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Novel Metal Oxides with Promising High-Temperature Thermoelectric Performance

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Detailed computations: method of verification

In the detailed calculations of ATa_2O_6 (A = Mg, Ca) and $SrTiO_3$, the PBEsol exchange-correlation functional[1] was used better to describe the structural properties. The LDA + *U* method of Dudarev *et al*.[2] with *U* - *J* = 5[3] and of Liechtenstein e*t al*.[4] with *U* = 5 eV and *J* = 0.64 eV[5] were used for the Ta 5*d* states of ATa_2O_6 (A = Mg, Ca) and the Ti 3*d* states of $SrTiO_3$, respectively. Considering the underestimation of the size of the bandgap in GGA-based calculations, the Heyd-Scuseria-Ernzerhof (HSE06) hybrid functional[6], with accurate exchange and correlation energy, was applied to calculate the band gaps of ATa_2O_6 (A = Mg, Ca), as shown in Fig. S1a and Fig. S1c . Our results coincide with the results of other theoretical calculations[3] and experimental results.[7, 8] Moreover, the spin-orbit coupling (SOC) effects on the electronic structure of ATa_2O_6 (A = Mg, Ca) and $SrTiO_3$ were also studied (see Fig. S1b, Fig. S1d and Fig. S2a) but there are no obvious changes. Therefore, SOC effects are not considered in the following calculations. To accurately estimate the electronic-transport properties, fine *k*-point meshes of 18×18×12 for $MgTa_2O_6$, 20×20×20 for $CaTa_2O_6$ and 27×27×27 for $SrTiO_3$ were used. Meanwhile, the scissor operator was also applied to correct the bandgap but leave the band dispersion unchanged. For $CaTa_2O_6$, the phonon dispersion was calculated with a 2×2×2 supercell and a 2×2×2 *k*-point mesh. For the thermal-conductivity calculation of $MgTa_2O_6$, the linearized phonon version of the

Bolztmann transport equation was solved, considering only two- and three-phonon scattering processes, using the ShengBTE code.[9] The second-order interatomic force constants (IFCs) were obtained via a 2×2×2 supercell with a 2×2×2 *k*-point mesh using density-functional perturbation theory (DFTP), as implemented in Phonopy.[10] The third-order IFCs were calculated using a 2×2×2 supercell and a 1×1×1 *k*-point mesh with only the gamma point, where interactions further than third neighbors in the supercell were neglected.

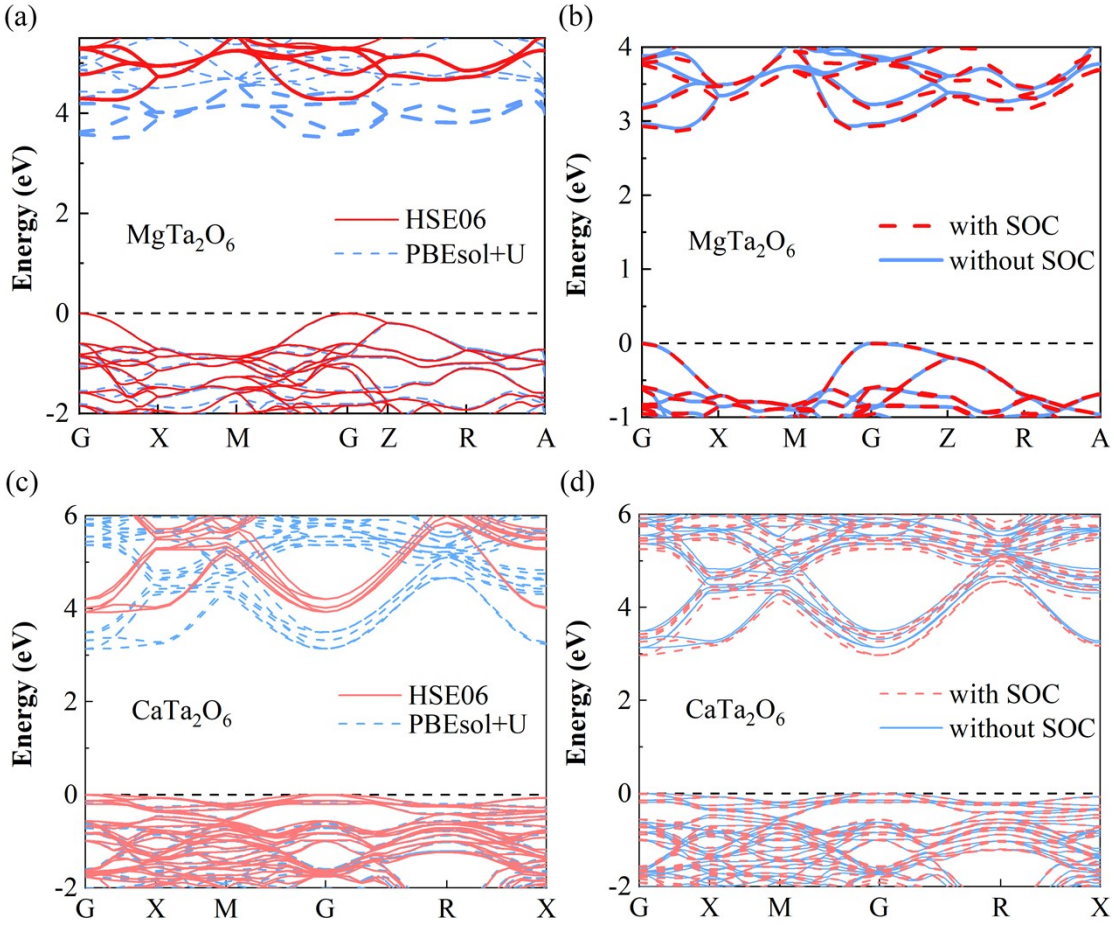

Fig S1. The effects of: (a) exchange-correlation functional; (b) spin-orbit coupling (SOC), on the electronic band structure of $MgTa_2O_6$ calculated with the PBEsol exchange-correlation functional and without using the LDA +*U* correction.

