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Supplemental Material

Ultralow thermal conductivity and anisotropy thermoelectric performance in layered materials LaMOCh (M=Cu, Ag; Ch=S, Se)

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1. Test of vdW interactions

TABLE S1. Calculated lattice constants by different vdW interactions.

Compound	vdW interactions	a&b (Å)	c (Å)
LaCuOS	Expt.[1]	3.99	8.52
	no vdW	4.00	8.55
	optB86b	4.11	8.75
	optB88	3.97	8.43
	DFT-D3	3.95	8.49
LaCuOSe	Expt. [1]	4.07	8.80
	no vdW	4.07	8.86
	optB86b	4.17	9.22
	optB88	4.05	8.70
	DFT-D3	4.02	8.79
LaAgOS	Expt. [2]	4.07	9.10
	no vdW	4.09	9.09
	optB86b	4.15	9.38
	optB88	4.05	8.93
	DFT-D3	4.04	9.03

The optimized lattice constants without the van der Waals (vdW) interactions are in the best agreement with the experimental values. Using optB86b overestimates the lattice constants while using optB88 and DFT-D3 underestimates them.

2. Heat Transport Properties

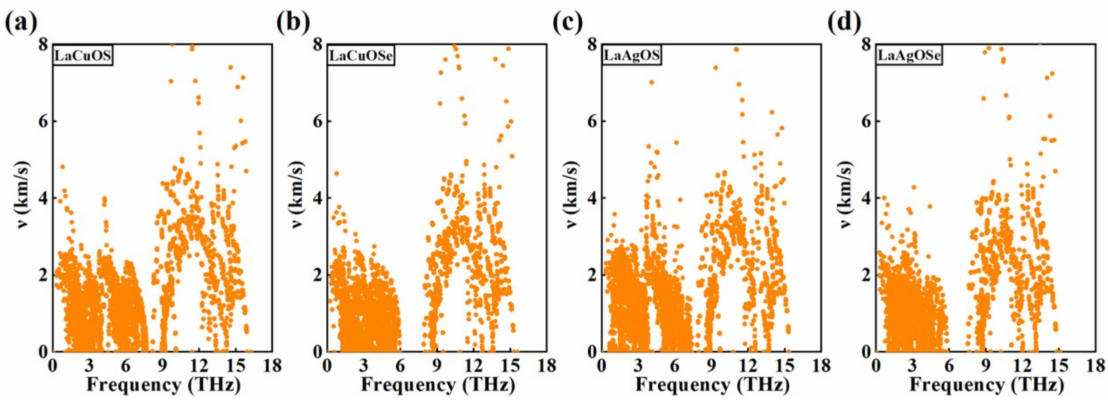

Figure S1. Calculated phonon group velocity (a) - (d) of La*MOCh* at 300 K.

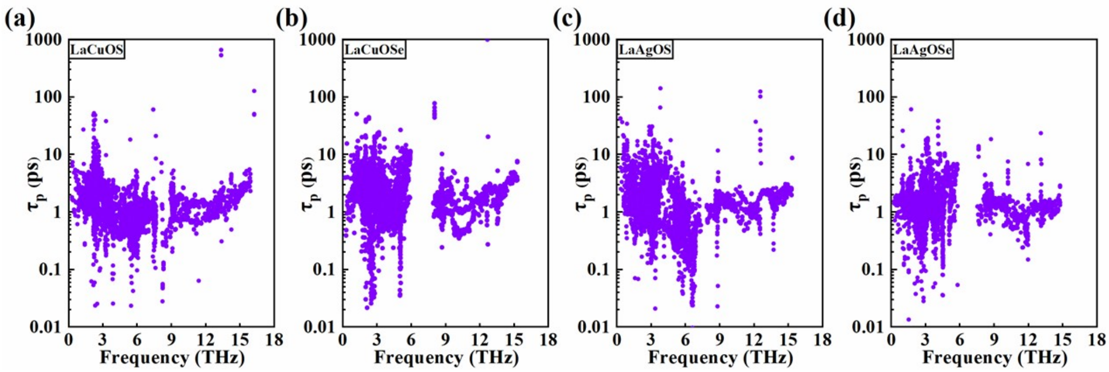

Figure S2. Calculated phonon relaxation time (a) - (d) of La*M*O*Ch* at 300 K.

