Supplemental information

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Table 1: Compounds with the $CaAl_2Si_2$ structure type.

compound	ref	compound	ref	compound	ref
$BaCd_2As_2$	[1, 2]	$CaZn_2Sb_2$	[3]	$SrMg_2Bi_2$	[4]
$BaCd_2P_2$	[1, 2]	$EuCd_2As_2$	[5]	$SrMg_2N_2$*	[6]
$BaCd_2Sb_2$	[7]	$EuCd_2P_2$	[8]	$SrMg_2Sb_2$	[4]
$BaMg_2As_2$	[1, 4]	$EuCd_2Sb_2$	[8]	$SrMn_2As_2$	[9, 10]
$BaMg_2Bi_2$	[4]	$EuMg_2Bi_2$	[11]	$SrMn_2P_2$	[9]
$BaMg_2P_2$	[1]	$EuMg_2Sb_2$	[12]	$SrMn_2Sb_2$	[13]
$BaMg_2Sb_2$	[4]	$EuMn_2As_2$	[14]	$SrZn_2As_2$	[15]
$CaCd_2As_2$	[16]	$EuMn_2P_2$	[14]	$SrZn_2P_2$	[1], [2]
$CaCd_2P_2$	[16]	$EuMn_2Sb_2$	[14, 5]	$SrZn_2Sb_2$	[3]
$CaCd_2Sb_2$	[3]	$EuZn_2As_2$	[2]	$YbCd_2Sb_2$	[17, 8]
$CaMg_2As_2$	[4]	$EuZn_2P_2$	[2]	$YbMg_2Bi_2$	[11]
$CaMg_2Bi_2$	[4, 11]	$EuZn_2Sb_2$	[5, 2]	$YbMg_2Sb_2$	[12]
$CaMg_2N_2$*	[6]	$Mg(MgMn)_2As_2$	[18]	$YbMn_2As_2$	[14]
$CaMg_2Sb_2$	[4]	$MgMg_2As_2$	[18]	$YbMn_2Sb_2$	[5, 19]
$CaMn_2As_2$	[9, 10]	$MgMg_2Bi_2$	[20]	$YbZn_2As_2$	[2, 21]
$CaMn_2Bi_2$	[13]	$MgMg_2Sb_2$	[20, 22]	$YbZn_2P_2$	[1, 23]
$CaMn_2P_2$	[9]	$SrCd_2As_2$	[15]	$YbZn_2Sb_2$	[2, 5, 17]
$CaMn_2Sb_2$	[13]	$SrCd_2P_2$	[1], [2]	$SmMg_2Bi_2$	[24]
$CaZn_2As_2$	[16]	$SrCd_2Sb_2$	[3]	$SmMg_2Sb_2$	[24]
$CaZn_2P_2$	[16]	$SrMg_2As_2$	[4]		
compound	ref	compound	ref	compound	ref
$CaAl_2Ge_2$	[25]	$MgAl_2Ge_2$	[26]	$YbAl_2Ge_2$	[27]
$CaAl_2Si_2$	[25]	$MgAl_2Si_2$	[28]	$YbAl_2Si_2$	[27]
$EuAl_2Ge_2$	[29]	$SrAl_2Ge_2$	[25]		
$EuAl_2Si_2$	[30], [27]	$SrAl_2Si_2$	[25]		
compound	ref	compound	ref	compound	ref
$CeAgZnAs_2$	[31]	$LaAgZnP_2$	[32]	$SmAgZnAs_2$	[31]
$CeAgZnP_2$	[31]	$LaCuZnP_2$	[32]	$SmAgZnP_2$	[32]
$CeCuZnAs_2$	[31]	$LuCuZnP_2$	[33]	$SmCuZnAs_2$	[31]
$CeCuZnP_2$	[32]	$NdAgZnAs_2$	[31]	$SmCuZnP_2$	[32]
$DyCuZnAs_2$	[31]	$NdAgZnP_2$	[31]	$TbAgZnAs_2$	[31]
$DyCuZnP_2$	[33]	$NdCuZnAs_2$	[31]	$TbCuZnAs_2$	[31]
$ErCuZnP_2$	[33]	$NdCuZnP_2$	[33]	$TbCuZnP_2$	[33]
$GdAgZnAs_2$	[31]	$PrAgZnAs_2$	[31]	$TmCuZnP_2$	[33]
$GdCuZnP_2$	[33]	$PrAgZnP_2$	[31]	$YbCuZnP_2$	[34]
$HoCuZnP_2$	[33]	$PrCuZnP_2$	[33]	$YbMnCuP_2$	[15]
$LaAgZnAs_2$	[31]	$ScCuZnP_2$	[32]	$YCuZnP_2$	[32, 2]

