ADVANCED FUNCTIONAL MATERIALS

Supporting Information

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Giant Anomalous Hall and Nernst Conductivities in Magnetic All-*d* Metal Heusler Alloys

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Supplementary Material

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I. Data from High-Throughput

TABLE S1: Results obtained from the high-throughput calculation of the Heusler materials displaying theoretical lattice constants (a and c/a), space group (SG), number of valence electrons (N_v), AHC and ANC values (at Fermi-level), maximum AHC and ANC values within $\in$ [-0.25,0.25] eV of the Fermi-level and the total magnetic moment of the primitive cell. The ANC is calculated at 300 K.

Material	a (Å)	c/a	SG	N_v	AHC (S/cm)	ANC (A/mK)	$AHC_{max}(\Delta E)$ (S/cm(eV))	$ANC_{max}(\Delta E)$ (A/mK(eV))	M_{tot} (μ_B)
Au_2CdMn	6.61	1.00	225	41	-653	0.0	-681 (0.030)	1.5 (0.250)	4.0
Au_2CuMn	5.96	1.19	139	40	-422	-1.1	-801 (0.220)	1.7 (0.250)	4.0
Au_2HfMn	6.61	1.00	225	33	-58	-1.0	-544 (0.120)	1.6 (0.150)	3.9
Au_2NbMn	5.77	1.40	139	34	-126	1.6	-1305 (-0.250)	7.6 (-0.240)	2.3
Au_2ScMn	6.62	1.00	225	32	758	-1.1	1179 (-0.160)	-1.4 (-0.070)	4.0
Au_2TiFe	5.65	1.41	139	34	-227	3.4	-1064 (-0.250)	3.4 (0.000)	1.8
Au_2TiMn	5.72	1.40	139	33	-923	0.8	-1045 (-0.090)	-4.4 (-0.180)	2.4
Au_2ZnMn	6.39	1.00	225	41	-390	0.9	-607 (-0.250)	0.9 (0.010)	3.9
Au_2ZrMn	6.66	1.00	225	33	-312	-2.4	587 (-0.250)	-2.9 (-0.030)	4.0
Cd_2PtCr	5.90	1.39	139	40	-80	0.3	-126 (-0.190)	0.3 (0.040)	3.8
Cd_2PtMn	5.85	1.41	139	41	162	-1.0	307 (-0.250)	-1.0 (0.020)	3.9
Cd_2RhMn	5.77	1.44	139	40	353	0.1	386 (0.060)	0.5 (-0.250)	4.2
Cd_2ScMn	6.83	1.00	225	34	-1	0.7	-486 (-0.150)	2.2 (0.250)	3.6
Co_2FeTi	5.82	1.00	225	30	-9	0.5	519 (0.130)	-1.9 (0.170)	5.3
Co_2HfFe	6.02	1.00	225	30	-771	-4.3	-2311 (0.210)	-6.8 (0.070)	5.2
Co_2HfIr	5.40	1.40	139	31	-278	-4.6	1993 (-0.250)	-8.1 (-0.200)	1.7
Co_2HfV	6.08	1.00	225	27	-57	1.7	-443 (0.250)	-2.3 (0.160)	3.0
Co_2MnFe	5.72	1.00	225	33	659	-2.1	967 (-0.020)	-2.7 (0.030)	9.0
Co_2MnHf	6.04	1.00	225	29	348	0.6	576 (0.140)	-4.5 (0.250)	5.0
Co_2MnTa	5.96	1.00	225	30	-871	1.3	-1106 (-0.020)	-4.4 (-0.210)	5.7
Co_2MnTi	5.84	1.00	225	29	128	0.6	594 (0.140)	-2.3 (0.230)	4.9
Co_2MnV	5.00	1.42	139	30	313	3.2	623 (0.130)	3.2 (-0.010)	0.9
Co_2NbMn	5.96	1.00	225	30	-1210	-1.7	-1317 (0.010)	-5.6 (-0.050)	5.9
Co_2PdTa	5.43	1.34	139	33	-332	-0.5	-530 (0.110)	2.3 (-0.210)	1.3
Co_2PtNi	5.14	1.45	139	38	1412	3.8	1646 (0.020)	-8.9 (0.250)	5.0
Co_2RhPt	5.37	1.36	139	37	371	5.4	-837 (-0.150)	-6.8 (-0.190)	4.9
Co_2ScFe	5.97	1.00	225	29	293	0.1	369 (-0.250)	-2.3 (-0.250)	5.0
Co_2ScMn	5.97	1.00	225	28	40	-0.0	274 (0.250)	1.6 (0.240)	4.3
Co_2ScNb	6.20	1.00	225	26	-137	-1.5	-389 (0.060)	-1.5 (0.000)	1.8
Co_2ScV	6.02	1.00	225	26	-40	-0.5	-330 (0.160)	-1.4 (0.140)	2.0
Co_2TaCr	5.96	1.00	225	29	-187	-0.3	765 (-0.250)	-3.9 (0.250)	4.7
