Supplementary Material

First-principles prediction of large thermoelectric efficiency in superionic $Li_2Sn$$X_3$($X$=S,Se)

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S. 1. Structural properties

The fully optimized fractional atomic coordinates of both compounds are listed in Table S1. The computed values are in well agreement with experimental values.

Table S1: Optimized fractional atomic coordinates of $Li_2Sn$$X_3$

Compound	Atom	Site	Calc. (PBE)	Experimental [1,2]
Li_2SnS_3	Li	8f	(0.2411, 0.0860, 0.9998)	(0.2466, 0.0840, 0.9997)
	Li	4e	(0.0000, 0.4168, 0.2500)	(0.0000, 0.4173, 0.2500)
	Li	4d	(0.2500, 0.2500, 0.5000)	(0.2500, 0.2500 0.5000)
	Sn	4e	(0.0000, 0.0832, 0.2500)	(0.0000, 0.0833, 0.2500)
	Sn	4e	(0.0000, 0.7495, 0.2500)	(0.0000, 0.7499, 0.2500)
	S	8f	(0.1126, 0.0830, 0.6298)	(0.1115, 0.0831, 0.6312)
	S	8f	(0.1345, 0.2426, 0.1296)	(0.1355, 0.2418, 0.1311)
	S	8f	(0.3657, 0.0917, 0.3723)	(0.3651, 0.0920 0.3708)
Li_2SnSe_3	Li	4a	(0.5573, 0.9372, 0.1502)	(0.5610, 0.9350, 0.1600)
	Li	4a	(0.3823, 0.4102, 0.1202)	(0.3720, 0.4110, 0.1030)
	Sn	4a	(0.2408, 0.9152, 0.1554)	(0.2428, 0.9165, 0.1571)
	Se	4a	(0.1008, 0.0787, 0.2660)	(0.1031, 0.0776, 0.2685)
	Se	4a	(0.4341, 0.0974, 0.2763)	(0.4349, 0.0993, 0.2788)
	Se	4a	(0.2653, 0.5834, 0.2499)	(0.2668, 0.5857, 0.2508)

S. 2. Transport properties

Fig. S1. Demonstrates carrier concentration dependent anisotropic electrical conductivity of Li_2SnS_3 (top panel) and Li_2SnSe_3 (bottom panel). Electrical conductivity of both compounds shows highly anisotropic behavior. For n-type carrier in both compounds the electrical conductivity along c-axis is higher compared to other axes.

