Supplementary file

TableS1. The calculated lattice thermal conductivity (LTC) κ_l ($Wm^{-1} \cdot k^{-1}$) of Al-TM_{Al} supercell at various temperatures, as plotted in Fig. 2 (b).

	100K	200K	300K	400K	500K	600K	700K	800K	900K	1000K
Al	25.48	12.00	7.38	5.04	3.63	2.69	2.02	1.52	1.14	0.83
V_{Al}	25.84	12.17	7.48	5.11	3.68	2.73	2.05	1.54	1.15	0.84
Sc_{Al}	26.51	12.51	7.71	5.29	3.83	2.86	2.16	1.64	1.24	0.93
Ti_{Al}	27.82	13.16	8.14	5.61	4.08	3.06	2.33	1.79	1.37	1.04
V_{Al}	28.06	13.27	8.22	5.66	4.12	3.09	2.36	1.81	1.39	1.05
Cr_{Al}	28.00	13.25	8.20	5.65	4.11	3.08	2.35	1.80	1.38	1.05
Mn_{Al}	27.87	13.18	8.15	5.61	4.08	3.06	2.33	1.79	1.37	1.03
Fe_{Al}	27.58	13.04	8.06	5.54	4.03	3.01	2.29	1.75	1.34	1.01
Co_{Al}	27.13	12.81	7.91	5.44	3.94	2.95	2.24	1.70	1.29	0.97
Ni_{Al}	26.45	12.48	7.69	5.27	3.81	2.84	2.15	1.63	1.23	0.91
Cu_{Al}	25.66	12.08	7.44	5.08	3.67	2.72	2.05	1.54	1.16	0.85
Zn_{Al}	25.19	11.85	7.28	4.97	3.58	2.65	1.99	1.50	1.11	0.81
Y_{Al}	25.92	12.22	7.53	5.16	3.73	2.78	2.10	1.59	1.20	0.89
Zr_{Al}	27.49	12.99	8.04	5.53	4.02	3.02	2.30	1.76	1.35	1.02
Nb_{Al}	28.11	13.31	8.24	5.68	4.14	3.11	2.38	1.83	1.40	1.07
Mo_{Al}	28.30	13.40	8.30	5.72	4.17	3.14	2.40	1.85	1.42	1.08
Tc_{Al}	28.16	13.33	8.25	5.69	4.14	3.11	2.38	1.83	1.40	1.07
Ru_{Al}	27.74	13.12	8.12	5.59	4.06	3.05	2.32	1.78	1.36	1.03
Rh_{Al}	27.12	12.81	7.92	5.44	3.95	2.95	2.24	1.71	1.30	0.98
Pd_{Al}	26.30	12.40	7.65	5.24	3.79	2.82	2.14	1.62	1.22	0.91
Ag_{Al}	25.31	11.91	7.33	5.01	3.61	2.68	2.01	1.52	1.13	0.83
Cd_{Al}	24.94	11.73	7.21	4.92	3.54	2.62	1.97	1.48	1.10	0.80
Hf_{Al}	27.25	12.88	7.97	5.48	3.99	2.99	2.28	1.75	1.34	1.01
Ta_{Al}	27.99	13.25	8.21	5.66	4.13	3.11	2.38	1.83	1.41	1.07
W_{Al}	28.21	13.36	8.28	5.71	4.17	3.14	2.40	1.85	1.43	1.09
Re_{Al}	27.98	13.24	8.20	5.66	4.12	3.10	2.37	1.82	1.40	1.07
Os_{Al}	27.69	13.09	8.11	5.58	4.07	3.05	2.33	1.79	1.37	1.04
Ir_{Al}	27.11	12.81	7.92	5.44	3.95	2.96	2.25	1.72	1.31	0.99
Pt_{Al}	26.36	12.44	7.67	5.27	3.82	2.85	2.16	1.64	1.25	0.93
Au_{Al}	25.33	11.93	7.34	5.02	3.62	2.69	2.03	1.53	1.15	0.85
Hg_{Al}	24.57	11.55	7.09	4.84	3.48	2.58	1.93	1.45	1.08	0.79

TableS2. The calculated electronic thermal conductivity (ETC) κ_l ($Wm^{-1}\cdot k^{-1}$) of Al-TM_{Al} supercell at various temperatures, as plotted in Fig. 2 (d).