Co_2TaFe	5.27	1.37	139	31	355	-2.5	1601 (-0.150)	-4.1 (-0.100)	3.2
Co_2TaSc	6.18	1.00	225	26	135	-1.2	817 (-0.200)	-3.0 (-0.140)	1.5
Co_2TiCr	5.85	1.00	225	28	43	-0.2	363 (-0.080)	2.0 (-0.120)	4.0
Co_2TiRh	5.17	1.49	139	31	-479	3.6	-1088 (-0.040)	-6.1 (-0.180)	2.8
Co_2TiZr	6.18	1.00	225	26	-135	-3.2	-560 (0.050)	-3.2 (-0.010)	1.7

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Co_2VFe	5.07	1.39	139	31	252	-2.9	1132 (-0.090)	-3.8 (-0.050)	3.1
Co_2VTi	5.88	1.00	225	27	-122	0.0	-310 (0.250)	-1.7 (0.220)	5.6
Co_2ZrFe	6.06	1.00	225	30	-363	-1.3	-999 (0.210)	-4.7 (-0.180)	5.4
Co_2ZrHf	6.34	1.00	225	26	-419	-0.3	-641 (-0.020)	-2.7 (-0.060)	1.6
Co_2ZrIr	5.45	1.40	139	31	-677	2.0	-1012 (-0.170)	-7.3 (-0.220)	2.6
Co_2ZrMn	6.08	1.00	225	29	212	0.6	506 (-0.180)	-2.2 (0.250)	5.2
Co_2ZrV	6.11	1.00	225	27	39	-0.3	243 (-0.076)	-2.8 (0.240)	3.1
Cr_2PtMn	5.18	1.46	139	29	64	-1.4	-864 (-0.210)	4.0 (-0.150)	0.5
Cu_2AuMn	5.45	1.40	139	40	-300	0.3	-326 (-0.250)	1.0 (0.180)	3.9
Cu_2HfMn	5.36	1.49	139	33	-825	1.7	-1237 (-0.100)	4.4 (0.120)	2.0
Cu_2ScMn	6.25	1.00	225	32	85	0.2	439 (0.240)	1.1 (0.170)	3.7
Cu_2ZrMn	5.39	1.49	139	33	-366	1.8	549 (0.180)	2.8 (0.050)	2.2
Fe_2AuZr	5.61	1.42	139	31	291	1.3	644 (0.150)	-2.8 (0.210)	4.1
Fe_2CuPt	5.21	1.47	139	37	-22	-2.9	-765 (0.170)	6.0 (0.220)	6.0
Fe_2NbMn	5.92	1.00	225	28	237	0.5	837 (-0.250)	-3.9 (-0.210)	4.9
Fe_2NiCo	5.13	1.34	139	35	1043	-2.1	1636 (-0.110)	6.4 (-0.190)	7.6
Fe_2NiCr	5.05	1.42	139	32	203	-1.2	376 (-0.160)	-1.3 (0.020)	2.4
Fe_2PdNi	5.20	1.43	139	36	47	-0.5	261 (-0.220)	1.9 (-0.250)	6.5
Fe_2PdPt	5.46	1.37	139	36	1209	2.1	1423 (0.110)	-4.8 (0.220)	6.8
Fe_2PtAu	5.49	1.41	139	37	126	-3.1	703 (-0.230)	-3.4 (0.030)	6.3
Fe_2PtCo	5.27	1.39	139	35	815	-4.1	2525 (-0.140)	-6.6 (-0.060)	7.4
Fe_2PtCr	5.10	1.44	139	32	-747	-3.3	-1437 (0.050)	6.1 (-0.230)	2.3
Fe_2PtNi	5.23	1.42	139	36	919	0.6	1467 (0.250)	-2.9 (0.250)	6.5
Fe_2ReTa	6.05	1.00	225	28	-483	-0.8	-522 (0.010)	-2.8 (-0.130)	3.8
Fe_2RhNi	5.24	1.38	139	35	315	1.4	1279 (-0.250)	-8.2 (-0.170)	6.7
Fe_2RhPd	5.49	1.32	139	35	352	-2.3	848 (-0.060)	-2.6 (-0.020)	6.9
Fe_2TaMn	5.91	1.00	139	28	305	1.9	1181 (0.250)	4.0 (0.220)	4.5
Fe_2TaNb	6.13	1.00	225	26	-198	-1.2	-837 (0.250)	-2.3 (0.200)	1.9
Fe_2TaV	5.96	1.00	225	26	-190	-0.9	-1298 (0.220)	-5.5 (0.170)	1.8
Fe_2TiMo	5.97	1.00	225	26	336	-1.7	687 (-0.100)	2.7 (-0.160)	1.9
Fe_2TiRe	5.95	1.00	225	27	834	-6.2	1606 (-0.190)	-7.6 (0.030)	2.8
Fe_2TiZn	5.86	1.00	225	32	537	-0.9	807 (-0.170)	1.0 (-0.250)	1.9
Fe_2VNb	5.97	1.00	225	26	-105	-2.3	928 (-0.200)	-3.8 (-0.140)	1.9
Fe_2WTi	5.97	1.00	225	26	280	-0.6	662 (-0.180)	2.0 (-0.230)	1.8
Hf_2CrFe	6.37	1.00	225	22	421	1.8	-694 (-0.250)	5.6 (-0.210)	1.7
Hf_2CrMn	6.41	1.00	225	21	693	2.6	733 (0.010)	4.6 (-0.050)	2.5
Hf_2MoMn	6.55	1.00	225	21	-231	2.8	-543 (-0.090)	-3.6 (-0.130)	2.2
Hf_2OsCr	6.50	1.00	225	22	313	0.9	697 (0.100)	7.7 (-0.250)	1.7
Hf_2ReCr	6.56	1.00	225	21	307	4.1	-630 (-0.130)	5.0 (-0.030)	2.5