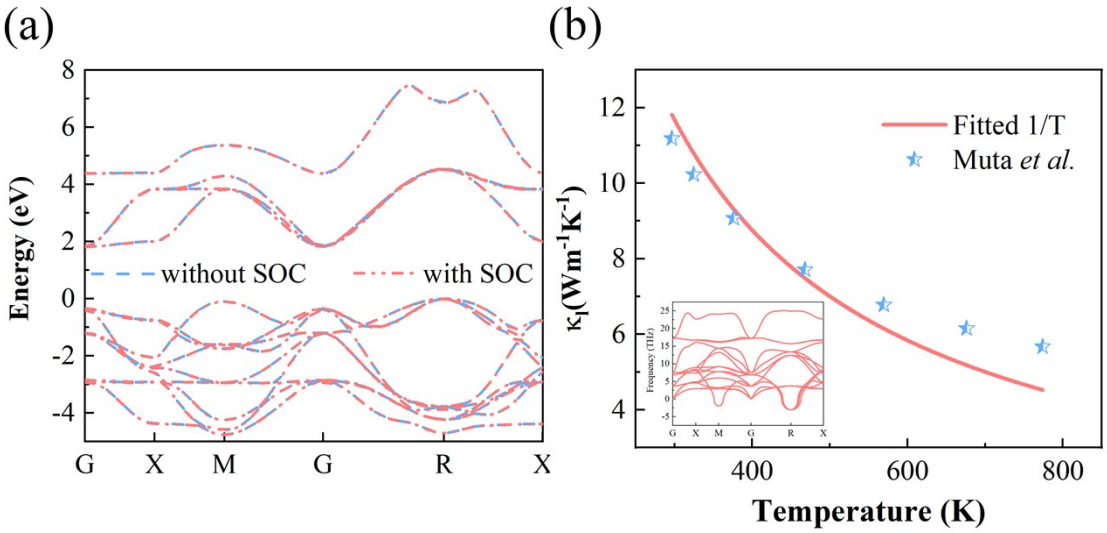

Fig S2 (a) The effects of spin-orbit coupling (SOC) on the electronic band structure of $SrTiO_3$ calculated with the PBEsol exchange-correlation functional. (b) The fitting curve plotting for $SrTiO_3$ with the $\kappa_l \sim 1/T$ relation in which the data points for the temperature dependence of the lattice thermal conductivity are extracted from the experimental results of Muta *et al.*[11] The inset shows the phonon-dispersion curves for $SrTiO_3$ calculated at 0 K.

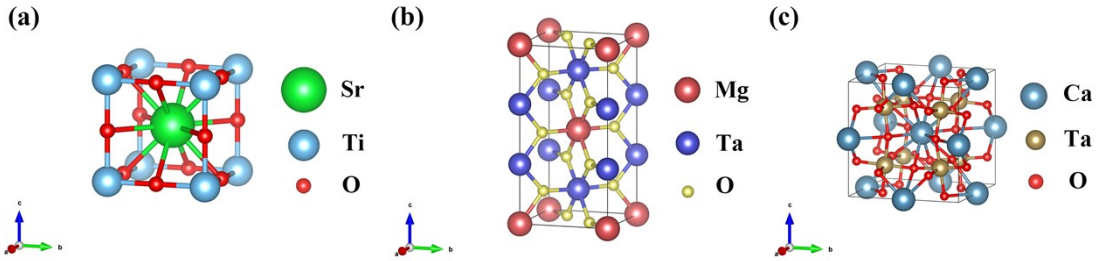

Fig S3 Crystal structure of: (a) $SrTiO_3$; (b) $MgTa_2O_6$; (c) $CaTa_2O_6$.

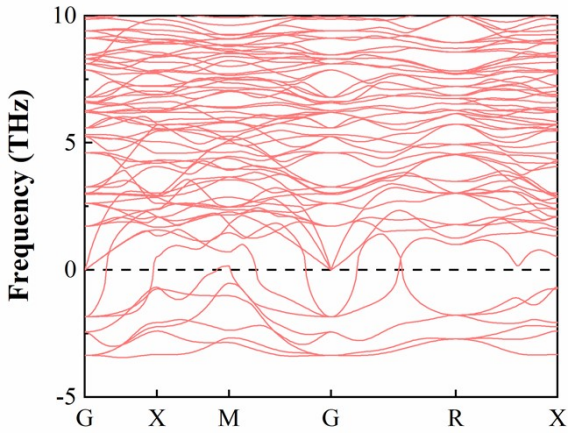

Fig S4 The phonon-dispersion curves for $CaTa_2O_6$.