	100K	200K	300K	400K	500K	600K	700K	800K	900K	1000K
Al	203.34	217.81	223.61	226.07	227.01	227.09	226.61	225.72	224.51	223.06
V_{Al}	202.33	176.88	178.95	179.68	179.25	178.16	176.69	174.98	173.12	171.18
Sc_{Al}	163.58	171.63	176.13	177.64	177.58	176.69	175.33	173.69	171.86	169.91
Ti_{Al}	196.70	177.43	181.60	183.28	183.40	182.67	181.44	179.89	178.14	176.25
V_{Al}	191.26	172.96	177.43	179.98	181.13	181.33	180.85	179.86	178.50	176.88
Cr_{Al}	188.33	173.21	178.41	180.87	181.79	181.82	181.25	180.22	178.87	177.27
Mn_{Al}	204.36	174.78	176.13	178.09	179.39	179.90	179.71	178.93	177.69	176.10
Fe_{Al}	168.79	175.68	178.67	179.91	180.14	179.69	178.77	177.52	212.57	192.20
Co_{Al}	211.37	177.23	177.65	179.68	181.30	182.19	182.37	181.95	181.04	179.76
Ni_{Al}	210.28	181.50	183.41	185.65	187.06	187.64	187.51	186.82	185.71	184.27
Cu_{Al}	193.08	178.10	184.12	186.62	187.38	187.24	186.52	185.40	183.99	182.37
Zn_{Al}	222.46	200.25	205.54	207.79	208.24	207.73	206.67	205.26	203.62	201.80
Y_{Al}	190.42	161.99	161.69	161.20	160.05	158.47	156.67	154.77	152.82	150.86
Zr_{Al}	191.31	158.35	158.06	159.55	160.70	161.20	161.06	160.40	159.34	157.97
Nb_{Al}	186.42	157.63	158.30	159.97	161.22	161.83	161.82	161.28	160.33	159.06
Mo_{Al}	171.61	157.33	162.37	164.83	165.79	165.85	165.30	164.32	163.02	161.49
Tc_{Al}	173.46	150.78	153.81	156.60	158.37	159.19	159.22	158.62	157.54	156.09
Ru_{Al}	174.22	148.47	150.51	153.08	154.88	155.80	155.93	155.44	154.44	153.08
Rh_{Al}	166.34	149.85	153.73	155.97	157.10	157.42	157.12	156.32	155.14	153.68
Pd_{Al}	154.74	138.19	140.95	142.31	142.85	142.85	142.44	141.68	140.65	139.42
Ag_{Al}	172.29	145.77	144.98	144.09	142.68	140.93	139.01	137.01	135.00	133.02
Cd_{Al}	210.75	190.17	194.94	196.47	196.23	195.14	193.63	191.86	189.93	187.91
Hf_{Al}	184.32	170.32	175.14	176.75	176.81	176.08	174.86	173.33	171.58	169.69
Ta_{Al}	197.84	172.59	174.88	176.10	176.16	175.50	174.37	172.93	171.29	169.51
W_{Al}	167.59	156.71	162.70	165.63	166.97	167.32	166.98	166.10	164.82	163.25
Re_{Al}	166.85	153.19	158.10	160.64	161.84	162.17	161.86	161.06	159.87	158.40
Os_{Al}	169.58	148.59	151.66	153.88	155.03	155.38	155.13	154.42	153.36	152.05
Ir_{Al}	161.99	140.51	142.88	144.74	145.74	146.07	145.87	145.27	144.35	143.18
Pt_{Al}	133.77	114.18	115.51	117.07	118.27	119.10	119.57	119.70	119.53	119.11
Au_{Al}	143.74	125.29	127.02	127.82	127.65	126.84	125.63	124.16	122.57	120.90
Hg_{Al}	209.44	187.31	191.10	192.32	192.10	191.18	189.84	188.24	186.45	184.53

TableS3. The calculated total thermal conductivity (TC) κ_l ($Wm^{-1}\cdot k^{-1}$) of Al-TM_{Al} supercell at various temperatures, as plotted in Fig. 2 (d).