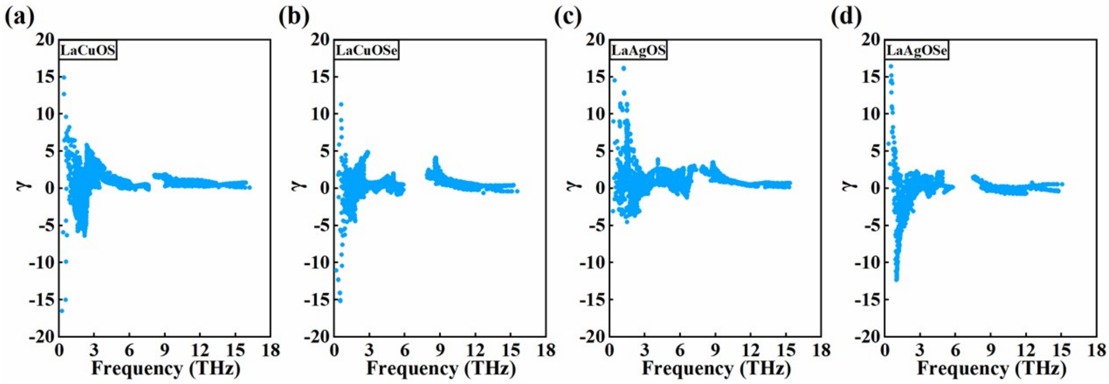

Figure S3. Calculated Grüneisen parameters (a) - (d) of La*M*O*Ch* at 300 K.

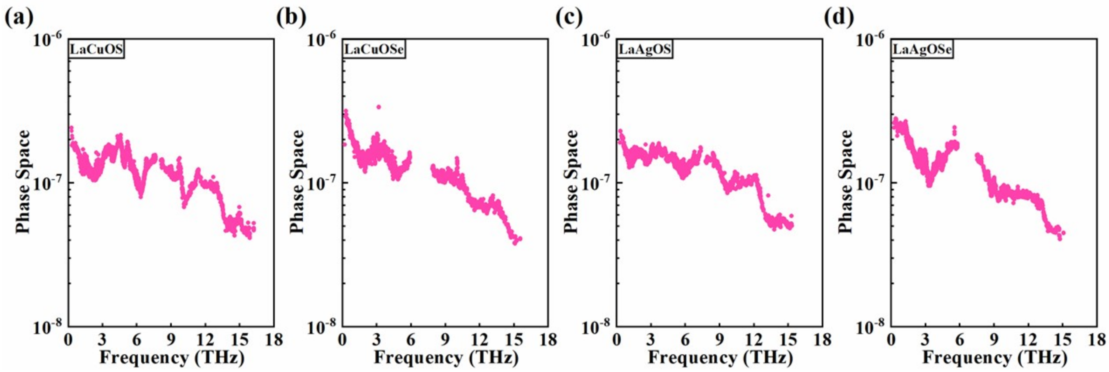

Figure S4. Calculated three phonon scattering phase space (a) - (d) of La*M*O*Ch* at 300 K.

3. Electronic Transport Properties

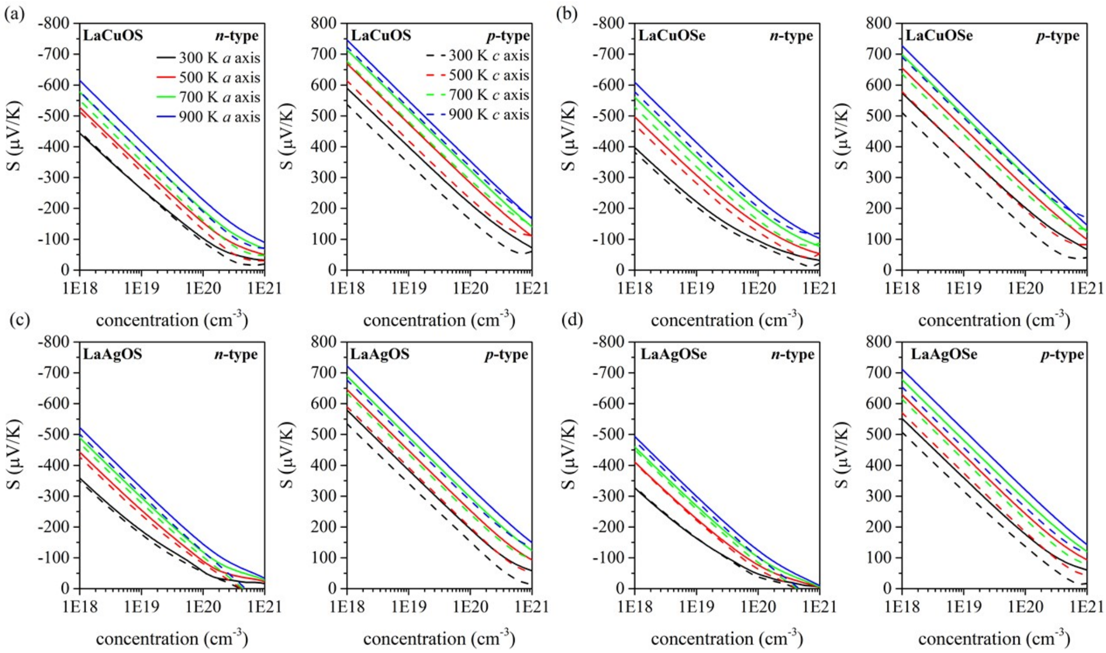

Figure S5. Calculated Seebeck coefficients (a) - (d) of La*M*O*Ch*.