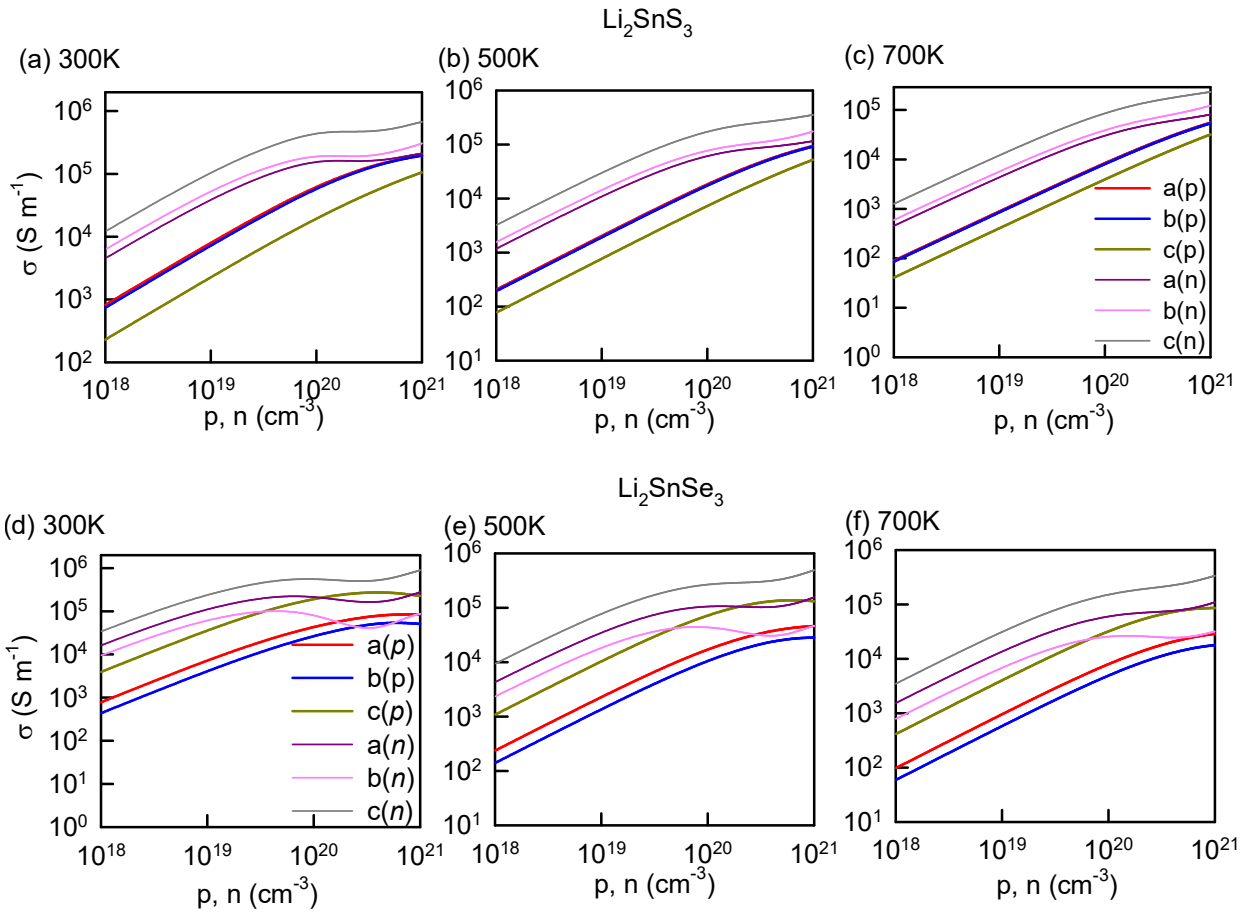

Fig. S1. Anisotropic electrical conductivity of Li_2SnS_3 (top panel) and Li_2SnSe_3 (bottom panel) as a function of carrier concentration.

The computed electronic part of the thermal conductivity of both compounds is shown in Fig. S2.

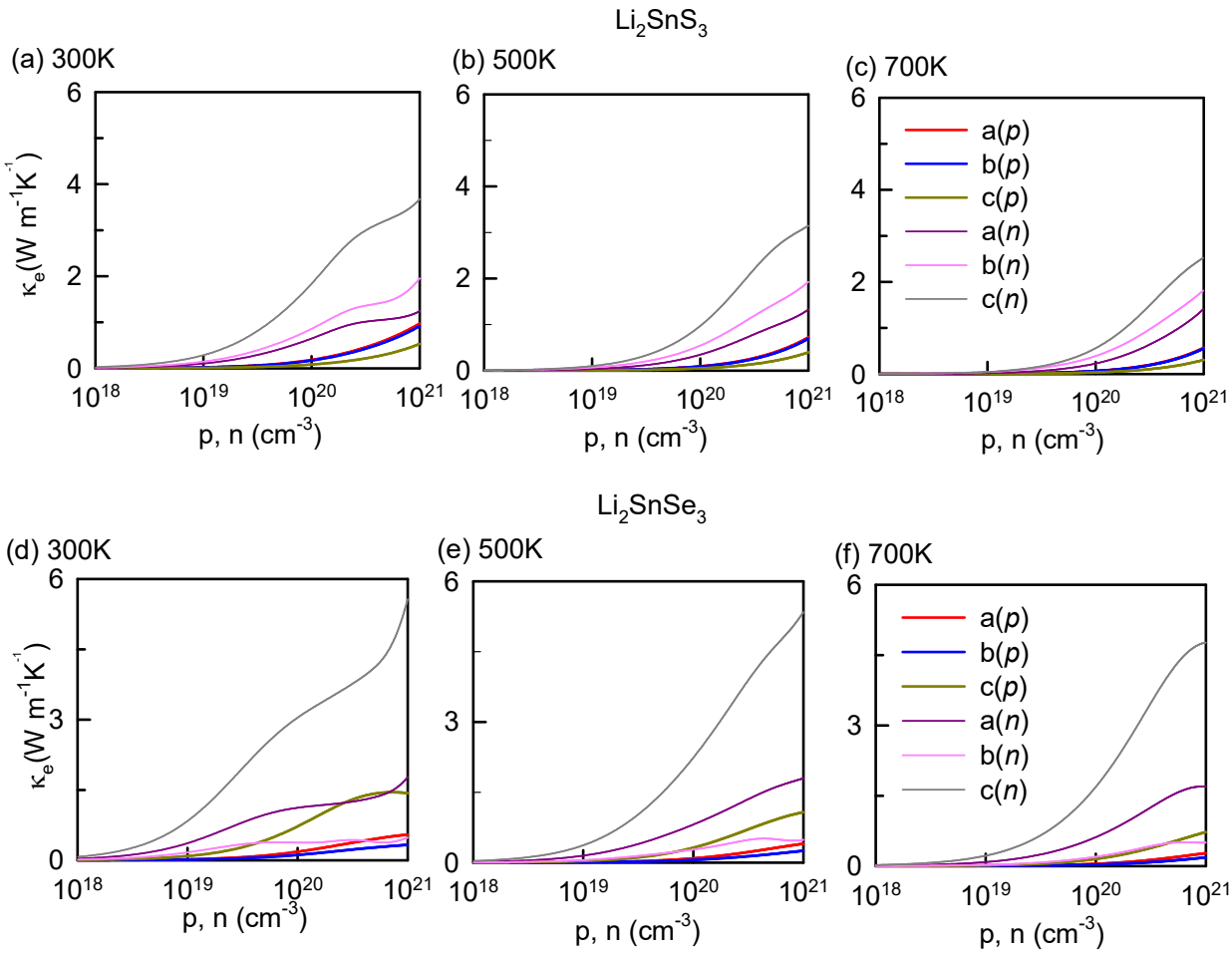

Fig. S2. Carrier concentration dependent of anisotropic electronic part of the thermal conductivity of Li_2SnS_3 (top panel) and Li_2SnSe_3 (bottom panel). The symbols a, b, and c indicate the crystallographic directions (x, y, z) and *p*, and *n* indicate the type of carrier.

At high carrier concentration, both compounds exhibit anisotropic electronic thermal conductivity. Although electronic thermal conductivity of Li_2SnS_3 is lower than that of Li_2SnSe_3, the lattice thermal conductivity is higher, resulting in the suppression of *zT*.

References

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