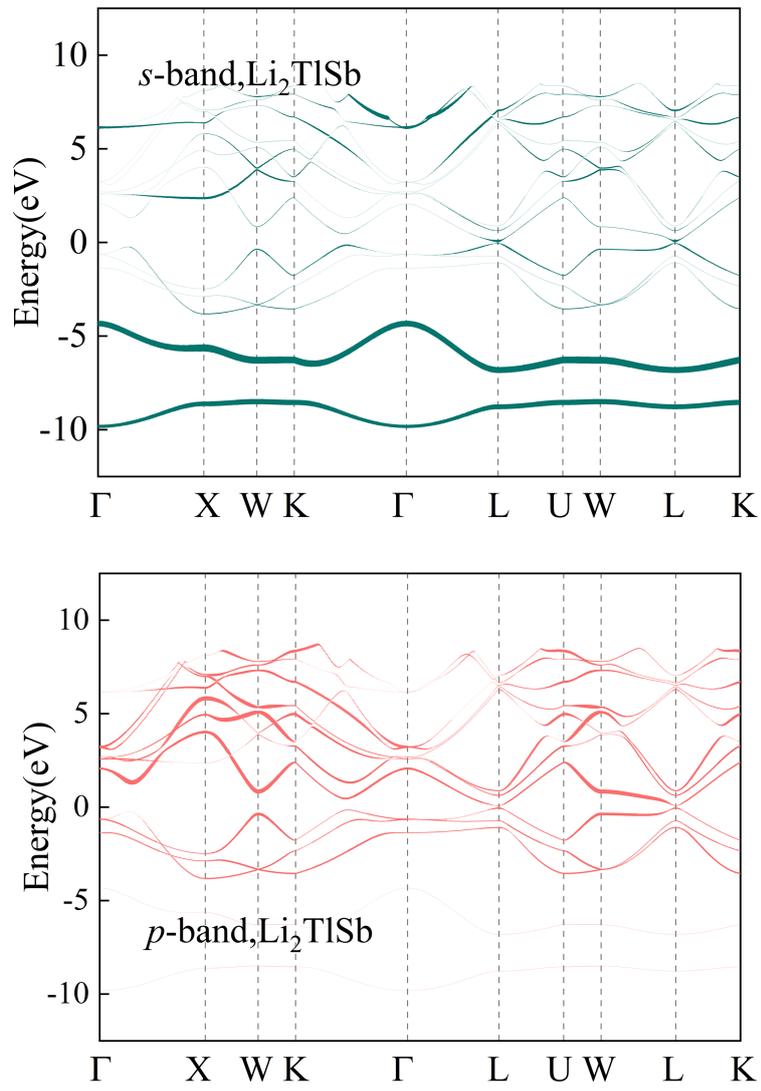


Figure S3: Weak s - p hybridization in Li_2TlSb , k -resolution projection band.

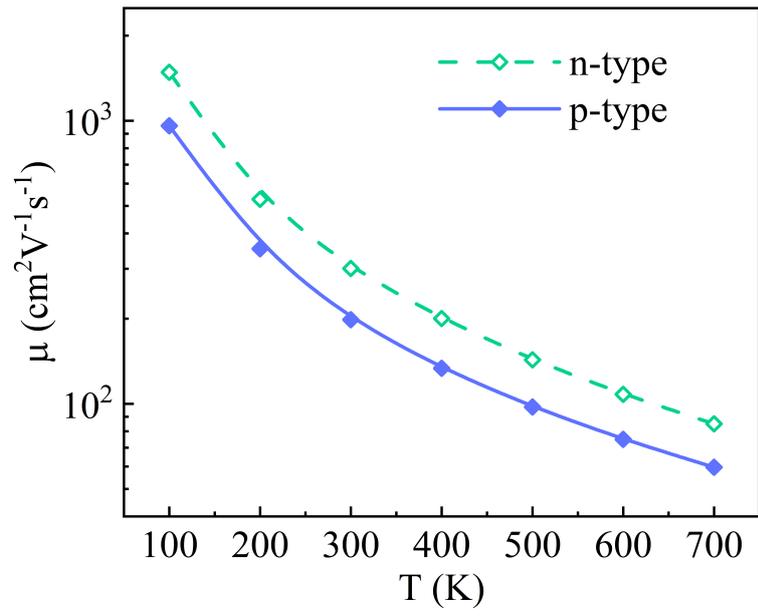


Figure S4: The function of carrier mobility with temperature was calculated, and the selected carrier concentration was $2.04 \times 10^{18} \text{ cm}^{-3}$.

