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Designing of Magnetic MAB Phases for Energy Applications

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Supporting Information

Computational details and supported figures and tables (a list of figures and tables in the supporting information at page 3)

Computational details

All calculations are carried out using the Vienna ab initio simulation package (VASP) code (version 5.4.4)[1,2] and associated pseudopotential library version. The exchange-correlation functional under the generalized gradient approximation (GGA) is implemented, as parameterized by Perdew, Burke, and Ernzerhof (PBE)[3]. The plane-wave energy cutoff and k-mesh density are set as 500 eV and 50 $Å^{-1}$, respectively. The structure optimization is performed in a two step manner, as detailed in our previous work[4].

After the optimization of atomic structures, the maximum residual force on each atom is less than 0.001 $eVÅ^{-1}$. For thermodynamical stability evaluation, we considered only the ferromagnetic configuration, which should be sufficient to evaluate the stabilities, whereas the magnetic ground state will be studied in a succeeding work. The lattice dynamics of targeted phases is studied in the framework of the harmonic approximation, where the phonon spectra are obtained using the frozen phonon approach with the Phonopy[5] and VASP[1,2] codes. Within this scheme, the forces on every atom are calculated on the basis of the Hellmann-Feynman theorem by explicitly displacing atoms. To calculate the force constant matrix, 3×3×3 supercells are used.

For the thermodynamical stable phases, the MAE is calculated using the force theorem[6] by implementing in full-potential local-orbital (FPLO)[7] with a k-mesh density of 60 $Å^{-1}$ to guarantee fine convergence. Finally, we used a simple computational proxy[8] based on performing nonmagnetic and magnetic density functional theory calculations to study the MCE of MAB phases and Non-MAB phases. This proxy, which Joshua termed the magnetic deformation Σ_M, is a measure of how much the unit cell deforms comparing with the relaxed structures with and without the inclusion of spin polarization. Σ_M appears to correlate very well with experimentally measured magnetic entropy change values, which can be used for screening magnetocaloric compounds. Hence, the calculations for all stable phases are carried out on both the nonmagnetic (NM) and the ferromagnetic (FM) states. For each considered compound, the magnetic deformation Σ_M was calculated following the procedure given in Ref[8]. And all the MAB and Non-MAB phases are presented as $M_xA_yB_z$ in the following parts.

List of figures and tables in the supporting information

Description: The thermodynamic stability information are listed in the Table (S1 and S10) and Figure (S1 and S4). The dynamic stability of unreported MAB and Non-MAB phases are shown in Figure S2. The results of effect of magnetic ground state are listed in the Table (S2 and S3) and Figure S0. The information of stability trends and bonding based on the Hume-Rothery rules and COPH are shown in Table (S4 and S5) and Figure (S5, S6, S7, and S8). The information of MAE of MAB and Non-MAB phases are shown in Table (S6, S7, and S8). The information of MCE of MAB and Non-MAB phases are shown in Table S9 and Figure S9. The DOS of predicted non-magnetic MAB phases are shown in Figure S3.

Table S1: The novel MAB and Non-MAB phases with convex hull distance < 0.1 eV/atom. Magnetic moment has the unit as μB per magnetic atom)