Hf_2ReMn	6.49	1.00	225	22	-184	1.3	386 (0.220)	2.2 (0.050)	1.5
Hf_2RuCr	6.48	1.00	225	22	374	3.1	1011 (0.080)	8.1 (-0.250)	1.6
Hg_2ScMn	6.85	1.00	225	34	36	1.3	831 (0.190)	2.9 (0.120)	3.8
Ir_2CoV	5.39	1.36	139	32	341	-1.9	812 (-0.200)	4.4 (-0.250)	1.1
Ir_2CuMn	5.45	1.32	139	36	-480	1.2	747 (0.220)	-6.0 (-0.190)	2.1
Ir_2FeV	5.43	1.35	139	31	237	0.6	-433 (-0.250)	-4.7 (0.240)	2.1
Ir_2HfCo	5.60	1.38	139	31	861	-6.8	1636 (-0.040)	11.4 (-0.230)	1.7
Ir_2HfMn	6.34	1.00	225	29	-214	2.8	-494 (-0.130)	3.1 (0.030)	4.6
Ir_2MnV	5.43	1.35	139	30	655	-1.9	706 (-0.010)	5.1 (-0.180)	1.7
Ir_2MoCo	5.44	1.39	139	33	261	0.8	1157 (-0.170)	-4.9 (-0.110)	1.3
Ir_2MoFe	5.47	1.39	139	32	282	-6.4	1867 (-0.080)	-7.1 (-0.020)	2.2
Ir_2MoMn	5.47	1.39	139	31	77	3.2	857 (0.130)	3.9 (0.060)	1.8
Ir_2NbCo	5.51	1.38	139	32	-37	-2.4	1683 (-0.190)	-6.1 (-0.110)	1.4
Ir_2NbFe	5.57	1.36	139	31	50	1.1	-659 (-0.250)	4.1 (-0.250)	2.5
Ir_2NbMn	5.65	1.32	139	30	57	1.8	1075 (0.250)	3.2 (0.150)	2.9
Ir_2OsFe	5.37	1.43	139	34	297	3.2	1247 (0.240)	3.3 (-0.020)	2.3
Ir_2OsMn	5.38	1.42	139	33	-20	5.4	-1067 (-0.100)	-6.9 (-0.250)	1.9
Ir_2ScFe	6.25	1.00	225	29	-546	-4.8	-1277 (0.130)	-4.8 (0.010)	4.5
Ir_2TaCo	5.52	1.38	139	32	-104	-1.8	1483 (-0.230)	-5.1 (-0.140)	1.5
Ir_2TaCr	5.59	1.36	139	29	-16	3.6	-774 (-0.200)	3.7 (-0.020)	1.6
Ir_2TaFe	5.59	1.35	139	31	220	1.7	378 (0.030)	3.0 (-0.060)	2.6
Ir_2TaMn	5.75	1.28	139	30	25	-1.4	-858 (-0.250)	4.6 (-0.170)	3.5
Ir_2TiCr	5.65	1.28	139	28	115	-3.6	771 (0.250)	6.0 (0.170)	2.4
Ir_2TiFe	5.68	1.25	139	30	-1898	-0.1	-1931 (-0.010)	6.7 (0.120)	3.5
Ir_2TiMn	6.17	1.00	225	29	-65	1.4	-482 (-0.250)	1.4 (0.020)	4.6

Ir_2WCo	5.45	1.38	139	33	218	-2.0	1332 (-0.210)	-3.6 (-0.150)	1.4
Ir_2WFe	5.48	1.38	139	32	660	-5.7	1341 (-0.170)	-5.8 (0.010)	2.3
Ir_2WMn	5.48	1.38	139	31	1185	4.9	2166 (0.250)	5.1 (0.020)	1.8
Ir_2ZnFe	6.04	1.00	225	38	497	-0.8	1073 (-0.210)	-2.1 (-0.120)	4.0
Ir_2ZrCo	5.60	1.39	139	31	742	-3.0	1132 (-0.060)	10.3 (-0.250)	1.7
Mn_2AgPt	6.33	1.00	225	35	1601	-1.5	1846 (-0.100)	3.6 (-0.240)	8.2
Mn_2AuPd	6.34	1.00	225	35	147	0.5	376 (0.170)	0.9 (0.050)	8.2
Mn_2CrCo	5.74	1.00	225	29	337	0.4	425 (0.050)	-1.4 (0.100)	4.8
Mn_2CrIr	5.99	1.00	225	29	888	-0.7	1263 (-0.190)	-4.4 (0.150)	4.7
Mn_2IrMo	6.05	1.00	225	29	553	1.5	831 (0.080)	-5.6 (0.250)	4.9
Mn_2IrPd	6.16	1.00	225	33	486	4.4	-1150 (-0.250)	4.7 (-0.030)	8.4
Mn_2IrRh	6.07	1.00	225	32	-356	-4.4	1589 (-0.090)	-9.1 (-0.060)	7.8
Mn_2IrTi	6.03	1.00	225	27	1723	2.0	1979 (0.060)	11.0 (-0.190)	4.4
Mn_2IrV	5.99	1.00	225	28	1045	-0.9	1630 (-0.190)	5.8 (-0.250)	4.1
Mn_2NbPd	6.17	1.00	225	29	848	-0.2	1238 (0.200)	2.2 (0.150)	5.0
Mn_2NbPt	6.16	1.00	225	29	1371	3.1	1482 (0.040)	-4.7 (0.200)	5.1
Mn_2NiPt	5.77	1.16	139	34	1015	0.9	1587 (0.110)	2.4 (0.060)	8.4
Mn_2PdRh	6.17	1.00	225	33	677	0.3	677 (0.000)	2.3 (-0.150)	8.7
Mn_2PdV	6.07	1.00	225	29	441	1.9	1307 (0.180)	-3.2 (0.250)	4.7
Mn_2PtPd	5.98	1.13	139	34	575	0.2	839 (-0.210)	1.8 (0.250)	8.5