Table 2: Compounds with the $CaAl_2Si_2$ structure type, continued. Compounds with * are not included in phase map in figure 3(d).

compound	ref	compound	ref	compound	ref
$CeLi_2As_2$	[35]	$LaLi_3P_2$	[36]	$PrLi_xCu_{2-y}P_2$*	[37]
$CeLi_3Bi_2$	[38]	$LaLi_3Sb2$	[36]	$SmLi_3Bi_2$	[38]
$CeLi_3Sb_2$	[39]	$LaLixCu_{2-y}P_2$*	[37]	$SmLi_3Sb_2$	[39]
$DyLi_3Sb_2$	[39]	$MdLixCu_{2-y}P_2$*	[37]	$TbLi_3Bi_2$	[38]
$ErLixCu_{2-y}P_2$*	[37]	$NdLi_3As_2$	[36]	$TbLi_3Sb_2$	[39]
$GdLi_3Bi_2$	[38]	$NdLi_3Bi_2$	[38]	YLi_3Bi_2	[36]
$GdLixCu_{2-y}P_2$*	[37]	$NdLi_3Sb_2$	[39]	YLi_3Sb_2	[36]
$HoLi_3Sb_2$	[39]	$PrLi_3Bi_2$	[38]		
$LaLi_3Bi_2$	[38]	$PrLi_3Sb_2$	[39]		
compound	ref	compound	ref	compound	ref
$NaCd_{1.5}Sn0.5As_2$	[40]	$NaZn_{1.5}Sn0.5As_2$	[40]	$RbCd_{1.5}Sn0.5As2$	[40]
$NaZn_{1.5}Ge0.5As_2$	[40]	$KZn_{1.5}Sn0.5As_2$	[40]		
$NaZn_{1.5}Si0.5As_2$	[40]	$KCd_{1.5}Sn0.5As_2$	[40]		
compound	ref	compound	ref	compound	ref
$NaFe_{1.6}S_2$	[41]				
compound	ref	compound	ref	compound	ref
$CeAl_2Ge_2$	[42, 43]	$LuAl_2Ge_2$	[44]	$TbAl_2Si_2$	[45]
$DyAl_2Si_2$	[45]	$NdAl_2Ge_2$	[44]	YAl_2Ge_2	[46, 44]
$GdAl_2Ge_2$	[44]	$PrAl_2Si_2$	[47]	YAl_2Si_2	[46, 45]
$GdAl_2Si_2$	[48]	$SmAl_2Si_2$	[45]		
$LaAl_2Ge_2$	[42, 44]	$TbAl_2Ge_2$	[44]		
$GdAlZnGe_2$	[45]				

Table 3: Compounds with VEC=16 forming the $ThCr_2Si_2$ structure type.

compound	ref	compound	ref	compound	ref
$BaMn_2As_2$	[10]	$BaPd_2As_2$	[49]	$KZn_{1.5}Si_{0.5}As_2$	[50]
$BaMn_2Bi_2$	[51]	$BaZn_2P_2$	[52]	$RbZn_{1.5}Ge_{0.5}As_2$	[50]
$BaMn_2P_2$	[9]	KFe_2AsSe	[53]		
$BaMn_2Sb_2$	[7]	$KZn_{1.5}Ge_{0.5}As_2$	[50]		