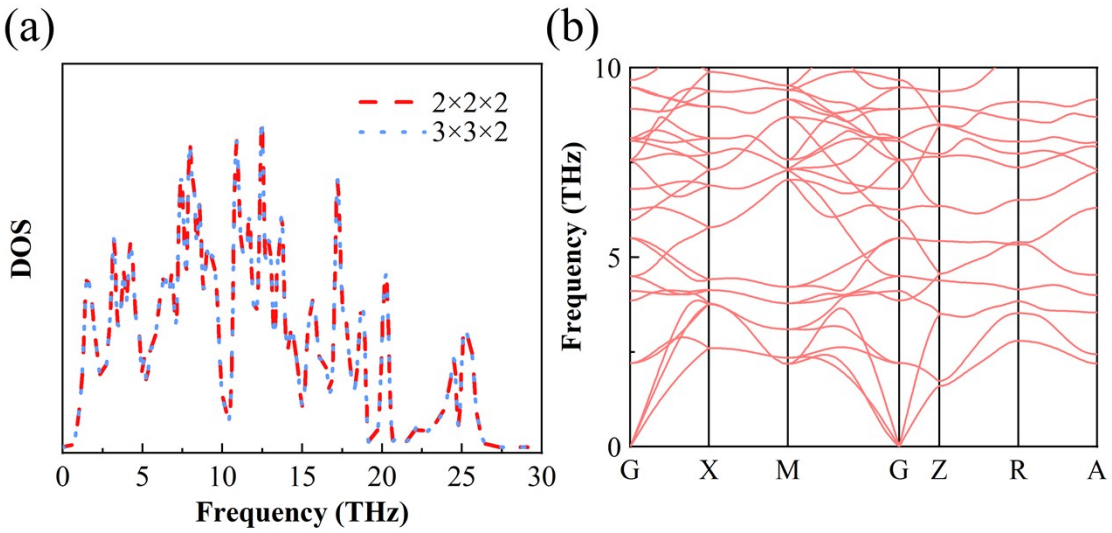

Fig. S5. (a) The phonon density of states of $MgTa_2O_6$ computed from supercell expansions of 2×2×2 and 3×3×2. (b) The phonon-dispersion curves for $MgTa_2O_6$.

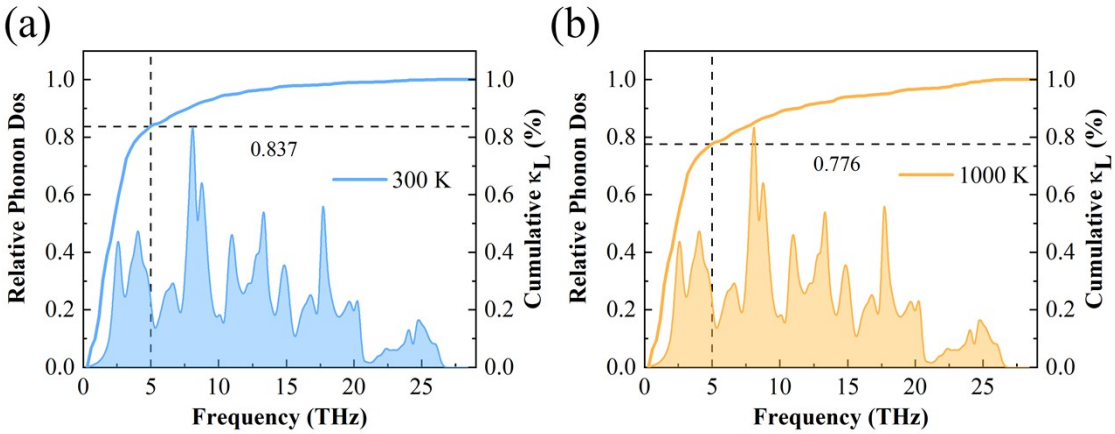

Fig. S6. The normalized phonon DOS and cumulative lattice thermal conductivity of $MgTa_2O_6$ at: (a) 300 K; (b) 1000 K.

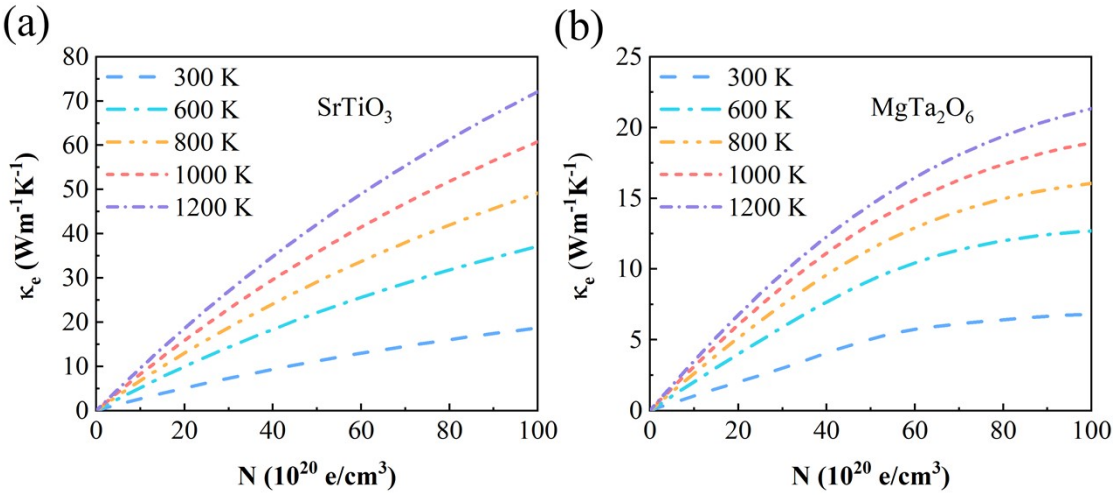

Fig. S7. Temperature-dependent electronic thermal conductivity of: (a) $SrTiO_3$; and (b) $MgTa_2O_6$, as a function of carrier concentration.

