Supplementary Information - Phonon engineering through crystal chemistry

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Compound	Exp. κ_L (W/mK)	N (primitive cell)	$V^{1/3}$ (Å)	θ_D (K)	γ	Calc. κ_L (W/mK)	References
AlSb	56	2	2.83	265	0.6	57	[1, 2]
BaO	2.3	2	2.76	290	1.5	7.1	[2]
BP	350	2	2.27	844	0.75	250	[2]
CdTe	7.5	2	3.24	151	0.52	24	[1, 2]
GaAs	45	2	2.81	277	0.75	39	[2]
GaP	100	2	2.72	346	0.75	52	[2]
GaSb	40	2	3.05	265	0.75	47	[1, 2]
Ge	65	2	2.83	296	0.76	46	[2, 3]
HgTe	2.5	2	3.23	141	1.9	2.5	[4, 5]
InAs	30	2	3.03	208	0.57	38	[2]
InP	93	2	2.92	277	0.6	60	[2]
InSb	16.5	2	3.24	202	0.56	45	[1, 2]
PbS	2.9	2	2.97	230	2	6.4	[2, 3, 6]
PbSe	2	2	3.06	126	1.5	2.4	[2, 7]
PbTe	2	2	3.21	132	1.45	3.5	[2, 8]
Si	166	2	2.70	498	0.56	140	[2, 3]
SnTe	1.5	2	3.15	155	2.1	2.1	[4, 9]
SrO	12	2	2.57	340	1.52	13	[2]
ZnTe	18	2	3.05	195	0.97	13	[2]
ZnS	27	2	2.66	290	0.75	30	[2]
ZnSe	33	2	2.83	239	0.75	26	[2, 3]
Mg_2Ge	13	3	2.79	332	1.38	11	[3]
Mg_2Si	7	3	2.78	476	1.32	22	[3, 10]
Mg_2Sn	16	3	2.95	224	1.27	5.9	[3]
CdS	16	4	2.92	214	0.75	15	[2]
CdSe	4.4	4	3.04	164	0.6	14	[2, 4]
InSe	6.9	4	3.07	190	1.2	6.3	[4]
ZnO	60	4	2.29	481	0.75	72	[2]
Bi_2Te_3	1.6	5	3.24	155	1.49	3.7	[4, 11]
Sb_2Te_3	2.4	5	3.15	160	1.49	3.2	[4]
$CuGaTe_2$	2.2	8	3.00	226	1.46	5.6	[4, 12]
InTe	1.7	8	3.17	186	1	7.8	[4, 13]
La_2Te_3	1.2	14	3.17	208	1.76	3.6	[14]
$CoSb_3$	10	16	2.85	307	0.95	49	[15]
$IrSb_3$	16	16	2.91	308	1.42	13	[16]
$CeFe_4Sb_{12}$	1.9	17	2.82	287	1.42	8.7	[17]
$Ba_8Ga_{16}Ge_{30}$	1.1	54	2.86	300	1.6	4.6	[18, 19]
$Yb_{14}AlSb_{11}$	0.6	104	3.07	160	1.5	1.2	[20]
$Yb_{14}MnSb_{11}$	0.5	104	3.07	160	1.5	1.2	[20]

TABLE I: Summary of the data which was used to calculate Figure 5 and 7 in the text. Our survey of the literature suggests fairly few compounds are sufficiently characterized for calculation of κ_L. Here, the calculated κ_L is the sum of κ_a and κ_o. The κ_a is obtained by solving Eq. 2 for a combination of Umklapp and boundary scattering (d =1 μm) limit with $\omega_m ax = \omega_a$ and $C_s(\omega) = C_{s,HT}(\omega)$. The κ_o is determined from Eq. 12.

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