Compounds	Space Group	Lattice Constant (Å)			Convex Hull (eV/atom)	Formation Energy (eV/atom)	Magnetic moment (μB/Mag)
		a	b	c			
FeBeB	63	2.925	2.648	12.164	0.000	-0.326	0.422
MnBeB	63	2.809	2.811	12.252	0.000	-0.378	0.002
CrAlB	63	2.969	3.004	13.881	0.011	-0.377	0.011
CoBeB	63	3.058	2.539	12.098	0.014	-0.284	0.087
CoPtB	63	3.133	2.822	14.347	0.037	-0.250	0.092
FeMgB	63	2.902	2.871	17.037	0.040	-0.211	0.908
FeCrB	63	2.912	2.926	13.261	0.041	-0.310	2.254
FeZnB	63	2.904	2.857	14.631	0.045	-0.206	1.151
Cr_2B	63	2.900	2.892	13.469	0.047	-0.328	0.002
NiPtB	63	3.053	3.024	14.015	0.048	-0.227	0.002
NiLiB	63	2.996	2.714	15.995	0.052	-0.149	0.003
CrReB	63	2.881	2.905	15.108	0.052	-0.299	0.003
NiCuB	63	3.037	2.881	13.038	0.054	-0.111	0.000
FeMnB	63	2.912	2.904	13.354	0.057	-0.301	3.889
CrBeB	63	2.860	2.860	12.584	0.060	-0.291	0.012
FeIrB	63	2.896	2.856	14.896	0.061	-0.190	1.451
MnIrB	63	2.926	2.925	14.755	0.062	-0.271	1.992
FePtB	63	2.951	2.974	14.720	0.063	-0.242	1.887
CrNiB	63	2.927	2.983	12.697	0.066	-0.297	0.020
MnAlB	63	2.988	2.953	13.908	0.066	-0.329	0.997
FeAlB	63	2.856	2.729	15.972	0.067	-0.281	0.644
Fe_2B	63	2.919	2.868	13.357	0.068	-0.244	4.078
CrPtB	63	2.850	3.124	14.749	0.069	-0.330	0.100
NiAuB	63	3.057	2.995	15.082	0.070	-0.095	0.002
NiPdB	63	3.044	2.965	14.116	0.070	-0.211	0.003
FeLiB	63	2.837	2.797	15.498	0.071	-0.180	0.356
CoMgB	63	2.930	2.834	16.933	0.072	-0.201	0.001
MnPtB	63	2.954	3.071	14.596	0.073	-0.340	2.441
CrTcB	63	2.888	2.915	14.819	0.075	-0.289	0.002
CrRhB	63	2.869	2.892	15.040	0.077	-0.295	0.005
NiZnB	63	2.973	2.788	14.808	0.078	-0.132	0.002
NiIrB	63	3.164	2.828	13.941	0.079	-0.139	0.016
CoPdB	63	3.017	2.847	14.528	0.081	-0.217	0.185
CoRhB	63	2.988	2.811	14.250	0.084	-0.191	0.006
MnCoB	63	2.930	2.891	13.195	0.084	-0.255	3.540
NiMnB	63	2.950	2.942	12.894	0.086	-0.278	2.448
CoLiB	63	2.962	2.679	15.351	0.087	-0.186	0.031
CoIrB	63	2.950	2.845	14.489	0.087	-0.186	0.000
MnZnB	63	2.872	2.868	14.626	0.087	-0.246	0.039
FePdB	63	2.946	2.938	14.740	0.088	-0.216	1.739
MnRhB	63	2.938	2.950	14.468	0.089	-0.273	2.236
MnPdB	63	2.958	3.015	14.701	0.090	-0.296	2.435
CrPdB	63	2.913	2.982	14.950	0.091	-0.270	0.185