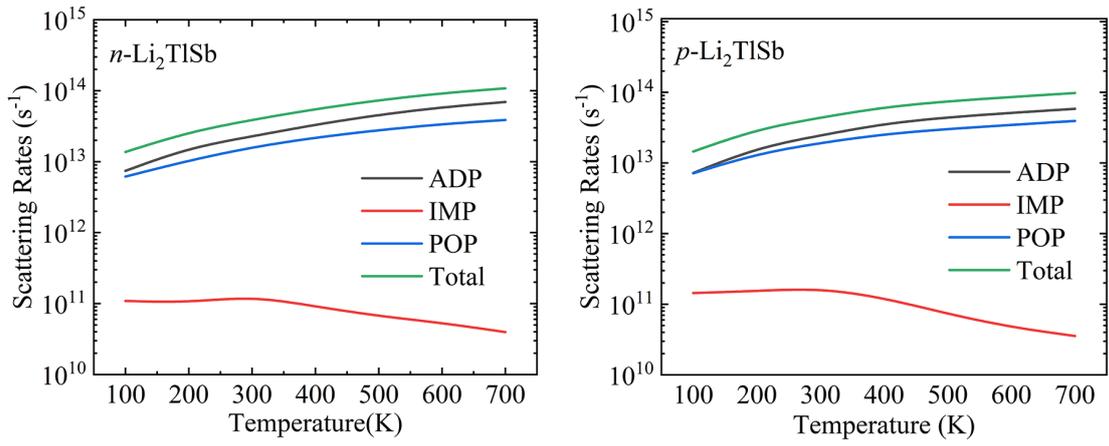


Figure S5: The ADP scattering rate, IMP scattering rate, and POP scattering rate calculated using the amset code as a function of temperature curves, and the selected doped carrier concentration is $2.04 \times 10^{18} \text{ cm}^{-3}$.

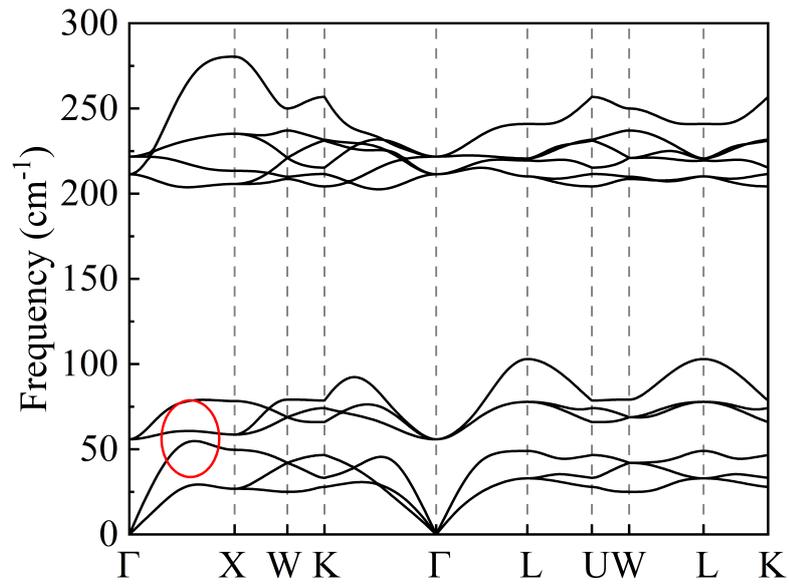


Figure S6: Calculate the phonon dispersion curve for the harmonic approximation, using $3 \times 3 \times 3$ cells, the red circle in the figure is the anti-crossing point along the Γ -X direction.

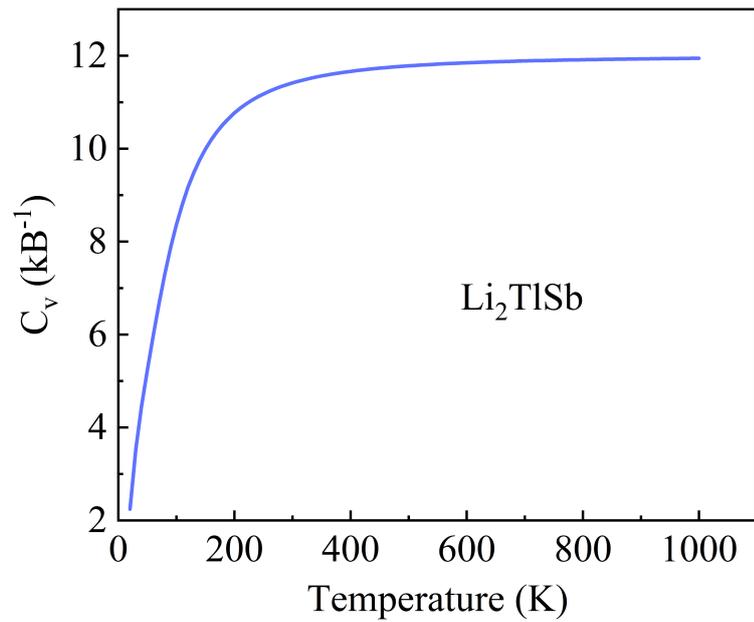


Figure S7: Calculates the heat capacity as a function of temperature for Li_2TlSb .