Table 4: Compounds with VEC=16 forming the $BaCu_2S_2$ structure type.

compound	ref	compound	ref	compound	ref
$BaAl_2Si_2$	[54]	α-$BaCu_2S_2$	[55]	$BaAl_2Ge_2$	[56]
$BaZn_2As_2$	[52]	α-$BaCu_2Se_2$	[55]		
$BaZn_2Sb_2$	[7]	α-$BaCu_2Te_2$	[57]		

Table 5: Source data for Figure 8b) and Figure 9. The room temperature Seebeck coefficients, α, electrical conductivity, σ, Hall mobility, μ_H, and total thermal conductivity as κ_{total}, are obtained from the literature. The Lorenz numbers, L, are estimated using an effective mass model. The electronic thermal conductivity, κ_e, and lattice thermal conductivity, κ_L, are calculated from the Wiedemann–Franz law using the corresponding σ. The transverse and longitudinal speed of sound (v_t and v_l) are from the predicted elastic modulus [58] and density. The mean speed of sound, v_s calc, is obtained through $(2v_t+v_l)/3$.

Ref.	Compound	α $\mu V K^{-1}$	L×10^8 $W\Omega K^{-2}$	σ S/m	κ_e $W/(mK)$	κ_{total} $W/(mK)$	κ_L $W/(mK)$	v_s calc. m/s	μ_H $cm^2/(Vs)$
[59]	Mg_3Sb_2	193	1.58	2.11×10^2	9.8×10^{-4}	1.33	1.3	2790	
[60]	$YbCd_2Sb_2$	115	1.75	4.56×10^4	2.40×10^{-1}	2.04	1.80	2160	73
	$CaCd_2Sb_2$	261	1.55	2.50×10^2	1.16×10^{-3}	1.06	1.06	2381	
[61]	$YbZn_2Sb_2$	48	2.3	3.13×10^5	2.16	4.25	2.09	2379	130
	$CaZn_2Sb_2$	120	1.81	4.22×10^4	2.29×10^{-1}	2.60	2.37	2480	83
[62]	$YbCd_2Sb_2$	124	1.82	4.90×10^4	2.68×10^{-1}	2.25	1.99	2117	72
	$YbCd_{1.95}Mn_{0.25}Sb_2$	138	1.75	4.25×10^3	2.23×10^{-2}	1.95	1.93	2117	73
	$YbMn_2Sb_2$	10	2.4	6.25×10^3	4.50×10^{-2}	2.75	2.71	2055	
[63]	$CaZn_2Sb_2$	115	1.75	8.00×10^4	4.20×10^{-1}	2.91	2.49	2480	
	$YbZn_2Sb_2$	100	1.9	1.33×10^5	7.58×10^{-1}	2.60	1.84	2379	
[64]	$EuMg_2Bi_2$	102	1.9	9.35×10^4	5.33×10^{-1}	4.72	4.19	2228	
	$CaMg_2Bi_2$	288	1.54	5.30×10^3	2.45×10^{-2}	2.93	2.91	2486	143
	$YbMg_2Bi_2$	209	1.6	1.33×10^4	6.38×10^{-2}	2.68	2.62	2133	119
[65]	$SrZn_2Sb_2$	159	1.69	2.22×10^4	1.13×10^{-1}	2.05	1.94	2366	