	100K	200K	300K	400K	500K	600K	700K	800K	900K	1000K
Al	228.82	229.81	230.99	231.11	230.64	229.78	228.63	227.24	225.65	223.89
V_{Al}	228.17	189.04	186.43	184.78	182.93	180.89	178.74	176.52	174.27	172.02
Sc_{Al}	190.09	184.14	183.85	182.93	181.41	179.55	177.50	175.33	173.10	170.84
Ti_{Al}	224.52	190.59	189.75	188.89	187.48	185.73	183.77	181.68	179.51	177.29
V_{Al}	219.32	186.23	185.65	185.64	185.25	184.43	183.21	181.67	179.89	177.94
Cr_{Al}	216.34	186.46	186.61	186.51	185.90	184.91	183.60	182.03	180.25	178.32
Mn_{Al}	232.23	187.96	184.28	183.70	183.47	182.96	182.04	180.72	179.06	177.14
Fe_{Al}	196.37	188.71	186.73	185.46	184.17	182.71	181.07	179.27	213.91	193.21
Co_{Al}	238.50	190.05	185.57	185.12	185.24	185.13	184.61	183.65	182.34	180.73
Ni_{Al}	236.73	193.98	191.10	190.92	190.87	190.47	189.65	188.45	186.94	185.18
Cu_{Al}	218.74	190.18	191.55	191.70	191.05	189.96	188.57	186.95	185.15	183.22
Zn_{Al}	247.65	212.11	212.82	212.77	211.82	210.38	208.66	206.76	204.73	202.61
Y_{Al}	216.35	174.21	169.22	166.36	163.78	161.25	158.77	156.36	154.02	151.76
Zr_{Al}	218.80	171.35	166.09	165.08	164.73	164.22	163.36	162.16	160.69	158.99
Nb_{Al}	214.54	170.93	166.54	165.65	165.36	164.94	164.19	163.11	161.74	160.13
Mo_{Al}	199.90	170.73	170.67	170.56	169.96	168.98	167.70	166.16	164.44	162.58
Tc_{Al}	201.62	164.10	162.06	162.29	162.52	162.31	161.60	160.45	158.94	157.16
Ru_{Al}	201.96	161.59	158.62	158.67	158.94	158.84	158.26	157.22	155.80	154.11
Rh_{Al}	193.47	162.67	161.65	161.41	161.04	160.37	159.36	158.04	156.45	154.66
Pd_{Al}	181.04	150.60	148.60	147.55	146.65	145.68	144.57	143.30	141.88	140.33
Ag_{Al}	197.60	157.68	152.30	149.10	146.29	143.61	141.02	138.53	136.14	133.85
Cd_{Al}	235.69	201.90	202.15	201.39	199.77	197.77	195.59	193.34	191.04	188.72
Hf_{Al}	211.57	183.19	183.10	182.23	180.80	179.07	177.14	175.08	172.92	170.71
Ta_{Al}	225.83	185.83	183.09	181.76	180.29	178.60	176.74	174.76	172.70	170.59
W_{Al}	195.80	170.06	170.98	171.35	171.14	170.46	169.38	167.95	166.25	164.34
Re_{Al}	194.83	166.43	166.30	166.30	165.96	165.27	164.23	162.88	161.27	159.47
Os_{Al}	197.26	161.68	159.76	159.47	159.10	158.43	157.46	156.21	154.73	153.09
Ir_{Al}	189.09	153.32	150.80	150.19	149.70	149.03	148.12	146.99	145.66	144.17
Pt_{Al}	160.14	126.62	123.19	122.34	122.09	121.95	121.72	121.34	120.78	120.04
Au_{Al}	169.08	137.22	134.36	132.84	131.28	129.53	127.65	125.70	123.72	121.75
Hg_{Al}	234.00	198.86	198.19	197.16	195.59	193.75	191.77	189.69	187.53	185.32

TableS4. The calculated total thermal conductivity (TC) κ_l ($Wm^{-1}\cdot k^{-1}$) of the second phase particle $L1_2$-Al_3TM with 1% solute atoms TM added at 300K and 600K.

	300K	600K
Al_3Sc	224.03	223.13
Al_3Ti	224.45	223.19
Al_3V	224.60	223.23
Al_3Cr	224.71	223.25
Al_3Mn	224.73	223.25
Al_3Fe	224.67	223.20
Al_3Co	224.33	222.98
Al_3Ni	224.11	222.98
Al_3Cu	224.01	223.31
Al_3Zn	223.95	223.73
Al_3Y	223.42	222.77
Al_3Zr	224.31	223.13
Al_3Nb	224.76	223.33
Al_3Mo	224.80	223.31
Al_3Tc	224.81	223.30
Al_3Ru	224.79	223.30
Al_3Rh	224.55	223.31
Al_3Pd	223.90	223.08
Al_3Ag	223.65	223.27
Al_3Cd	223.76	223.56
Al_3Hf	223.75	222.90
Al_3Ta	224.49	223.25
Al_3W	224.51	223.21
Al_3Re	224.68	223.29
Al_3Os	224.72	223.34
Al_3Ir	224.65	223.43
Al_3Pt	224.06	223.24
Al_3Au	223.58	223.13
Al_3Hg	223.40	223.32

TableS5. The calculated total thermal conductivity (TC) κ_l ($Wm^{-1}\cdot k^{-1}$) of Al-TM_{Al} solid solution with 1% solute atoms TM added at 300K and 600K.