Mn_2PtV	6.07	1.00	225	29	530	-0.7	1079 (-0.190)	3.9 (-0.250)	4.8
Mn_2RhAu	5.95	1.16	139	34	652	-1.1	971 (0.170)	2.1 (0.120)	8.4
Mn_2RhCr	5.99	1.00	225	29	617	0.3	861 (0.220)	-4.0 (0.250)	4.7
Mn_2RhV	5.99	1.00	225	28	287	-4.4	1827 (-0.100)	-6.5 (-0.050)	4.2
Mn_2RhW	6.04	1.00	225	29	1350	0.3	1354 (0.004)	-4.2 (0.210)	5.0
Mn_2ScTa	6.21	1.00	225	22	-182	1.2	-723 (-0.210)	2.3 (0.170)	1.5
Mn_2TiHf	6.17	1.00	225	22	231	-1.0	625 (0.220)	-1.8 (-0.050)	1.4
Mn_2VCo	5.77	1.00	225	28	68	-1.6	823 (-0.120)	-2.7 (-0.070)	4.4
Mn_2ZnIr	6.10	1.00	225	35	941	3.4	1819 (0.100)	4.9 (0.040)	7.3
Mn_2ZnTa	6.02	1.00	225	31	1341	0.8	1481 (0.040)	5.3 (-0.120)	2.9
Mn_2ZnV	5.87	1.00	225	31	485	0.3	946 (0.150)	-4.7 (0.210)	2.9
Mn_2ZrHf	6.37	1.00	225	22	-20	0.3	1195 (-0.230)	-4.0 (-0.120)	1.5
Mn_2ZrTi	6.19	1.00	225	22	166	-1.7	682 (-0.050)	-2.0 (-0.020)	1.4
Mo_2IrMn	5.42	1.46	139	28	-146	-0.4	-441 (0.160)	3.2 (0.230)	1.7
Mo_2PtCr	5.43	1.49	139	28	447	-1.6	-578 (0.180)	3.3 (0.230)	1.9
Nb_2CoMn	6.14	1.00	225	26	-128	-1.0	-455 (-0.250)	1.6 (-0.210)	1.6
Nb_2IrFe	5.69	1.33	139	27	195	-0.9	1064 (-0.250)	-5.2 (-0.250)	1.2
Nb_2OsCo	6.01	1.14	139	27	249	-5.5	1120 (-0.130)	-5.6 (0.010)	1.2
Nb_2OsFe	6.29	1.00	225	26	631	-0.9	633 (0.010)	-3.6 (0.060)	1.7
Nb_2PtCr	5.58	1.49	139	26	-118	0.7	1821 (-0.250)	-9.6 (-0.170)	2.3
Nb_2PtMn	5.54	1.51	139	27	15	-0.5	713 (0.200)	4.4 (0.160)	2.6
Nb_2ReCo	6.31	1.00	225	26	-40	-4.5	1052 (-0.250)	-4.5 (0.000)	1.6
Nb_2RuCo	5.89	1.18	139	27	-272	1.2	-557 (-0.240)	2.4 (-0.240)	0.8
Nb_2RuFe	6.27	1.00	225	26	875	1.1	905 (0.060)	-5.3 (0.140)	1.7
Ni_2AuMn	5.40	1.35	139	38	344	2.3	-817 (-0.200)	-9.8 (-0.240)	4.3
Ni_2CoMn	5.02	1.43	139	36	134	1.5	903 (-0.240)	-4.5 (-0.160)	5.7
Ni_2CuMn	5.19	1.34	139	38	138	-0.8	1623 (-0.190)	-4.6 (-0.130)	4.0
Ni_2FeCo	4.96	1.46	139	37	162	0.5	417 (0.230)	1.8 (0.170)	5.7
Ni_2FeV	4.97	1.49	139	33	236	-0.3	310 (-0.020)	-1.1 (0.190)	1.8
Ni_2MoFe	5.04	1.50	139	34	465	0.2	797 (-0.170)	-2.9 (0.110)	1.5
Ni_2MoMn	5.08	1.49	139	33	-252	0.0	-282 (-0.010)	-1.5 (-0.100)	2.0
Ni_2NbFe	5.15	1.47	139	33	-290	-2.4	507 (0.220)	3.7 (0.190)	1.9
Ni_2NbMn	5.18	1.47	139	32	-441	1.5	1043 (-0.210)	-5.4 (-0.160)	2.3
Ni_2PdPt	5.43	1.33	139	40	-1103	-4.7	-2675 (0.220)	-9.1 (-0.250)	2.2
Ni_2RhFe	5.12	1.45	139	37	240	-1.9	-986 (0.250)	-6.1 (0.230)	5.1
Ni_2ScMn	6.09	1.00	225	30	205	-0.3	330 (-0.190)	2.6 (-0.250)	4.2
Ni_2TaFe	5.15	1.47	139	33	-168	-2.6	656 (-0.200)	3.2 (0.180)	1.8
Ni_2TaMn	5.19	1.46	139	32	382	0.9	982 (-0.230)	-3.7 (-0.150)	2.3
Ni_2TiFe	5.10	1.45	139	32	110	0.3	310 (0.170)	-2.0 (0.250)	2.3
Ni_2VMn	5.01	1.48	139	32	-594	-2.5	-857 (-0.230)	4.3 (-0.160)	2.1
Ni_2VTi	5.23	1.41	139	29	25	1.3	-295 (-0.020)	-1.4 (-0.080)	0.3
Ni_2WFe	5.04	1.50	139	34	76	1.1	905 (0.130)	-4.8 (0.210)	1.4
Ni_2WMn	5.09	1.48	139	33	-363	-2.7	1154 (-0.230)	-3.8 (-0.040)	1.9
Ni_2ZnCr	5.33	1.27	139	38	287	2.1	1956 (0.090)	4.9 (0.040)	2.9

Ni_2ZnFe	5.24	1.31	139	40	154	2.3	690 (0.180)	-2.3 (0.250)	3.8