	$CaZn_2Sb_2$	120	1.81	4.22×10^4	2.29×10^{-1}	2.60	2.37	2480	
	$YbZn_2Sb_2$	48	2.3	3.13×10^5	2.16	4.25	2.09	2379	
	$EuZn_2Sb_2$	120	1.81	1.14×10^5	6.17×10^{-1}	2.50	1.88	2401	
[66]	$YbCd_2Sb_2$	118	1.75	4.60×10^4	2.42×10^{-1}	2.10	1.86	2160	73
	$YbZn_2Sb_2$	45	2.2	2.16×10^5	1.43	3.80	2.37	2379	119
[67]	$CaZn_2Sb_2$	120	1.81	3.20×10^4	1.74×10^{-1}	3.89	3.72	2480	63.6
[68]	$YbZn_2Sb_2$	53	2.19	1.58×10^5	1.04	3.23	2.20	2379	85
[69]	$EuZn_2Sb_2$	120	1.81	1.13×10^4	6.14×10^{-2}	2.62	2.56	2401	
[70]	$EuCd_2Sb_2$	229	1.58	1.11×10^4	5.26×10^{-2}	1.40	1.35	2133	
[71]	$EuCd_2Sb_2$	222	1.59	1.16×10^4	5.53×10^{-2}	1.40	1.35	2133	
	$CaCd_2Sb_2$	262	1.55	6.67×10^4	3.10×10^{-1}	1.06	0.75	2381	
[72]	$SrZn_2Sb_2$	167	1.69	3.50×10^3	1.77×10^{-2}	2.20	2.18	2366	
[73]	$YbCd_2Sb_2$	169	1.69	3.30×10^4	1.67×10^{-1}	2.08	1.91	2160	
[74]	$YbZn_2Sb_2$	58	2.16	2.10×10^5	1.36	4.13	2.76	2379	
	$La_{0.01}Yb_{0.99}Zn_2Sb_2$	63	2.14	1.67×10^5	1.07	3.50	2.43	2379	
[75]	$YbZn_2Sb_2$	130	1.52	4.55×10^4	2.07×10^{-1}	2.90	2.69	2379	115
	$Yb_{0.99}Zn_2Sb_2$	65	2.14	1.67×10^5	1.07	2.40	1.33	2379	90
[76]	Mg_3Sb_2	313	1.5	9.52×10^2	4.29×10^{-3}	1.40	1.40	2790	28.3
	$Mg_{2.995}Ag_{0.005}Sb_2$	162	1.68	1.22×10^4	6.15×10^{-2}	1.45	1.39	2790	50.1
	$Mg_{2.990}Ag_{0.010}Sb_2$	177	1.65	1.04×10^4	5.16×10^{-2}	1.35	1.30	2790	47.6
	$Mg_{2.985}Ag_{0.015}Sb_2$	177	1.65	1.18×10^4	5.82×10^{-2}	1.25	1.19	2790	47.3
	$Mg_{2.980}Ag_{0.020}Sb_2$	165	1.68	1.03×10^4	5.20×10^{-2}	1.30	1.24	2790	48.9
[77]	Mg_3Sb_2	1000	1.5	1.00	4.50×10^{-6}	1.40	1.35	2790	23.2
	$Mg_{2.994}Na_{0.006}Sb_2$	110	1.9	1.04×10^4	5.94×10^{-2}	1.60	1.60	2790	16.7
	$Mg_{0.975}Na_{0.0125}Sb_2$	100	1.9	2.08×10^4	1.19×10^{-1}	1.70	1.64	2790	15.9
[78]	$CaMg_2Sb_2$						4.55	3207	

Table 6: Source data for figure 8a). Hall carrier concentration, n_H, Seebeck coefficient, α, and Hall mobility, μ_H, for p-type AM_2X_2 compounds.