Table S1 The formula, space-group symbols (SG), space-group numbers (SN), bandgap (E_g), semiconductor type (n-type or p-type), and the corresponding carrier concentration (n_{max}, p_{max}), effective conductivity mass (m_c) and Seebeck mass (m_s), Fermi-surface complexity factors ($N_v^*K^*$) calculated at the maximum *PF* of the binary and ternary oxides at 1000 K. The table of electrical-transport properties from $KCoO_2$ onwards are left blank as their bandgaps are less than 0.1 eV (the bandgap screening criterion).

formula	SG	SN	E_g	type	n_{max}, p_{max} (10^{20} cm^{-3})	m_s (PF_{max})	m_c (PF_{max})	$N_v^*K^*$ (PF_{max})	PF_{max} (μW/(cmK^2)
Al_2O_3	$R\bar{3}c$	167	5.868	p	50.000	6.387	6.266	1.029	65.655
As_2O_3	$Fd\bar{3}m$	227	4.026	n	10.000	2.566	2.419	1.093	40.648
As_2O_5	$P4_12_12$	92	1.357	n	100.000	5.139	12.894	0.252	22.852
B_2O_3	$P3_121$	152	6.347	n	25.000	3.133	4.030	0.686	43.850
Ba_2ZrO_4	$I4/mmm$	139	3.156	p	25.000	5.503	6.700	0.744	55.952
$Ba_3Mn_2O_8$	$R\bar{3}m$	166	1.592	n	10.000	2.531	7.825	0.184	15.272
$Ba_3Y_4O_9$	$R32$	155	3.214	n	100.000	6.864	17.465	0.246	31.175
$Ba_4Nb_2O_9$	$P6_3/m$	176	3.518	n	10.000	2.668	5.681	0.322	18.188
$Ba_5Ta_4O_{15}$	$P\bar{3}m1$	164	3.083	n	10.000	1.708	85.310	0.003	44.049
$Ba_8V_7O_{22}$	$R\bar{3}m$	166	0.438	p	10.000	2.480	43460.545	0.000	6.200
$BaCoO_2$	$P3_121$	152	1.129	n	7.500	1.449	2.123	0.564	23.531
$BaHgO_2$	$R\bar{3}m$	166	2.301	p	25.000	5.325	4.317	1.370	71.597
$BaMnO_3$	$P6_3/mmc$	194	1.932	p	25.000	4.494	5.488	0.741	44.279
$BaMoO_4$	$I4_1/a$	88	4.375	p	25.000	6.377	13.730	0.317	26.510
BaO_2	$I4/mmm$	139	2.218	n	50.000	2.410	1.054	3.458	238.158

$BaTa_2O_6$	$P6/mmm$	191	2.079	n	10.000	1.283	19.220	0.017	34.519
$BaTiO_3$	$Pm\bar{3}m$	221	1.676	p	50.000	5.436	2.284	3.671	141.781
BaV_6O_{11}	$P6_3mc$	186	0.603	p	10.000	2.838	14.050	0.091	9.105
$BaWO_4$	$I4_1/a$	88	0.970	p	25.000	5.892	23.310	0.127	13.606
$BaZnO_2$	$P3_121$	152	2.246	p	25.000	5.305	13.006	0.261	22.059
$BaZrO_3$	$Pm\bar{3}m$	221	3.121	p	50.000	5.298	2.362	3.358	132.278
$Ca_2Hf_7O_{16}$	$R\bar{3}$	148	4.303	p	7.500	3.443	29.249	0.040	11.757
Ca_2MnO_4	$I4_1/acd$	142	0.395	n	100.000	2.179	14.500	0.058	26.745
$Ca_2Nb_2O_7$	$Fd\bar{3}m$	227	1.434	n	5.000	1.489	3.069	0.338	14.466
$Ca_2Ta_2O_7$	$Fd\bar{3}m$	227	2.317	n	5.000	1.742	3.898	0.299	13.788
$CaCrO_4$	$I4_1/amd$	141	2.429	p	50.000	6.235	9.109	0.566	44.297
$CaMoO_4$	$I4_1/a$	88	3.769	p	25.000	6.180	13.213	0.320	37.637
CaO	$Fm\bar{3}m$	225	3.641	p	100.000	5.725	2.222	4.135	157.859
CaO_2	$I4/mmm$	139	2.784	n	75.000	4.278	5.283	0.729	201.574
$CaTa_2O_6$	$Pm\bar{3}$	200	2.455	n	10.000	1.876	0.651	4.889	100.692
$CaTa_4O_{11}$	$P6_322$	182	3.573	n	25.000	3.765	17.276	0.102	30.429
CaV_4O_9	$P4/n$	85	2.447	n	25.000	5.405	43.869	0.043	7.783
$CdIn_2O_4$	$Fd\bar{3}m$	227	0.880	p	75.000	8.541	20.114	0.277	30.753
CdO_2	$Pa\bar{3}$	205	1.241	p	50.000	4.330	1.707	4.041	136.635
CoO_2	$P\bar{3}m1$	164	0.982	p	50.000	5.465	2.385	3.468	141.242
Cr_2O_3	$R\bar{3}c$	167	2.401	n	10.000	2.755	4.805	0.434	22.446