	300K	600K
Sc_{Al}	180.08	176.98
Ti_{Al}	186.45	175.53
V_{Al}	182.02	182.20
Cr_{Al}	183.06	180.80
Mn_{Al}	180.55	181.32
Fe_{Al}	183.19	179.22
Co_{Al}	181.94	178.94
Ni_{Al}	187.91	181.56
Cu_{Al}	188.40	187.33
Zn_{Al}	211.37	186.77
Y_{Al}	164.27	208.83
Zr_{Al}	160.90	155.77
Nb_{Al}	161.38	158.97
Mo_{Al}	165.85	159.75
Tc_{Al}	156.55	164.12
Ru_{Al}	152.83	156.91
Rh_{Al}	156.10	153.17
Pd_{Al}	142.00	154.82
Ag_{Al}	146.01	138.95
Cd_{Al}	199.84	136.71
Hf_{Al}	179.27	195.21
Ta_{Al}	179.26	175.01
W_{Al}	166.18	174.51
Re_{Al}	161.13	165.72
Os_{Al}	154.06	160.11
Ir_{Al}	144.38	152.72
Pt_{Al}	114.56	142.57
Au_{Al}	126.63	113.32
Hg_{Al}	195.57	121.51

TableS6. The optimized Al-W is taken as an example to export a copy of the extxyz file with lattice parameters and atomic positions.

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Lattice="12.1340300578217981 0.0 0.0 0.0 12.1334160840703511 0.0 0.0 0.0 12.1334160840703511"Properties=species:S:1:pos:R:3 pbc="T T T"

Al	-0.000576616538445	0.000000000000000	0.000000000000000
Al	0.000057694741742	2.021937325776550	2.021937325776550
Al	2.022174393543756	0.000000000000000	2.022698420778172
Al	2.022174393543756	2.022698420778172	0.000000000000000
Al	4.045048793975447	0.000000000000000	0.000000000000000
Al	4.044529617331508	2.021954132280426	2.021954132280426
Al	6.065817948289804	0.000000000000000	2.017824298090235
Al	6.065817948289804	2.017824298090235	0.000000000000000
Al	8.089223409402120	0.000000000000000	0.000000000000000
Al	8.089522458407775	2.005845171665302	2.005845171665302
Al	10.112963472307738	0.000000000000000	2.017434973060051
Al	10.112963472307738	2.017434973060051	0.000000000000000
Al	0.004614699598882	4.043042020458578	0.000000000000000
Al	0.016420562044235	6.066708042035176	2.005926473298810
Al	2.022336194567511	4.043170582302055	2.017728025933748
Al	2.022249268751801	6.066708042035176	0.000000000000000
Al	4.039921506216094	4.043441021221639	0.000000000000000
Al	4.028387683903896	6.066708042035176	2.005856396354352
Al	6.061589482003898	4.039036386095544	2.012961376931206
Al	6.067164176638882	6.066708042035176	0.000000000000000
Al	8.089250431817813	4.044769614889340	0.000000000000000
Al	8.089302796078950	6.066708042035176	2.018598851385362
Al	10.117170632589932	4.039215777728941	2.013052011947769
Al	10.111600735123769	6.066708042035176	0.000000000000000
Al	0.004614699598882	8.090374540631995	0.000000000000000
Al	0.000057694741742	10.111478042263432	2.021937325776550
Al	2.022336194567511	8.090245978788520	2.017728025933748
Al	2.022174393543756	10.110716947261812	0.000000000000000
Al	4.039921506216094	8.089975539868933	0.000000000000000
Al	4.044529617331508	10.111461235759556	2.021954132280426
Al	6.061589482003898	8.094380174995031	2.012961376931206
Al	6.065817948289804	10.115591069949746	0.000000000000000
Al	8.089250431817813	8.088646946201235	0.000000000000000
Al	8.089522458407775	10.127570196374679	2.005845171665302
Al	10.117170632589932	8.094200783361631	2.013052011947769
Al	10.112963472307738	10.115980394979930	0.000000000000000
Al	0.004614699598882	0.000000000000000	4.043042020458578