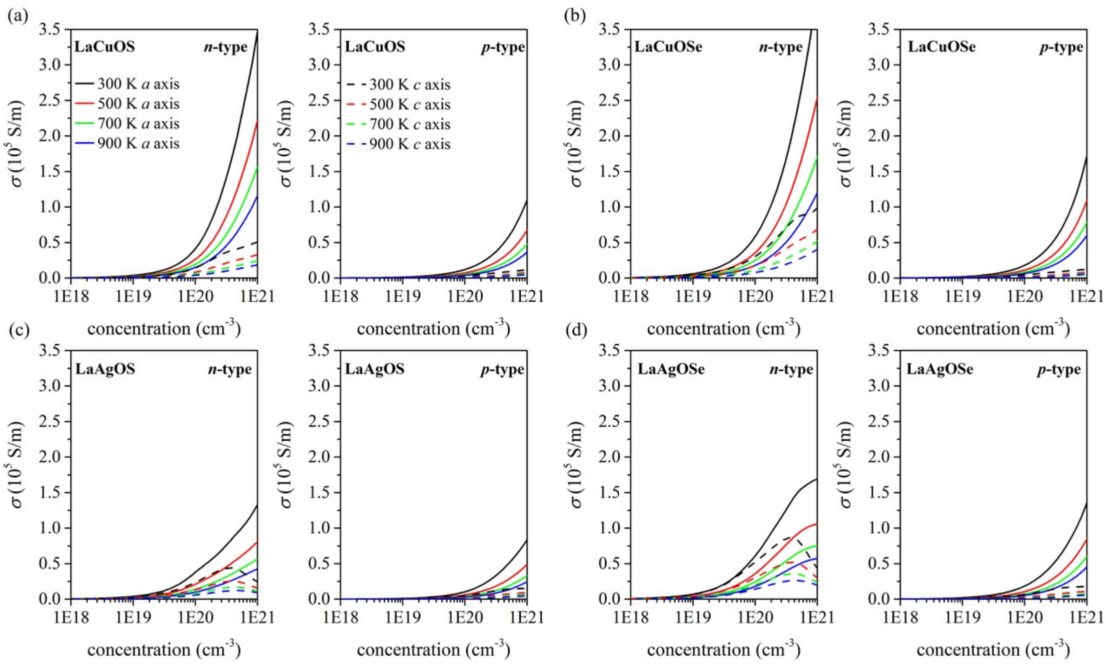

Figure S6. Calculated electrical conductivity (a) - (d) of La*M*O*Ch*.

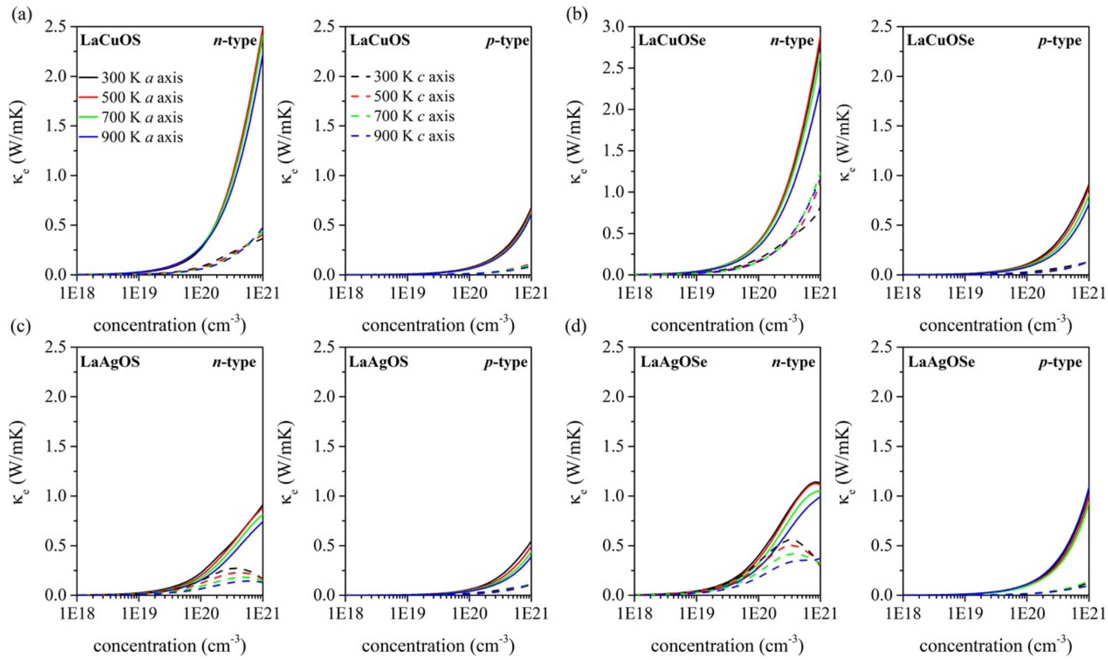

Figure S7. Calculated electrical thermal conductivity (a) - (d) of La*M*O*Ch*.