CoZnB	63	2.980	2.818	14.328	0.092	-0.181	0.002
FeRuB	63	2.863	2.854	14.744	0.095	-0.155	1.528
MnReB	63	2.832	2.790	15.606	0.096	-0.237	0.049
MnMgB	63	2.883	2.887	17.126	0.096	-0.237	0.265
FeNiB	63	2.957	2.896	12.742	0.097	-0.209	1.977
CoCrB	63	2.927	2.963	12.754	0.097	-0.254	1.379
FeRhB	63	2.913	2.866	14.666	0.098	-0.201	1.852
Fe_2BeB_2	65	2.749	2.904	9.947	0.000	-0.344	0.760
Mn_2BeB_2	65	2.815	2.846	9.969	0.000	-0.435	0.011
Fe_2AlB_2	65	2.851	2.916	11.019	0.000	-0.401	1.330
Mn_2AlB_2	65	2.831	2.894	11.080	0.000	-0.471	0.400
Cr_2AlB_2	65	2.932	2.924	11.051	0.000	-0.466	0.010
Cr_2SiB_2	65	2.931	2.923	10.441	0.029	-0.414	0.001
Cr_2BeB_2	65	2.911	2.895	9.911	0.034	-0.387	0.131
Cr_2ReB_2	65	2.916	2.885	11.474	0.034	-0.387	0.006
Fe_2MgB_2	65	2.849	2.895	12.019	0.035	-0.266	0.910
Co_2BeB_2	65	2.542	3.017	10.196	0.043	-0.300	0.016
Cr_2TcB_2	65	2.916	2.887	11.376	0.045	-0.385	0.005
Mn_2IrB_2	65	2.950	2.960	11.131	0.046	-0.354	2.068
Fe_2ZnB_2	65	2.853	2.905	11.158	0.054	-0.248	1.046
Cr_2IrB_2	65	2.933	2.876	11.456	0.055	-0.377	0.009
Ni_2LiB_2	65	2.667	2.999	11.874	0.058	-0.182	0.002
Ni_2PtB_2	65	2.962	3.028	10.878	0.060	-0.214	0.006
Co_2AlB_2	65	2.687	2.971	11.351	0.063	-0.347	0.149
Cr_2FeB_2	65	2.927	2.913	10.586	0.064	-0.357	1.334
Fe_2IrB_2	65	2.878	2.917	11.246	0.065	-0.236	1.684
Ni_2CuB_2	65	2.800	2.995	10.754	0.065	-0.133	0.001
Ni_2ZnB_2	65	2.819	2.977	11.145	0.066	-0.169	0.005
Cr_3B_2	65	2.884	2.901	10.773	0.066	-0.374	0.008
Fe_2PtB_2	65	2.914	2.974	11.188	0.067	-0.267	1.598
Cr_2WB_2	65	2.926	2.899	11.646	0.068	-0.353	0.007
Co_2MgB_2	65	2.795	2.932	12.069	0.069	-0.259	0.017
Cr_2MoB_2	65	2.929	2.903	11.593	0.071	-0.357	0.007
Mn_2CoB_2	65	2.909	2.934	10.500	0.071	-0.336	2.717
Mn_2FeB_2	65	2.906	2.926	10.588	0.071	-0.344	2.830
Mn_2RhB_2	65	2.947	2.961	11.070	0.071	-0.346	2.170
Fe_3B_2	65	2.840	2.931	10.679	0.074	-0.265	2.899
Cr_2RuB_2	65	2.917	2.882	11.312	0.075	-0.346	0.013
Cr_2OsB_2	65	2.916	2.883	11.372	0.077	-0.344	0.007
Mn_2PtB_2	65	3.015	2.984	11.158	0.067	-0.384	2.354
Fe_2GaB_2	65	2.877	2.944	10.995	0.078	-0.237	1.360
Ni_2BeB_2	65	2.712	2.964	10.174	0.080	-0.207	0.001
Ni_2PdB_2	65	2.928	3.019	10.958	0.080	-0.199	0.005
Mn_2SiB_2	65	2.734	2.937	10.668	0.081	-0.354	0.004
Mn_2ReB_2	65	2.907	2.926	11.306	0.081	-0.319	1.647
Cr_2RhB_2	65	2.934	2.877	11.407	0.082	-0.352	0.034
Cr_2VB_2	65	2.908	2.927	10.971	0.083	-0.475	0.005