Al	0.016420562044235	2.005926473298810	6.066708042035176
Al	2.022249268751801	0.000000000000000	6.066708042035176
Al	2.022336194567511	2.017728025933748	4.043170582302055
Al	4.039921506216094	0.000000000000000	4.043441021221639
Al	4.028387683903896	2.005856396354352	6.066708042035176
Al	6.067164176638882	0.000000000000000	6.066708042035176
Al	6.061589482003898	2.012961376931206	4.039036386095544
Al	8.089250431817813	0.000000000000000	4.044769614889340
Al	8.089302796078950	2.018598851385362	6.066708042035176
Al	10.111600735123769	0.000000000000000	6.066708042035176
Al	10.117170632589932	2.013052011947769	4.039215777728941
Al	0.008934738233151	4.039133747723120	4.039133747723120
Al	0.003513108383319	6.066708042035176	6.066708042035176
Al	2.022200768473422	4.044768844320469	6.066708042035176
Al	2.022200768473422	6.066708042035176	4.044768844320469
Al	4.035920843892439	4.039307035719194	4.039307035719194
Al	4.041104778967400	6.066708042035176	6.066708042035176
Al	6.019631059821107	3.996641657240182	6.066708042035176
Al	6.019631059821107	6.066708042035176	3.996641657240182
Al	8.089211446208632	3.996394979575352	3.996394979575352
Al	10.159349751720885	3.996902077821908	6.066708042035176
Al	10.159349751720885	6.066708042035176	3.996902077821908
Al	0.008934738233151	8.094282813367457	4.039133747723120
Al	0.016420562044235	10.127488894741171	6.066708042035176
Al	2.022200768473422	8.088647716770103	6.066708042035176
Al	2.022336194567511	10.115687342106234	4.043170582302055
Al	4.035920843892439	8.094109525371382	4.039307035719194
Al	4.028387683903896	10.127558971685628	6.066708042035176
Al	6.019631059821107	8.136774903850393	6.066708042035176
Al	6.061589482003898	10.120453991108775	4.039036386095544
Al	8.089211446208632	8.137021581515222	3.996394979575352
Al	8.089302796078950	10.114816516654621	6.066708042035176
Al	10.159349751720885	8.136514483268664	6.066708042035176
Al	10.117170632589932	10.120363356092215	4.039215777728941
Al	0.004614699598882	0.000000000000000	8.090374540631995
Al	0.000057694741742	2.021937325776550	10.111478042263432
Al	2.022174393543756	0.000000000000000	10.110716947261812
Al	2.022336194567511	2.017728025933748	8.090245978788520
Al	4.039921506216094	0.000000000000000	8.089975539868933
Al	4.044529617331508	2.021954132280426	10.111461235759556
Al	6.065817948289804	0.000000000000000	10.115591069949746
Al	6.061589482003898	2.012961376931206	8.094380174995031
Al	8.089250431817813	0.000000000000000	8.088646946201235
Al	8.089522458407775	2.005845171665302	10.127570196374679

Al	10.112963472307738	0.000000000000000	10.115980394979930
Al	10.117170632589932	2.013052011947769	8.094200783361631
Al	0.008934738233151	4.039133747723120	8.094282813367457
Al	0.016420562044235	6.066708042035176	10.127488894741171
Al	2.022336194567511	4.043170582302055	10.115687342106234
Al	2.022200768473422	6.066708042035176	8.088647716770103
Al	4.035920843892439	4.039307035719194	8.094109525371382
Al	4.028387683903896	6.066708042035176	10.127558971685628
Al	6.061589482003898	4.039036386095544	10.120453991108775
Al	6.019631059821107	6.066708042035176	8.136774903850393
Al	8.089211446208632	3.996394979575352	8.137021581515222
Al	8.089302796078950	6.066708042035176	10.114816516654621
Al	10.117170632589932	4.039215777728941	10.120363356092215
Al	10.159349751720885	6.066708042035176	8.136514483268664
Al	0.008934738233151	8.094282813367457	8.094282813367457
Al	0.000057694741742	10.111478042263432	10.111478042263432
Al	2.022336194567511	8.090245978788520	10.115687342106234
Al	2.022336194567511	10.115687342106234	8.090245978788520
Al	4.035920843892439	8.094109525371382	8.094109525371382
Al	4.044529617331508	10.111461235759556	10.111461235759556
Al	6.061589482003898	8.094380174995031	10.120453991108775
Al	6.061589482003898	10.120453991108775	8.094380174995031
Al	8.089211446208632	8.137021581515222	8.137021581515222
Al	8.089522458407775	10.127570196374679	10.127570196374679
Al	10.117170632589932	8.094200783361631	10.120363356092215
Al	10.117170632589932	10.120363356092215	8.094200783361631
W	8.089388500543768	6.066708042035176	6.066708042035176