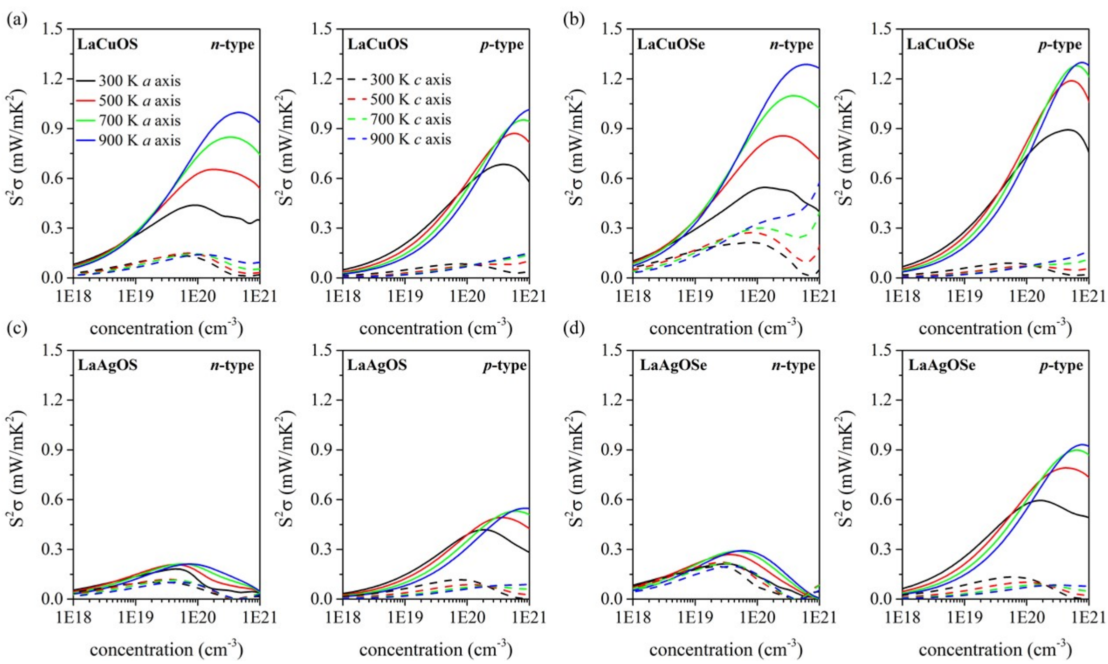

Figure S8. Calculated power factor (a) - (d) of La*M*O*Ch*.

4. Figure of Merit

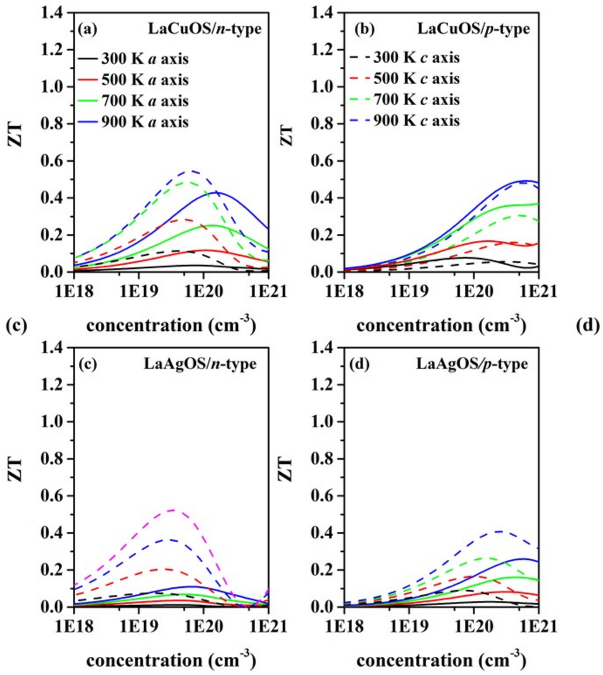

Figure S9. ZT value as function of carrier concentrations for La*M*OS.

Reference

[1] K. Ueda and H. Hosono, Thin Solid Films **411**, 115 (2002).

[2] M. Palazzi, C. Carcaly, and J. Flahaut, J. Solid State Chem. **35**, 150 (1980).