Ni_2ZrFe	5.34	1.43	139	32	53	0.0	-379 (0.230)	-2.6 (0.200)	2.4
Os_2CrV	6.03	1.00	225	27	501	-9.3	-1754 (0.150)	-11.4 (0.030)	2.6
Os_2MnV	6.03	1.00	225	28	-809	2.4	-1386 (-0.250)	2.6 (-0.030)	3.5
Os_2NbMn	6.22	1.00	225	28	-415	1.6	-1471 (-0.230)	4.5 (-0.070)	3.7
Os_2TaCr	6.23	1.00	225	27	-291	-9.7	-1401 (0.100)	-9.7 (0.000)	2.8
Os_2TaFe	6.21	1.00	225	29	-12	-0.2	-806 (0.250)	-3.9 (0.200)	4.3
Os_2TaMn	6.23	1.00	225	28	-647	2.3	-1499 (-0.190)	3.9 (-0.110)	3.7
Os_2TiMn	6.10	1.00	225	27	-1082	2.0	-1991 (-0.110)	-7.7 (-0.180)	3.0
Pd_2AgFe	5.70	1.31	139	39	226	-1.1	316 (-0.110)	-1.2 (0.040)	3.7
Pd_2AgMn	5.85	1.26	139	38	88	0.4	135 (-0.230)	-0.5 (-0.140)	4.3
Pd_2AuFe	5.64	1.36	139	39	40	-0.1	252 (0.120)	-1.6 (0.170)	3.8
Pd_2CdFe	5.28	1.28	139	40	259	0.3	487 (0.140)	3.4 (-0.060)	3.5
Pd_2CuFe	5.59	1.27	139	39	215	-1.5	326 (-0.060)	-1.6 (0.020)	3.7
Pd_2CuMn	6.12	1.00	225	38	134	0.0	166 (0.190)	0.1 (-0.250)	4.3
Pd_2FeNi	5.44	1.35	139	38	658	0.2	737 (0.010)	-3.1 (-0.140)	4.3
Pd_2HgFe	5.77	1.34	139	40	75	-0.3	638 (0.180)	3.1 (0.150)	3.5
Pd_2MnFe	5.61	1.31	139	35	92	0.0	-437 (0.100)	2.6 (0.170)	7.4
Pd_2NbFe	5.46	1.47	139	33	98	-0.7	451 (-0.240)	0.8 (-0.250)	2.1
Pd_2NbMn	5.52	1.46	139	32	-5	-0.7	350 (-0.110)	-1.2 (-0.050)	2.6
Pd_2RhFe	5.42	1.45	139	37	1223	-0.0	1354 (-0.010)	-6.7 (0.240)	5.1
Pd_2ScFe	5.75	1.33	139	31	-98	0.7	605 (-0.190)	-2.3 (0.250)	2.8
Pd_2ScMn	6.43	1.00	225	30	172	0.7	958 (0.210)	2.2 (0.160)	4.0
Pd_2TaFe	5.44	1.47	139	33	175	0.1	484 (-0.240)	-1.3 (-0.200)	2.0
Pd_2TaMn	5.49	1.46	139	32	607	-0.2	818 (-0.020)	3.3 (-0.080)	2.6
Pd_2TiCo	5.44	1.42	139	33	229	-0.9	431 (-0.040)	-1.8 (0.250)	1.4
Pd_2TiFe	5.48	1.41	139	32	85	0.0	413 (0.100)	-1.7 (0.130)	2.3
Pd_2VFe	5.38	1.44	139	33	-205	-0.2	-725 (0.250)	2.8 (-0.250)	1.6
Pd_2YMn	6.68	1.00	225	30	319	-0.2	632 (-0.200)	1.5 (-0.240)	4.1
Pd_2ZnFe	5.66	1.26	139	40	503	-0.1	572 (-0.030)	2.8 (-0.060)	3.5
Pd_2ZrFe	5.62	1.43	139	32	289	-0.2	307 (0.010)	-1.1 (0.150)	2.5
Pt_2AgFe	5.65	1.36	139	39	600	-0.1	654 (-0.200)	0.8 (-0.250)	3.8
Pt_2AgMn	5.68	1.37	139	38	731	-1.2	1766 (-0.250)	-4.2 (-0.200)	4.1
Pt_2AuCr	5.64	1.40	139	37	1589	-3.1	2040 (-0.030)	5.4 (-0.190)	2.7
Pt_2AuFe	5.64	1.38	139	39	632	-0.4	734 (0.200)	3.1 (-0.250)	3.8
Pt_2CdCo	5.65	1.38	139	41	-22	-0.9	1037 (-0.100)	-5.3 (-0.060)	2.2
Pt_2CdFe	5.75	1.34	139	40	704	0.3	809 (0.070)	-4.2 (0.200)	3.7
Pt_2CrFe	5.38	1.41	139	34	96	1.1	958 (0.160)	-3.9 (-0.250)	3.9
Pt_2CuCo	5.47	1.34	139	40	226	-6.4	1342 (-0.090)	-6.5 (0.010)	2.5
Pt_2CuCr	5.53	1.34	139	37	155	-4.1	1649 (0.200)	8.0 (0.140)	2.5
Pt_2CuFe	5.56	1.30	139	39	885	0.9	1000 (0.100)	0.9 (-0.020)	3.8
Pt_2CuMn	5.60	1.31	139	38	581	-0.1	1152 (-0.150)	-2.4 (-0.110)	3.9
Pt_2FeNi	5.46	1.35	139	38	-911	-0.1	-1847 (0.060)	-10.5 (-0.180)	4.3
Pt_2HfCo	5.57	1.44	139	33	661	1.9	1073 (0.220)	-8.2 (0.250)	1.5
Pt_2HfFe	5.61	1.42	139	32	18	-2.0	513 (-0.140)	2.0 (0.250)	2.5
Pt_2MnCo	5.47	1.38	139	36	1686	1.2	1839 (0.030)	7.2 (-0.250)	5.9