Ni_2AuB_2	65	2.958	3.044	11.262	0.084	-0.114	0.014
Cr_2CoB_2	65	2.934	2.904	10.520	0.085	-0.336	1.111
Cr_2NiB_2	65	2.971	2.917	10.347	0.085	-0.344	0.009
Co_2PtB_2	65	2.819	3.059	11.026	0.085	-0.252	0.307
Cr_2MnB_2	65	2.885	2.878	10.698	0.087	-0.360	0.034
Fe_2ReB_2	65	2.826	2.870	11.552	0.088	-0.232	1.386
Fe_2NiB_2	65	2.862	2.941	10.376	0.090	-0.244	1.537
Mn_2ScB_2	65	2.891	2.873	12.668	0.092	-0.432	0.323
Cr_2PtB_2	65	3.061	2.881	11.283	0.093	-0.357	0.185
Fe_2RhB_2	65	2.886	2.911	11.204	0.095	-0.248	1.899
Mn_2RuB_2	65	2.929	2.938	11.061	0.096	-0.304	1.798
Mn_2NiB_2	65	2.910	2.953	10.404	0.096	-0.322	2.096
Mn_2WB_2	65	2.790	2.833	12.067	0.099	-0.328	0.006
Mn_2TcB_2	65	2.899	2.927	11.270	0.099	-0.320	1.605
Cr_3AlB_4	47	2.939	2.939	8.091	0.000	-0.445	0.049
Cr_3BeB_4	47	2.915	2.916	7.571	0.011	-0.403	0.006
Mn_3BeB_4	47	2.911	2.830	7.591	0.025	-0.364	0.636
Cr_3SiB_4	47	2.954	2.918	7.787	0.035	-0.392	0.010
Mn_3AlB_4	47	2.937	2.834	8.164	0.038	-0.396	0.758
Fe_3BeB_4	47	2.953	2.792	7.586	0.047	-0.240	1.198
Fe_3AlB_4	47	2.961	2.818	8.149	0.065	-0.27975	1.255
Cr_3IrB_4	47	2.911	2.911	8.359	0.067	-0.37507	0.007
Cr_3GaB_4	47	2.948	2.950	8.100	0.071	-0.34263	0.099
Cr_3ZnB_4	47	2.932	2.944	8.162	0.083	-0.33128	0.200
Cr_3PtB_4	47	2.921	2.968	8.335	0.086	-0.36613	0.245
Fe_3ZnB_4	47	2.953	2.851	8.198	0.088	-0.19442	1.364
Fe_3IrB_4	47	2.949	2.854	8.245	0.091	-0.19070	1.436
Fe_3MgB_4	47	2.940	2.855	8.675	0.092	-0.21718	1.259
Mn_3IrB_4	47	2.963	2.966	8.165	0.093	-0.32952	2.219
Mn_3PtB_4	47	2.976	3.011	8.176	0.094	-0.33546	2.258
Mn_3SiB_4	47	2.982	2.824	7.826	0.095	-0.31629	0.975
Cr_3B_5	47	2.922	2.920	7.239	0.095	-0.33817	0.013
Mn_3MgB_4	47	2.911	2.887	8.683	0.098	-0.30260	0.526
Mn_3GaB_4	47	2.940	2.838	8.228	0.099	-0.29042	0.791
Cr_3NiB_4	47	2.936	2.944	7.785	0.099	-0.36333	0.019
Cr_3ReB_4	47	2.916	2.902	8.358	0.099	-0.37916	0.011
Fe_3PtB_4	47	2.961	2.888	8.264	0.099	-0.21703	1.450
$Fe_3Al_2B_2$	65	2.872	2.912	16.537	0.033	-0.393	0.735
$Mn_3Al_2B_2$	65	2.832	2.853	17.788	0.007	-0.406	0.962
Cr_5B_2	65	2.881	2.889	16.320	0.044	-0.277	0.006
$Cr_3Al_2B_2$	65	2.950	2.936	17.311	0.046	-0.326	1.024
$Mn_3Ir_2B_2$	65	3.012	2.979	17.063	0.050	-0.302	2.731
$Mn_3Rh_2B_2$	65	3.022	2.981	16.960	0.052	-0.299	2.968
$Co_3Al_2B_2$	65	2.781	2.931	16.884	0.056	-0.412	0.006
Fe_5B_2	65	2.854	2.914	16.253	0.057	-0.211	3.519
$Ni_3Pt_2B_2$	65	2.969	3.077	16.525	0.059	-0.202	0.161

