Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Ultralow Lattice Thermal Conductivity of Binary Compounds A_2B (A=Cs, Rb & B=Se, Te) with Higher-Order Anharmonicity Correction

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TABLE SI. The interatomic distances of the symmetrically independent atoms in the binary compounds A_2B (A=Cs, Rb & B=Se, Te). In the A_2B system, there are three unequal atoms, denoted by A1, A2 and B1, whose coordinates are (0.0, 0.0, 0.0), (0.333, 0.667, 0.250) and (0.333, 0.667, 0.750), respectively. The distances between A1 and A2, A1 and B1 and A2 and B1 are denoted by d_{12}, d_{13} and d_{23} respectively.

Material	d_{12}	d_{13}	d_{23}
Cs_2Se	3.942	3.942	3.425
Cs_2Te	4.155	4.155	3.628
Rb_2Se	3.779	3.779	3.276
Rb_2Te	3.995	3.995	3.480

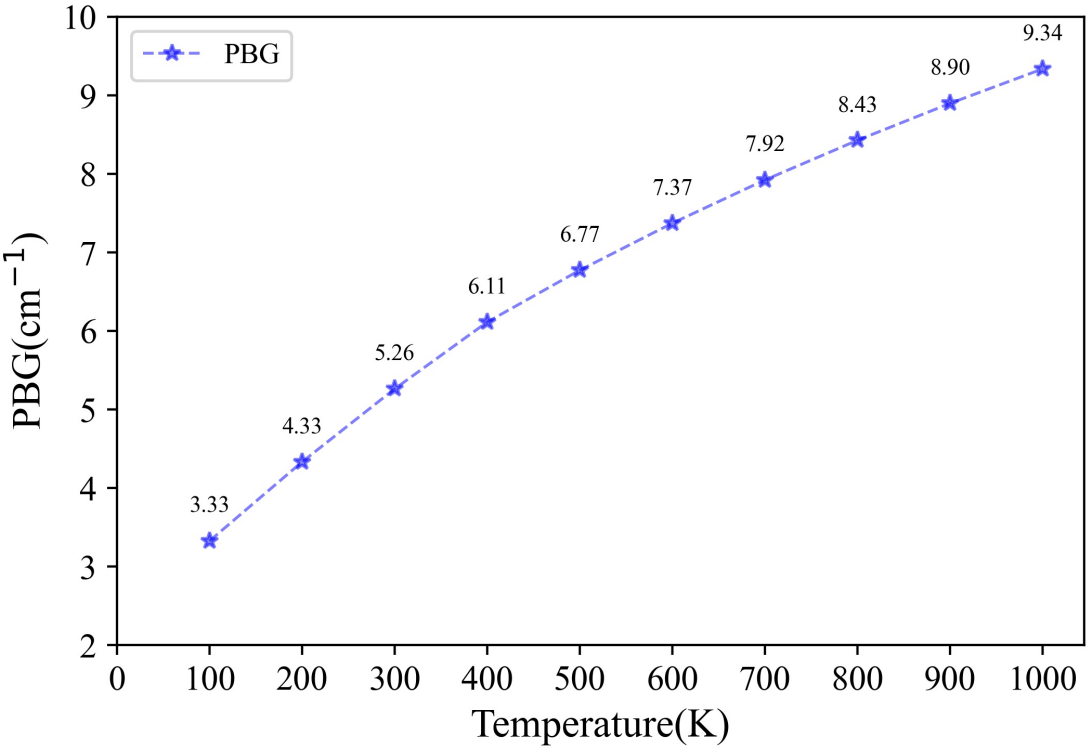

FIG. S1. The phonon band gap(PBG) of Cs_2Se at different temperature(K).

TABLE SII. The frequencies corresponding to the cumulative lattice thermal conductivity of 50%, 60%, 70%, 80%, and 90% are presented. Here, $\omega(a, b)$ represents the frequency corresponding to the a(b)-direction and $\omega(c)$ represents the frequency corresponding to the c-direction.

Material	Percentage	$\omega(a, b)$ cm^{-1}	$\omega(c)$ cm^{-1}
Cs_2Se	50%	26	21
	60%	33	24
	70%	41	28
	80%	52	42
	90%	63	58
Cs_2Te	50%	26	20
	60%	32	25
	70%	38	32
	80%	46	50
	90%	58	62
Rb_2Se	50%	30	26
	60%	34	30
	70%	46	36
	80%	59	53
	90%	70	74
Rb_2Te	50%	30	26
	60%	34	30
	70%	40	36
	80%	50	49
	90%	63	70