Pt_2MnFe	5.60	1.32	139	35	-71	-0.8	735 (0.240)	4.5 (0.160)	7.2
Pt_2MoFe	5.42	1.47	139	34	-1308	-0.2	-1345 (0.010)	-3.4 (-0.060)	2.2
Pt_2NbFe	5.50	1.45	139	33	127	-0.3	-491 (0.250)	-3.2 (0.190)	2.3
Pt_2NiCo	5.41	1.36	139	39	-1607	-6.3	-2158 (0.030)	-7.6 (-0.030)	3.5
Pt_2PdCo	5.47	1.42	139	39	-1616	-0.6	-1715 (0.030)	-8.8 (-0.240)	3.0
Pt_2PdFe	5.53	1.41	139	38	-1608	2.5	-1694 (-0.180)	9.2 (0.080)	4.0
Pt_2PdNi	5.48	1.41	139	40	-986	-4.7	-2050 (0.160)	-7.6 (-0.250)	1.3
Pt_2ReFe	5.38	1.48	139	35	-138	2.0	1120 (0.200)	4.4 (0.110)	2.3
Pt_2RhCo	5.43	1.42	139	38	-1259	-9.5	-2154 (0.040)	-10.2 (-0.020)	3.1
Pt_2RhCr	5.46	1.43	139	35	1966	7.5	2432 (0.050)	10.2 (-0.050)	1.4
Pt_2RhFe	5.46	1.43	139	37	308	-4.9	-1863 (0.140)	-9.7 (0.080)	4.3
Pt_2RuFe	5.42	1.44	139	36	609	2.9	1610 (0.180)	-5.9 (-0.120)	3.5
Pt_2RuMn	5.43	1.44	139	35	253	5.0	1154 (0.120)	-5.4 (0.150)	2.8
Pt_2ScCo	5.63	1.38	139	32	165	2.5	774 (0.090)	2.8 (0.020)	1.8
Pt_2ScFe	5.72	1.34	139	31	91	1.7	-797 (-0.210)	2.5 (-0.140)	3.0
Pt_2ScMn	5.91	1.26	139	30	135	-0.6	-448 (0.250)	-4.0 (0.230)	4.1
Pt_2TaFe	5.49	1.45	139	33	248	-0.1	461 (0.090)	-1.2 (0.110)	2.3
Pt_2TaMn	5.54	1.44	139	32	482	-0.7	1055 (-0.250)	-2.4 (-0.100)	2.7

Pt_2TiCo	5.46	1.41	139	33	340	2.6	645 (0.160)	3.3 (-0.050)	1.5
Pt_2TiFe	5.50	1.40	139	32	50	-3.3	710 (-0.080)	-3.4 (-0.010)	2.4
Pt_2TiMn	5.61	1.36	139	31	106	-0.9	-511 (0.250)	-2.5 (0.220)	3.2
Pt_2VFe	5.42	1.42	139	33	-166	-2.4	-985 (0.250)	5.6 (-0.250)	2.0
Pt_2WFe	5.41	1.47	139	34	-644	-4.7	-1577 (0.050)	6.7 (0.100)	2.0
Pt_2WMn	5.45	1.46	139	33	-18	-0.1	-622 (0.240)	-2.1 (-0.180)	2.4
Pt_2ZnFe	5.63	1.29	139	40	506	0.2	746 (-0.250)	-6.0 (0.250)	3.7
Pt_2ZrCo	5.58	1.45	139	33	491	1.3	1229 (0.220)	-8.2 (0.250)	1.5
Pt_2ZrFe	5.63	1.43	139	32	-77	-2.1	542 (-0.130)	-2.3 (-0.020)	2.6
Re_2TaMn	6.23	1.00	225	26	2011	-3.2	2031 (0.003)	-8.2 (0.060)	2.3
Rh_2FeCo	5.87	1.00	225	34	177	0.0	795 (-0.240)	2.6 (0.190)	8.6
Rh_2HfCo	5.67	1.31	139	31	-460	-2.4	-990 (0.070)	2.5 (0.120)	2.0
Rh_2HfCr	6.33	1.00	225	28	49	-1.8	428 (-0.070)	2.9 (-0.230)	3.9
Rh_2HfFe	5.97	1.16	139	30	135	-0.2	-351 (-0.120)	-1.8 (-0.180)	3.7
Rh_2HfMn	6.32	1.00	225	29	-252	0.7	332 (0.180)	-1.7 (0.250)	4.5
Rh_2MoCo	5.39	1.40	139	33	82	1.8	-344 (-0.070)	2.0 (-0.020)	1.6
Rh_2MoFe	5.44	1.38	139	32	-442	-3.9	1258 (-0.210)	-6.5 (-0.040)	2.4
Rh_2NbCo	5.49	1.37	139	32	27	3.6	608 (0.060)	-3.7 (-0.150)	1.6
Rh_2NbCr	5.55	1.37	139	29	-17	2.9	420 (0.160)	2.9 (0.010)	1.7
Rh_2NbFe	5.58	1.34	139	31	69	0.9	318 (0.250)	1.1 (-0.030)	2.7
Rh_2NbMn	5.80	1.23	139	30	122	1.2	-290 (-0.230)	-1.7 (0.090)	3.9
Rh_2OsMn	5.35	1.43	139	33	1087	-4.6	2113 (-0.080)	-5.8 (0.160)	2.3
Rh_2ReCo	5.34	1.41	139	34	218	0.3	218 (0.000)	-3.7 (0.250)	1.3
Rh_2ScFe	6.23	1.00	225	29	-296	-3.5	-1273 (0.070)	8.4 (0.150)	4.4
Rh_2TaCo	5.51	1.36	139	32	-178	1.2	-712 (-0.130)	-3.3 (-0.190)	1.6
Rh_2TaFe	5.59	1.33	139	31	-329	1.7	-662 (-0.210)	2.3 (0.050)	2.8
Rh_2TaMn	5.85	1.20	139	30	-80	2.1	-458 (-0.240)	2.2 (0.020)	4.0