$Co_3Be_2B_2$	65	2.596	2.894	15.185	0.066	-0.287	0.076
$Fe_3Be_2B_2$	65	2.624	2.914	15.157	0.067	-0.266	0.879
$Mn_3Be_2B_2$	65	2.787	2.820	15.315	0.068	-0.321	0.950
$Mn_3Co_2B_2$	65	2.920	2.915	16.092	0.070	-0.248	3.321
$Mn_3Si_2B_2$	65	2.808	2.883	16.009	0.071	-0.391	0.022
$Co_3Pt_2B_2$	65	2.775	3.191	16.604	0.072	-0.195	0.477
$Fe_3Ir_2B_2$	65	2.883	2.912	17.631	0.074	-0.174	2.108
$Cr_3V_2B_2$	65	2.921	2.920	16.757	0.080	-0.397	0.002
$Cr_3W_2B_2$	65	2.980	2.985	17.281	0.082	-0.232	0.004
$Ni_3Zn_2B_2$	65	2.793	2.965	17.255	0.084	-0.174	0.004
$Cr_3Re_2B_2$	65	2.945	2.940	17.330	0.084	-0.230	0.260
$Mn_3Pt_2B_2$	65	2.946	2.940	18.452	0.087	-0.351	2.794
$Ni_3Al_2B_2$	65	2.831	2.961	16.872	0.087	-0.368	0.000
$Cr_3Tc_2B_2$	65	2.942	2.932	17.178	0.088	-0.229	0.234
$Fe_3Co_2B_2$	65	2.859	2.900	16.112	0.088	-0.182	3.101
$Cr_3Mo_2B_2$	65	2.977	2.976	17.263	0.089	-0.226	0.013
$Fe_3Zn_2B_2$	65	2.816	2.874	17.849	0.090	-0.156	1.484
$Fe_3Si_2B_2$	65	2.762	2.914	16.035	0.091	-0.315	0.819
$Cr_3Mn_2B_2$	65	2.881	2.878	16.063	0.094	-0.240	0.000
$Mn_3Ga_2B_2$	65	2.830	2.848	18.356	0.095	-0.249	1.111
$Fe_3Rh_2B_2$	65	2.795	2.841	17.976	0.096	-0.172	2.168
$Ni_3Be_2B_2$	65	2.615	2.945	15.349	0.100	-0.240	0.001
Fe_4BeB_4	71	2.821	2.918	17.513	0.000	-0.377	1.017
Fe_4AlB_4	71	2.870	2.927	18.565	0.000	-0.417	1.271
Mn_4BeB_4	71	2.878	2.899	17.591	0.000	-0.467	0.878
Fe_4MgB_4	71	2.875	2.932	19.626	0.000	-0.354	1.391
Cr_4AlB_4	71	2.939	2.920	18.856	0.000	-0.510	0.000
Mn_4AlB_4	71	2.889	2.929	18.591	0.000	-0.500	1.014
Ni_4ZnB_4	71	2.880	2.992	18.517	0.000	-0.261	0.000
Fe_4ZnB_4	71	2.872	2.931	18.726	0.000	-0.348	1.326
Ni_4CuB_4	71	2.875	2.992	18.125	0.000	-0.227	0.000
Ni_4PtB_4	71	2.960	2.995	18.351	0.000	-0.267	0.001
Ni_4AuB_4	71	2.950	3.012	18.793	0.000	-0.224	0.000
Fe_4GaB_4	71	2.883	2.939	18.557	0.000	-0.343	1.288
Ni_4PdB_4	71	2.931	2.996	18.453	0.000	-0.266	0.001
Fe_5B_4	71	2.880	2.932	18.163	0.001	-0.354	2.135
Ni_4CdB_4	71	2.914	3.004	19.570	0.001	-0.219	0.001
Fe_4IrB_4	71	2.887	2.930	18.791	0.003	-0.332	1.530
Cr_4BeB_4	71	2.919	2.896	17.837	0.003	-0.465	0.002
Mn_4IrB_4	71	2.966	2.959	18.716	0.005	-0.439	2.004
Fe_4NiB_4	71	2.878	2.938	17.924	0.007	-0.346	1.453
Fe_4PtB_4	71	2.914	2.950	18.827	0.009	-0.344	1.565
Ni_4AgB_4	71	2.904	2.997	19.167	0.009	-0.211	0.000
Cr_4SiB_4	71	2.925	2.932	18.249	0.010	-0.470	0.000
Mn_4FeB_4	71	2.929	2.940	18.189	0.013	-0.439	2.237
Ni_4BeB_4	71	2.828	2.969	17.582	0.013	-0.257	0.000
Mn_4CoB_4	71	2.932	2.949	18.134	0.013	-0.435	2.246