$Cs_2V_5O_{13}$	$I4mm$	107	1.551	p	50.000	8.620	217.699	0.008	45.311
Fe_2O_3	$R\bar{3}c$	167	1.565	p	25.000	4.548	9.615	0.325	24.718
Ga_2O_3	$R\bar{3}c$	167	2.329	p	100.000	7.829	16.793	0.318	34.658
GeO_2	$P3_121$	152	3.215	n	100.000	3.247	3.378	0.942	40.151
HfO_2	$Fm\bar{3}m$	225	3.804	p	25.000	2.798	0.824	6.252	146.918
In_2O_3	$Ia\bar{3}$	206	0.893	p	25.000	5.877	14.361	0.262	22.017
$K_2V_3O_8$	$P4bm$	100	2.000	p	50.000	16.569	355.152	0.010	15.828
$K_2Zn_6O_7$	$P4_2nm$	102	0.868	p	5.000	2.688	121.366	0.003	16.647
$K_4Zr_5O_{12}$	$P\bar{3}m1$	164	3.247	p	25.000	4.101	36.005	0.038	43.634
$K_5V_3O_{10}$	$P4_12_12$	92	3.058	p	10.000	3.138	108480.705	0.000	0.502
K_6CdO_4	$P6_3mc$	186	1.599	n	1.000	0.430	0.472	0.868	15.113
KO_3	$I4/mcm$	140	0.617	n	5.000	1.351	14.420	0.029	4.627
$KReO_4$	$I4_1/a$	88	3.969	p	25.000	6.732	35.779	0.082	10.417
Li_3CuO_3	$P4_2/mnm$	136	1.175	p	100.000	9.545	41.065	0.112	21.358
$Mg(RhO_2)_2$	$Fd\bar{3}m$	227	1.177	n	10.000	2.197	0.915	3.719	88.450
$Mg_2Mo_3O_8$	$P6_3mc$	186	1.641	p	10.000	2.863	25.763	0.037	16.388
$Mg_3Nb_6O_{11}$	$P\bar{3}m1$	164	0.237	p	25.000	2.484	7.398	0.195	35.124
$Mg_4Nb_2O_9$	$P\bar{3}c1$	165	3.419	p	25.000	4.197	16.616	0.127	23.757
Mg_6MnO_8	$Fm\bar{3}m$	225	2.312	p	25.000	5.365	12.657	0.276	22.543
$MgCr_2O_4$	$Fd\bar{3}m$	227	2.814	n	7.500	1.741	1.357	1.453	42.422
MgO_2	$Pa\bar{3}$	205	3.716	n	25.000	6.446	3.908	2.118	89.446

$MgTa_2O_6$	$P4_2/mnm$	136	2.857	n	10.000	2.541	2.361	1.116	48.630
$MgTiO_3$	$R\bar{3}$	148	3.519	p	50.000	6.681	11.957	0.418	39.771
Mn_3O_4	$I4_1/amd$	141	0.655	n	10.000	1.982	7.082	0.148	42.392
MnO	$Fm\bar{3}m$	225	0.120	p	25.000	3.937	1.138	6.436	171.612
$Na_{14}Cd_2O_9$	$P\bar{3}$	147	1.372	n	50.000	0.890	2.071	0.282	15.577
Na_2O_2	$P\bar{6}2m$	189	1.717	n	50.000	1.066	5.199	0.093	58.822
$Na_2Ta_4O_{11}$	$R\bar{3}c$	167	3.494	p	25.000	5.457	1850.255	0.000	22.424
Na_3CoO_2	$P4_2/mnm$	136	1.366	n	2.500	0.842	1.666	0.359	11.668
$Na_4Ti_5O_{12}$	$P\bar{3}$	147	2.502	n	25.000	4.057	29.237	0.052	60.598
$NaNbO_2$	$P6_3/mmc$	194	1.389	n	75.000	3.956	3.833	1.049	105.347
$NaNbO_3$	$R\bar{3}$	148	3.843	n	25.000	4.153	16.742	0.124	39.818
Nb_2O_5	$I4/mmm$	139	1.493	p	10.000	2.837	82826.358	0.000	13.573
NbO_2	$I4_1/a$	88	0.406	n	25.000	2.800	6.705	0.270	19.321
Pb_3O_4	$P4_2/mbc$	135	1.113	p	7.500	2.323	3.022	0.674	27.230
PoO_2	$Fm\bar{3}m$	225	1.916	n	7.500	1.388	0.365	7.406	115.424
Rb_3TaO_8	$I\bar{4}2m$	121	3.083	n	10.000	2.343	5.910	0.250	21.906
$Rb_3V_5O_{14}$	$P31m$	157	2.262	n	7.500	2.417	282.709	0.001	22.279
$RbScO_2$	$P6_3/mmc$	194	3.464	p	50.000	5.671	8.352	0.560	82.163
Rh_2O_3	$R\bar{3}c$	167	0.669	n	25.000	4.487	3.880	1.243	60.565

Sb_2O_3	$Fd\bar{3}m$	227	3.290	n	25.000	2.239	1.153	2.707	74.308
Sc_2O_3	$Ia\bar{3}$	206	3.826	p	10.000	3.800	6.207	0.479	24.558
SeO_2	$P4_2/mbc$	135	3.235	n	5.000	1.363	2.179	0.495	36.767
SiO_2	$P3_221$	154	5.727	p	25.000	6.469	9.033	0.606	51.325
SnO_2	$P4_2/mnm$	136	0.619	p	25.000	2.538	2.906	0.817	36.058
$Sr_3V_2O_7$	$I4/mmm$	139	0.534	p	25.000	1.689	1718.130	0.000	24.709
$Sr_6(CoO_3)_5$	$R32$	155	0.373	p	10.000	2.886	87.441	0.006	1.639
$SrMoO_4$	$I4_1/a$	88	4.061	p	25.000	6.151	13.779	0.298	30.262
SrO_2	$I4/mmm$	139	2.817	n	50.000	5.110	8.245	0.488	252.999
$SrTa_4O_{11}$	$P6_322$	182	3.550	n	25.000	3.678	13.727	0.139	27.717
$SrTiO_3$	$Pm\bar{3}m$	221	1.791	n	10.000	2.430	0.842	4.903	109.233
$SrV_{13}O_{18}$	$R\bar{3}$	148	0.108	n	50.000	1.503	61.895	0.004	1.033
$SrWO_4$	$I4_1/a$	88	0.687	p	25.000	5.429	7158.355	0.000	17.470
$SrZrO_3$	$Pm\bar{3}m$	221	3.307	p	100.000	5.604	2.138	4.244	158.530
Te_4O_9	$R\bar{3}$	148	2.211	p	10.000	3.751	8.141	0.313	19.040
TeO_3	$R\bar{3}c$	167	1.132	p	25.000	5.689	5.301	1.112	61.132
TiO_2	$P4_2/mnm$	136	1.789	n	50.000	5.375	1.772	5.282	182.470
V_2O_3	$Ia\bar{3}$	206	0.890	n	5.000	1.285	3.394	0.233	10.817
VO_2	$P4_2/mnm$	136	0.882	p	25.000	4.251	2.646	2.036	90.812