Rh_2TiCo	5.50	1.32	139	31	-154	-2.7	-738 (0.070)	3.5 (0.130)	1.8
Rh_2TiFe	5.82	1.15	139	30	-246	0.5	-363 (0.160)	1.4 (0.220)	3.8
Rh_2TiMn	6.15	1.00	225	29	-24	1.0	-310 (-0.220)	-1.3 (-0.250)	4.6
Rh_2VCo	5.37	1.35	139	32	-221	3.3	1194 (0.120)	5.7 (0.060)	1.5
Rh_2VCr	5.39	1.36	139	29	88	-0.8	370 (0.150)	-2.8 (-0.250)	1.1
Rh_2VFe	5.44	1.33	139	31	-23	1.8	424 (0.040)	1.8 (-0.010)	2.4
Rh_2WCo	5.40	1.39	139	33	-84	-1.0	499 (-0.240)	1.9 (0.250)	1.6
Rh_2WFe	5.44	1.38	139	32	231	-0.2	864 (-0.220)	-3.1 (-0.150)	2.5
Rh_2WMn	5.48	1.37	139	31	961	0.1	1535 (-0.180)	5.6 (-0.240)	2.6
Rh_2YMn	6.49	1.00	225	28	-56	0.0	-87 (0.060)	0.5 (0.110)	4.4
Rh_2ZnFe	6.02	1.00	225	38	252	-0.8	1126 (-0.250)	-3.8 (-0.180)	4.2
Rh_2ZnMn	6.03	1.00	225	37	1024	2.5	1959 (0.230)	-5.1 (0.250)	3.2
Rh_2ZrCo	5.67	1.32	139	31	99	-3.0	-437 (0.060)	-3.1 (0.010)	2.0
Rh_2ZrFe	5.97	1.17	139	30	-170	-0.3	-412 (0.040)	-2.1 (-0.210)	3.7
Rh_2ZrMn	6.36	1.00	225	29	13	0.9	324 (0.130)	-1.8 (0.170)	4.5
Ru_2CrV	6.00	1.00	225	27	536	-1.0	998 (-0.080)	3.1 (-0.110)	2.7
Ru_2HfFe	6.24	1.00	225	28	675	-1.0	869 (-0.040)	3.0 (-0.110)	4.0
Ru_2HfMn	6.26	1.00	225	27	-3	-0.3	-1953 (-0.240)	6.3 (-0.170)	3.3
Ru_2MnV	6.01	1.00	225	28	50	-0.4	-939 (-0.140)	4.3 (-0.100)	3.8
Ru_2NbFe	6.17	1.00	225	29	15	0.0	243 (-0.080)	1.1 (-0.180)	4.6
Ru_2NbMn	6.19	1.00	225	28	-613	-2.9	-945 (0.050)	4.9 (-0.220)	3.9
Ru_2ScFe	6.17	1.00	225	27	520	-1.1	574 (-0.040)	-2.9 (0.110)	3.3
Ru_2TaCr	6.20	1.00	225	27	-212	1.5	-1061 (-0.050)	-5.1 (-0.180)	2.9
Ru_2TaFe	6.18	1.00	225	29	-113	-0.8	-377 (0.020)	-4.4 (-0.250)	4.5
Ru_2TaMn	6.20	1.00	225	28	-669	-1.6	-1028 (-0.240)	4.5 (-0.160)	3.9
Ru_2TiFe	6.06	1.00	225	28	-33	1.8	-942 (-0.130)	-3.8 (-0.170)	4.0
Ru_2TiMn	6.08	1.00	225	27	-280	0.9	-1283 (-0.170)	4.1 (0.200)	3.1
Ru_2VFe	5.99	1.00	225	29	168	0.1	-571 (0.250)	-2.8 (-0.210)	4.3
Ru_2ZrFe	6.27	1.00	225	28	-84	-1.7	-362 (0.250)	-1.8 (0.010)	4.1
Ru_2ZrMn	6.30	1.00	225	27	-162	-0.1	-1557 (-0.250)	5.2 (-0.190)	3.5
Sc_2AgMn	6.91	0.94	139	24	-352	-1.8	-865 (-0.150)	4.0 (0.200)	2.4
Sc_2CdMn	6.74	1.07	139	25	100	1.1	748 (0.210)	2.7 (0.140)	2.6
Sc_2CuMn	6.69	0.94	139	24	-258	-0.3	-776 (-0.220)	4.5 (0.130)	2.2
Sc_2HgMn	6.59	1.13	139	25	-231	0.3	623 (0.130)	2.3 (-0.120)	2.6
Sc_2IrCr	6.55	1.00	225	21	342	-2.3	-740 (0.130)	-3.7 (0.070)	3.2
Sc_2IrMn	6.60	0.96	139	22	292	-2.7	598 (-0.140)	-3.4 (0.050)	2.7
Sc_2MnCo	6.52	0.96	139	22	11	-1.6	-602 (0.120)	-3.0 (0.070)	3.0

Sc_2OsCr	6.53	1.00	225	20	-167	0.3	-394 (-0.210)	0.8 (-0.140)	3.4
Sc_2OsFe	6.41	1.00	225	22	-140	3.5	-1059 (-0.180)	4.0 (-0.080)	1.5
Sc_2RhMn	6.62	0.95	139	22	-75	-1.7	-783 (0.160)	-3.5 (0.100)	2.3
Sc_2RuCr	6.54	1.00	225	20	-87	-0.1	-307 (-0.250)	0.4 (-0.190)	3.4
Sc_2ZnCr	6.72	1.00	225	24	48	0.1	217 (0.140)	0.5 (0.060)	3.3
Sc_2ZnMn	6.51	1.07	139	25	251	0.7	707 (0.160)	2.3 (0.120)	2.4
Ta_2CoMn	6.14	1.00	225	26	-225	-0.4	924 (0.220)	3.8 (0.160)	1.6
Ta_2OsFe	6.29	1.00	225	26	476	0.1	595 (0.120)	-3.5 (0.160)	1.6