Cr_4ReB_4	71	2.922	2.895	19.306	0.014	-0.454	0.001
Ni_4LiB_4	71	2.812	2.991	19.253	0.015	-0.252	0.000
Co_4MgB_4	71	2.823	2.994	19.214	0.019	-0.346	0.006
Cr_4FeB_4	71	2.925	2.914	18.438	0.019	-0.449	0.668
Mn_4RhB_4	71	2.966	2.962	18.697	0.019	-0.435	2.072
Fe_4RhB_4	71	2.887	2.933	18.798	0.020	-0.338	1.614
Mn_4GaB_4	71	2.906	2.946	18.573	0.021	-0.423	1.004
Mn_4SiB_4	71	2.885	2.974	17.913	0.022	-0.442	1.124
Cr_4IrB_4	71	2.927	2.895	19.312	0.023	-0.451	0.002
Co_4AlB_4	71	2.844	2.987	18.182	0.023	-0.387	0.001
Co_4BeB_4	71	2.787	2.999	17.096	0.024	-0.349	0.006
Cr_4TcB_4	71	2.924	2.898	19.231	0.024	-0.449	0.000
Fe_4SiB_4	71	2.869	2.938	17.935	0.025	-0.342	1.253
Ni_5B_4	71	2.884	2.984	17.819	0.025	-0.251	0.005
Fe_4PdB_4	71	2.901	2.941	18.845	0.025	-0.327	1.507
Fe_4ReB_4	71	2.871	2.898	19.036	0.026	-0.322	1.436
Co_4ZnB_4	71	2.817	3.010	18.275	0.027	-0.338	0.001
Mn_4NiB_4	71	2.943	2.959	18.024	0.027	-0.428	1.963
Cr_4NiB_4	71	2.947	2.908	18.228	0.027	-0.445	0.001
Cr_5B_4	71	2.903	2.905	18.629	0.028	-0.451	0.001
Fe_4CoB_4	71	2.882	2.933	18.044	0.028	-0.335	1.922
Mn_4ReB_4	71	2.932	2.947	18.884	0.028	-0.416	1.727
Cr_4CoB_4	71	2.932	2.912	18.356	0.029	-0.439	0.676
Cr_4WB_4	71	2.925	2.900	19.518	0.029	-0.439	0.000
Fe_4LiB_4	71	2.856	2.915	19.111	0.029	-0.306	1.385
Mn_4ZnB_4	71	2.919	2.918	18.694	0.030	-0.414	1.103
Co_4PtB_4	71	2.838	3.054	18.233	0.030	-0.339	0.001
Cr_4GaB_4	71	2.951	2.924	18.875	0.031	-0.437	0.000
Fe_4CuB_4	71	2.873	2.935	18.316	0.031	-0.304	1.437
Cr_4MoB_4	71	2.927	2.902	19.483	0.031	-0.442	0.001
Fe_4MnB_4	71	2.877	2.923	18.396	0.032	-0.351	2.163
Mn_4MgB_4	71	2.918	2.921	19.595	0.032	-0.412	0.983
Cr_4VB_4	71	2.916	2.919	18.857	0.033	-0.514	0.001
Mn_4PtB_4	71	2.989	2.978	18.796	0.034	-0.437	2.074
Fe_4TcB_4	71	2.875	2.904	18.986	0.036	-0.322	1.485
Cr_4RhB_4	71	2.930	2.893	19.287	0.036	-0.439	0.002
Cr_4OsB_4	71	2.923	2.896	19.189	0.038	-0.430	0.002
Cr_4MnB_4	71	2.906	2.893	18.541	0.038	-0.444	0.181
Fe_4RuB_4	71	2.882	2.922	18.768	0.038	-0.304	1.528
Mn_4RuB_4	71	2.956	2.953	18.649	0.039	-0.405	1.897
Cr_4RuB_4	71	2.924	2.895	19.153	0.039	-0.429	0.003
Mn_4OsB_4	71	2.953	2.953	18.676	0.040	-0.404	1.867
Fe_4CdB_4	71	2.882	2.939	20.057	0.041	-0.294	1.418
Fe_4OsB_4	71	2.879	2.916	18.762	0.042	-0.293	1.410
Cr_4ZnB_4	71	2.944	2.912	18.995	0.042	-0.426	0.005
Ni_4GaB_4	71	2.931	3.005	18.282	0.043	-0.218	0.000
Ni_4IrB_4	71	2.922	2.984	18.389	0.045	-0.217	0.000
Ni_4MgB_4	71	2.883	2.986	19.384	0.045	-0.274	0.000