Y_2O_3	$Ia\bar{3}$	206	4.119	p	25.000	4.309	10.732	0.254	20.425
ZnO_2	$Pa\bar{3}$	205	2.113	p	50.000	4.169	1.662	3.974	132.473
ZrO_2	$P4_2/nmc$	137	4.045	p	50.000	7.532	3.302	3.446	167.613
$KCoO_2$	$I\bar{4}2d$	122	0.092						
$BaV_{13}O_{18}$	$R\bar{3}$	148	0.075						
$Sr_5(CoO_3)_4$	$P\bar{3}c1$	165	0.057						
$Ca_3(CoO_3)_2$	$R\bar{3}c$	167	0.039						
$Ba_3W_2O_9$	$R\bar{3}c$	167	0.018						
PbO_2	$P4_2/mnm$	136	0.015						
Mg_2VO_4	$Fd\bar{3}m$	227	0.008						
Ba_2Co_9O14	$R\bar{3}m$	166	0.000						
$Ba_2Nb_{15}O_{32}$	$R\bar{3}$	148	0.000						
$Ba_2Nb_5O_9$	$P4/mmm$	123	0.000						
$Ba_3Cr_2O_8$	$R\bar{3}m$	166	0.000						
$Ba_3Ta_5O_{15}$	$P4/mbm$	127	0.000						
$Ba_5Co_5O_{14}$	$P\bar{3}m1$	164	0.000						
$BaCoO_3$	$P6_3/mmc$	194	0.000						
$BaIrO_3$	$Pm\bar{3}m$	221	0.000						
$BaMoO_3$	$Pm\bar{3}m$	221	0.000						
$BaNb_4O_6$	$P4/mmm$	123	0.000						

$BaRhO_3$	$P6_3/mmc$	194	0.000
Bi_2O_3	$Pn\bar{3}m$	224	0.000
BiO_2	$Fm\bar{3}m$	225	0.000
Ca_2IrO_4	$P\bar{6}2m$	189	0.000
$CaMn_7O_{12}$	$Im\bar{3}$	204	0.000
CdO	$Fm\bar{3}m$	225	0.000
Co_3O_4	$Fd\bar{3}m$	227	0.000
Cr_3O	$Pm\bar{3}n$	223	0.000
CrO_2	$P4_2/mnm$	136	0.000
Cu_3TeO_6	$Ia\bar{3}$	206	0.000
FeO	$Fm\bar{3}m$	225	0.000
IrO_2	$Pa\bar{3}$	205	0.000
$K(IrO_2)_4$	$I4/m$	87	0.000
$K(Mo_2O_3)_2$	$P4/mbm$	127	0.000
$K_2Ta_{15}O_{32}$	$R\bar{3}$	148	0.000
$K_4(CoO_2)_7$	$P6_3/m$	176	0.000
KCr_4O_8	$I4/m$	87	0.000
$KIrO_3$	$Pn\bar{3}$	201	0.000
KO_2	$I4/mmm$	139	0.000

KV_4O_8	$I4/m$	87	0.000	
$MgTi_2O_4$	$Fd\bar{3}m$	227	0.000	
MgV_2O_4	$Fd\bar{3}m$	227	0.000	
Mn_2O_3	$Ia\bar{3}$	206	0.000	
MnO_2	$P4_2/mnm$	136	0.000	
MoO_2	$P4_2/mnm$	136	0.000	
$Na(Mo_2O_3)_2$	$P4/mbm$	127	0.000	
$NaMn_7O_{12}$	$Im\bar{3}$	204	0.000	
NaO_2	$Pa\bar{3}$	205	0.000	
$NaTi_8O_{13}$	$R\bar{3}$	148	0.000	
NaV_6O_{11}	$P6_3mc$	186	0.000	
$NaWO_3$	$Pm\bar{3}m$	221	0.000	
Nb_4O_5	$P4_2/nmc$	137	0.000	
$Rb_2Ta_{15}O_{32}$	$R\bar{3}$	148	0.000	
$Rb_4Nb_{11}O_{30}$	$R\bar{3}m$	166	0.000	
ReO_2	$P4_2/mnm$	136	0.000	
ReO_3	$Im\bar{3}$	204	0.000	
RhO_2	$P4_2/mnm$	136	0.000	
Sb_2O_5	$Fd\bar{3}m$	227	0.000	

SbO_2	$Fd\bar{3}m$	227	0.000	
Sr_2IrO_4	$I4_1/acd$	142	0.000	
$Sr_2Nb_5O_9$	$P4/mmm$	123	0.000	
Sr_2TcO_4	$I4/mmm$	139	0.000	
Sr_2VO_4	$I4/mmm$	139	0.000	
$Sr_3(CoO_3)_2$	$R\bar{3}c$	167	0.000	
$Sr_4Cr_3O_9$	$P3$	143	0.000	
Sr_4IrO_6	$R\bar{3}c$	167	0.000	
Sr_4RhO_6	$R\bar{3}c$	167	0.000	
$Sr_4V_3O_{10}$	$I4/mmm$	139	0.000	
$Sr_7Nb_6O_{21}$	$R\bar{3}$	148	0.000	
$SrCo_{12}O_{19}$	$P6_3/mmc$	194	0.000	
$SrCo_6O_{11}$	$P6_3/mmc$	194	0.000	
$SrMoO_3$	$Pm\bar{3}m$	221	0.000	
$SrNbO_3$	$Pm\bar{3}m$	221	0.000	
SrV_6O_{11}	$P6_3/mmc$	194	0.000	
TaO_2	$P4_2/mnm$	136	0.000	
TeO_2	$P4_2/mnm$	136	0.000	
Ti_2O_3	$R\bar{3}c$	167	0.000	