Ta_2PtCr	5.63	1.46	139	26	513	-2.4	939 (-0.250)	-3.9 (0.050)	2.1
Ta_2PtMn	5.59	1.46	139	27	-286	2.0	633 (0.250)	-3.1 (-0.200)	2.0
Ta_2ReCo	6.30	1.00	225	26	568	0.4	633 (0.050)	-2.1 (0.120)	1.6
Ta_2RuCo	5.90	1.18	139	27	11	-1.3	436 (-0.230)	-2.3 (-0.170)	0.7
Ta_2RuFe	6.26	1.00	225	26	553	-1.3	650 (-0.040)	-2.6 (0.120)	1.6
Ti_2CoV	6.09	1.00	225	22	103	0.8	440 (0.130)	2.7 (-0.230)	1.7
Ti_2CrFe	6.01	1.00	225	22	-4	0.7	-305 (-0.210)	3.1 (0.240)	1.5
Ti_2IrCo	6.13	1.00	225	26	385	1.7	593 (0.110)	-3.3 (0.140)	1.6
Ti_2MnCr	6.06	1.00	225	21	60	-0.6	336 (-0.250)	-1.9 (-0.250)	2.4
Ti_2MnV	6.13	1.00	225	20	-126	0.7	-366 (-0.120)	-2.2 (-0.210)	2.3
Ti_2OsCr	6.16	1.00	225	22	-255	0.0	284 (-0.210)	-1.9 (-0.090)	1.5
Ti_2ReCr	6.21	1.00	225	21	-107	0.4	-862 (-0.210)	3.1 (-0.090)	2.3
Ti_2RuCr	6.14	1.00	225	22	-97	0.6	-284 (-0.250)	1.2 (-0.220)	1.4
Ti_2VFe	6.10	1.00	225	21	-74	1.8	346 (0.060)	1.9 (0.020)	2.5
Ti_2ZnNi	6.18	1.00	225	30	-284	0.8	-774 (-0.170)	1.8 (-0.070)	1.8
V_2CoFe	5.41	1.20	139	27	2	0.6	-573 (-0.210)	1.6 (-0.170)	0.8
V_2MnCo	5.77	1.00	225	26	-103	1.2	-520 (0.250)	-2.4 (0.200)	1.7
V_2OsCo	5.94	1.00	225	27	-440	-1.2	-746 (0.250)	-2.4 (0.120)	2.5
V_2OsFe	5.94	1.00	225	26	517	-1.6	-856 (0.190)	-3.9 (0.090)	1.6
V_2PtFe	5.31	1.41	139	28	48	-2.0	612 (-0.210)	-2.1 (0.020)	0.5
V_2PtMn	5.26	1.50	139	27	-840	2.8	-988 (-0.030)	4.9 (0.060)	1.9
V_2RuCo	5.57	1.19	139	27	-116	-1.9	-800 (0.130)	2.7 (-0.190)	1.4
V_2RuFe	5.91	1.00	225	26	17	1.6	-800 (0.230)	-1.9 (0.140)	1.5
W_2IrMn	5.46	1.44	139	28	-51	-1.0	-597 (-0.250)	4.4 (-0.220)	1.6
Y_2AgMn	7.23	1.00	225	24	122	-0.9	759 (0.130)	2.7 (0.100)	3.3
Y_2CdMn	7.30	1.00	225	25	355	-0.5	-536 (0.150)	2.7 (0.250)	3.3
Y_2HgMn	7.42	0.95	139	25	10	-1.4	-753 (0.200)	-2.0 (0.170)	3.1
Y_2ZnMn	7.13	1.00	225	25	455	3.0	1103 (0.100)	3.0 (0.000)	3.1
Zn_2AuCr	5.80	1.26	139	41	26	0.0	87 (-0.250)	-0.3 (0.190)	3.5
Zn_2HfFe	5.36	1.55	139	36	56	-0.4	181 (-0.250)	0.5 (0.210)	0.6
Zn_2HfMn	5.55	1.45	139	35	86	2.0	359 (0.040)	2.0 (0.000)	1.5
Zn_2NiMn	5.44	1.29	139	41	194	0.1	238 (-0.110)	0.7 (-0.200)	3.5
Zn_2PtCr	5.64	1.31	139	40	-50	-0.1	-71 (0.030)	0.4 (0.240)	3.6
Zn_2RuMn	5.39	1.42	139	39	-24	-0.2	-81 (-0.250)	0.3 (0.250)	4.0
Zn_2ScFe	5.51	1.44	139	35	194	-2.9	722 (-0.080)	-3.0 (-0.010)	1.2
Zn_2ScMn	6.39	1.00	225	34	159	2.3	514 (0.060)	2.5 (-0.020)	3.3
Zn_2TiFe	5.22	1.54	139	36	306	-0.0	462 (-0.130)	1.1 (-0.170)	0.6
Zn_2TiMn	5.30	1.52	139	35	366	0.4	401 (-0.020)	1.2 (-0.050)	1.0
Zn_2YMn	6.66	1.00	225	34	-247	2.2	-533 (-0.110)	2.2 (0.000)	3.6
Zn_2ZrFe	5.62	1.39	139	36	94	0.8	931 (-0.240)	-3.7 (-0.170)	1.3
Zn_2ZrMn	6.38	1.00	225	35	149	2.0	656 (0.070)	-2.2 (0.250)	3.0
Zr_2OsCr	6.55	1.00	225	22	408	2.5	615 (0.130)	2.8 (-0.010)	1.6
Zr_2PdFe	6.55	1.00	225	26	170	0.8	673 (-0.250)	-2.0 (-0.140)	0.7
Zr_2ZnNi	6.57	1.00	225	30	-352	-1.9	-859 (-0.230)	3.4 (-0.190)	1.1

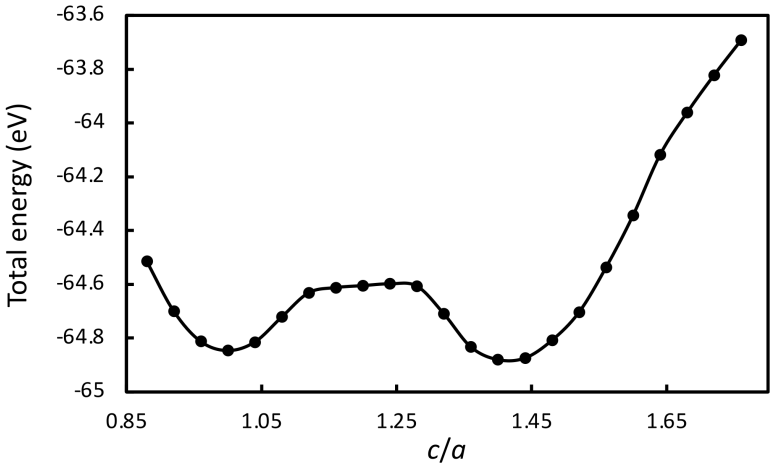

FIG. S1. Energy variation as a function of c/a in regular structure of Co_2MnV.