Compound [Ref.]	$n_H \times 10^{-19}$ carriers/cm^3	α μVK^{-1}	μ_H $cm^2/(Vs)$	Compound [Ref.]	$n_H \times 10^{19}$ carriers/cm^3	α μVK^{-1}	μ_H $cm^2/(Vs)$
$YbZn_{2-x}Mn_xSb_2$ [68]				$Yb_{1-x}Ca_xCd_2Sb_2$ [60]			
0	11.5	51	85	0	3.9	115	73
0.05	9	85	56	0.2	2.66	128	82
0.1	7.2	69	88	0.4	1.88	149	104
0.15	8.3	924	59	0.5	1.94	149	91
0.2	6.6	64	38	0.6	1.12	161	135
0.3	6	87	54	0.8	0.33	216	114
$Ca_{1-x}Eu_xZn_2Sb_2$ [67]				$Yb_{1-x}Zn_2Sb_2$ [75]			
0	3.04	120	63.6	0.98	2.38	131	120
0.1	3.29	112	117.4	0.99	2.04	121	115
0.3	3.59	110	120.8	1	3.09	118	90
0.7	3.81	111	123.6	1.025	9.06	62	75
0.9	3.83	111	140	1.05	15	40	92
1	2.94	112	186.2				
				$(Eu_{0.5}Yb_{0.5})_{1-x}Ca_xMg_2Bi_2$ [64]			
$YbCd_{2-x}Zn_xSb_2$ [66]				0	3.99	105	200
0	3.9	116	73	0.4	2.74	126	180
0.4	6	101	118	0.5	2.26	148	166
0.8	7.2	68	93	0.6	1.7	162	171
1	8.6	66	103	0.7	1.41	172	164
1.2	9.1	55	104	$EuMg_2Bi_2$	4.33	102	202
1.6	10.3	40	123	$Eu_{0.5}Ca_{0.5}Mg_2Bi_2$	3.07	128	159
2	11.4	45	119				
				$Mg_3Sb_{2-x}Bi_x$ [59]			
$Ca_{1-x}Na_xMg_2Bi_{1.98}$ [79]				0	11	192	30
0	0.35	256	138	0.1	19	275	25
0.0025	1.84	160	144	0.15	23	310	22.2
0.005	2.53	138	147	0.2	29	305	18.6
0.0075	4.4	103	154	0.25	42	237	13.9
				0.4	150	141	36.9
$Ca_{1-x}Yb_xMg_2Bi_2$ [80]				$Mg_{3-x}Ag_xSb_2$ [76]			
0	0.24	288	143	0	0.18	316	28.3
0.3	0.28	263	153	0.05	1.52	163	50.1
0.5	0.34	260	138	0.02	1.36	167	47.6
0.7	0.42	247	131	0.025	1.27	174	47.3
1	0.72	210	119	0.01	1.23	175	48.9
$YbCd_{2-x}Mn_xSb_2$ [62]				0.015	1.5	178	43.7
0	4.3	125	72				
0.05	3.6	139	73	$Mg_{3-x}Na_xSb_2$ [77]			
0.1	2.8	135	63	0.006	3.87	117	16.7
0.15	2.2	162	64	0.02	1.36	167	47.6
0.2	2.1	161	74	0.0125	8.41	89	15.9
0.4	1.7	181	54	0.025	17.1	73	12.6
0.6	1.1	192	53	0.015	1.5	177	43.7
$Ca_xYb_{1-x}Zn_2Sb_2$ [61]							
0	15	48	130				
0.25	8.9	58	72				
0.5	6.4	79	76				
0.75	5.7	96	50				
1	3.1	120	83				

Table 7: Hall carrier concentration, Seebeck coefficient and Hall mobility for all n-type AM_2X_2 compounds. Source data for figure 7(b) in the paper. Here, we define Hall carrier concentration as n_H, Seebeck coefficient as α, Hall mobility as μ_H.

Compound [Ref.]	$n_H \times 10^{-19}$ carriers/cm^3	α $\mu_H\, V K^{-1}$	n_H $cm^2/(Vs)$
$Mg_{3.07}Sb_{1.5}Bi_{0.5-x}Se_x$ [81]			
0.02	0.88	276	76
0.03	0.70	280	64
0.04	0.68	281	63
0.05	0.77	279	60
0.06	0.64	296	61
$Mg_3Sb_{1.5-0.5x}Bi_{0.5-0.5x}Te_x$ [82]			
0.04	2.21	208	
0.05	2.17	214	
0.08	2.06	221	
0.2	1.81	227	

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