Ti_4O_5	$I4/m$	87	0.000	
Ti_6O	$P\bar{3}1m$	162	0.000	
Tl_2O_3	$Ia\bar{3}$	206	0.000	
Tl_2TeO_6	$P321$	150	0.000	
$V_{13}O_{16}$	$I4_1/amd$	141	0.000	
$V_{16}O_3$	$I4/mmm$	139	0.000	
WO_2	$P4_2/mnm$	136	0.000	
Yb_2O_3	$Ia\bar{3}$	206	0.000	

Table S2 Bulk modulus, B_{vrh}, and shear modulus, G_{vrh}, calculated using the Voigt-Reuss-Hill approximation, the Grüneisen constant, γ, the Clarke thermal conductivity, κ_{Clarke}, the Cahill thermal conductivity, κ_{Cahill}, the Slack thermal conductivity, κ_{Slack}, and the maximum thermal conductivity, κ_{max}, between κ_{Clarke} and κ_{Slack} for the binary and ternary oxides at 1000 K.

formula	B_{vrh} (GPa)	G_{vrh} (GPa)	γ	κ_{Clarke} ($Wm^{-1}K^{-1}$)	κ_{Cahill} ($Wm^{-1}K^{-1}$)	κ_{Slack} ($Wm^{-1}K^{-1}$)	κ_{max} ($Wm^{-1}K^{-1}$)
Al_2O_3	234.343	144.074	1.476	2.737	2.991	5.864	5.864
As_2O_3	9.938	5.724	1.541	0.345	0.379	0.077	0.345
As_2O_5	93.753	51.418	1.591	1.213	1.333	1.248	1.248
B_2O_3	45.957	44.602	1.063	1.740	1.895	4.011	4.011
Ba_2ZrO_4	104.762	55.270	1.631	0.878	0.967	3.125	3.125
$Ba_3Mn_2O_8$	62.924	28.780	1.782	0.722	0.804	0.313	0.722
$Ba_3Y_4O_9$	99.925	47.869	1.733	0.857	0.951	0.626	0.857
$Ba_4Nb_2O_9$	72.579	30.955	1.858	0.700	0.784	0.341	0.700
$Ba_5Ta_4O_{15}$	113.227	60.231	1.623	0.888	0.978	1.313	1.313
$Ba_8V_7O_{22}$	45.029	27.719	1.474	0.706	0.772	0.214	0.706
$BaCoO_2$	77.419	27.762	2.050	0.666	0.760	0.483	0.666
$BaHgO_2$	45.633	8.740	2.747	0.284	0.358	0.049	0.284
$BaMnO_3$	72.401	12.480	2.858	0.519	0.667	0.076	0.519
$BaMoO_4$	52.397	24.352	1.765	0.659	0.733	0.367	0.659
BaO_2	70.113	35.462	1.675	0.742	0.820	1.682	1.682
$BaTa_2O_6$	160.878	84.962	1.630	1.086	1.197	0.776	1.086
$BaTiO_3$	163.849	107.202	1.415	1.444	1.574	12.889	12.889
BaV_6O_{11}	166.546	51.414	2.218	1.268	1.474	0.441	1.268
$BaWO_4$	49.562	22.915	1.771	0.556	0.618	0.489	0.556

$BaZnO_2$	79.781	32.948	1.893	0.707	0.795	0.740	0.740
$BaZrO_3$	148.340	93.162	1.455	1.211	1.322	10.226	10.226
$Ca_2Hf_7O_{16}$	188.244	91.240	1.720	1.184	1.312	0.895	1.184
Ca_2MnO_4	120.441	68.360	1.556	1.517	1.665	2.026	2.026
$Ca_2Nb_2O_7$	140.721	88.295	1.456	1.526	1.666	4.023	4.023
$Ca_2Ta_2O_7$	155.654	97.299	1.459	1.327	1.449	3.778	3.778
$CaCrO_4$	17.264	27.497	0.713	0.862	0.970	5.062	5.062
$CaMoO_4$	67.730	33.595	1.696	0.972	1.076	1.051	1.051
CaO	105.983	75.109	1.338	1.528	1.662	21.468	21.468
CaO_2	70.875	47.407	1.393	1.346	1.466	7.369	7.369
$CaTa_2O_6$	160.749	35.484	2.592	0.809	0.992	0.176	0.809
$CaTa_4O_{11}$	165.369	33.330	2.692	0.770	0.959	0.149	0.770
CaV_4O_9	42.214	37.634	1.133	1.077	1.171	1.728	1.728
$CdIn_2O_4$	122.470	45.614	2.008	0.864	0.982	0.850	0.864
CdO_2	107.251	36.554	2.107	0.868	0.997	0.617	0.868
CoO_2	43.671	6.573	2.997	0.502	0.664	0.056	0.502
Cr_2O_3	206.172	114.571	1.578	1.974	2.168	3.286	3.286
$Cs_2V_5O_{13}$	25.348	8.231	2.161	0.447	0.517	0.069	0.447
Fe_2O_3	191.441	85.539	1.808	1.678	1.872	1.619	1.678
Ga_2O_3	199.308	87.752	1.824	1.581	1.767	1.470	1.581
GeO_2	52.015	26.520	1.667	0.843	0.931	0.902	0.902
HfO_2	254.816	115.216	1.795	1.296	1.444	8.581	8.581
In_2O_3	118.390	55.450	1.757	0.979	1.088	0.692	0.979
$K_2V_3O_8$	40.422	19.441	1.729	0.787	0.872	0.347	0.787

$K_2Zn_6O_7$	70.566	27.503	1.957	0.827	0.935	0.292	0.827
$K_4Zr_5O_{12}$	128.410	54.349	1.867	1.152	1.291	1.211	1.211
$K_5V_3O_{10}$	5.491	1.795	2.153	0.238	0.274	0.003	0.238
K_6CdO_4	32.155	15.079	1.756	0.580	0.645	0.254	0.580
KO_3	21.848	6.988	2.178	0.539	0.623	0.076	0.539
$KReO_4$	29.160	7.627	2.404	0.381	0.454	0.058	0.381
Li_3CuO_3	50.888	36.284	1.333	1.370	1.490	1.138	1.370
$Mg(RhO_2)_2$	174.460	53.906	2.217	1.160	1.348	0.857	1.160
$Mg_2Mo_3O_8$	129.549	55.769	1.848	1.266	1.417	0.908	1.266
$Mg_3Nb_6O_{11}$	180.711	89.631	1.696	1.478	1.635	2.640	2.640
$Mg_4Nb_2O_9$	142.786	68.198	1.736	1.561	1.732	2.814	2.814
Mg_6MnO_8	131.662	100.013	1.274	2.093	2.275	8.164	8.164
$MgCr_2O_4$	159.369	77.780	1.713	1.692	1.874	3.008	3.008
MgO_2	122.826	82.654	1.388	2.093	2.280	6.261	6.261
$MgTa_2O_6$	182.312	94.648	1.648	1.314	1.450	2.817	2.817
$MgTiO_3$	159.352	81.970	1.658	1.869	2.062	2.131	2.131
Mn_3O_4	130.113	44.306	2.108	1.179	1.354	0.827	1.179
MnO	146.459	64.486	1.824	1.353	1.511	6.726	6.726
$Na_{14}Cd_2O_9$	44.199	27.897	1.450	0.940	1.026	0.802	0.940
Na_2O_2	52.683	29.695	1.563	1.201	1.318	1.259	1.259
$Na_2Ta_4O_{11}$	160.990	55.703	2.090	1.012	1.160	0.347	1.012
Na_3CoO_2	13.838	17.041	0.881	0.676	0.744	1.239	1.239
$Na_4Ti_5O_{12}$	128.665	61.167	1.741	1.572	1.745	1.656	1.656
$NaNbO_2$	125.719	97.398	1.256	1.567	1.703	10.082	10.082

$NaNbO_3$	79.316	35.171	1.816	1.020	1.139	0.511	1.020
Nb_2O_5	151.015	64.298	1.860	1.254	1.405	0.833	1.254
NbO_2	212.585	80.208	1.993	1.402	1.591	0.871	1.402
Pb_3O_4	37.066	10.815	2.281	0.312	0.365	0.047	0.312
PoO_2	163.502	73.207	1.805	0.927	1.034	4.868	4.868
Rb_3TaO_8	32.511	11.901	2.027	0.474	0.540	0.162	0.474
$Rb_3V_5O_{14}$	46.249	21.216	1.779	0.756	0.842	1.205	1.205
$RbScO_2$	94.065	57.446	1.482	1.119	1.223	3.934	3.934
Rh_2O_3	225.174	99.901	1.815	1.428	1.595	1.666	1.666
Sb_2O_3	13.380	9.099	1.377	0.354	0.385	0.160	0.354
Sc_2O_3	163.170	80.545	1.701	1.684	1.864	1.755	1.755
SeO_2	23.003	10.615	1.773	0.507	0.564	0.117	0.507
SiO_2	4.466	25.179	0.227	0.690	1.012	12.546	12.546
SnO_2	172.945	85.281	1.702	1.278	1.414	5.139	5.139
$Sr_3V_2O_7$	136.461	72.258	1.627	1.307	1.440	3.222	3.222
$Sr_6(CoO_3)_5$	42.500	47.417	0.954	0.977	1.069	3.453	3.453
$SrMoO_4$	63.350	31.011	1.710	0.825	0.913	0.906	0.906
SrO_2	74.651	40.367	1.606	0.958	1.053	3.780	3.780
$SrTa_4O_{11}$	173.097	24.156	3.071	0.643	0.866	0.070	0.643
$SrTiO_3$	169.469	109.170	1.430	1.674	1.826	5.317	5.317
$SrV_{13}O_{18}$	139.227	110.175	1.237	1.806	1.962	2.347	2.347
$SrWO_4$	53.623	28.202	1.635	0.670	0.739	0.750	0.750
$SrZrO_3$	148.877	81.159	1.597	1.271	1.398	7.293	7.293
Te_4O_9	37.347	18.330	1.707	0.582	0.644	0.347	0.582

TeO_3	99.154	97.622	1.051	1.395	1.520	13.642	13.642
TiO_2	213.729	111.104	1.647	2.051	2.262	9.814	9.814
V_2O_3	193.063	64.784	2.124	1.524	1.753	0.667	1.524
VO_2	234.644	117.597	1.685	2.089	2.309	9.701	9.701
Y_2O_3	137.879	64.126	1.765	1.141	1.269	1.064	1.141
ZnO_2	144.282	62.406	1.843	1.422	1.591	1.784	1.784
ZrO_2	165.676	52.087	2.197	1.150	1.335	1.485	1.485

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