Mn_4TcB_4	71	2.934	2.949	18.842	0.046	-0.411	1.717
Ni_4AlB_4	71	2.880	2.986	18.490	0.046	-0.273	0.000
Co_4NiB_4	71	2.804	3.033	17.487	0.046	-0.328	0.024
Fe_4AuB_4	71	2.903	2.952	19.333	0.047	-0.288	1.461
Co_4RhB_4	71	2.828	3.015	18.211	0.049	-0.316	0.024
Cr_4PtB_4	71	2.977	2.900	19.288	0.049	-0.435	0.003
Fe_4CaB_4	71	2.897	2.947	21.118	0.050	-0.285	1.278
Mn_5B_4	71	2.922	2.941	18.363	0.051	-0.417	2.127
Fe_4MoB_4	71	2.861	2.896	19.370	0.052	-0.331	1.380
Co_4GaB_4	71	2.860	3.006	18.043	0.053	-0.321	0.001
Ni_4NaB_4	71	2.823	3.024	20.975	0.053	-0.177	0.000
Co_4PdB_4	71	2.836	3.024	18.360	0.054	-0.319	0.003
Fe_4WB_4	71	2.864	2.890	19.388	0.057	-0.323	1.387
Co_4IrB_4	71	2.849	3.006	18.193	0.057	-0.308	0.016
Mn_4WB_4	71	2.858	2.903	19.560	0.057	-0.403	1.084
Ni_4InB_4	71	2.958	3.024	19.418	0.057	-0.163	0.000
Mn_4PdB_4	71	2.976	2.967	18.895	0.060	-0.402	2.017
Cr_4ScB_4	71	2.964	2.934	20.212	0.061	-0.468	0.007
Mn_4ScB_4	71	2.923	2.913	20.264	0.062	-0.487	0.981
Fe_4InB_4	71	2.891	2.947	19.867	0.063	-0.272	1.300
Ni_4HgB_4	71	2.945	3.018	19.498	0.066	-0.154	0.000
Fe_4B_5	71	2.839	2.938	16.717	0.066	-0.269	1.046
Fe_4AgB_4	71	2.882	2.933	19.644	0.066	-0.269	1.419
Ni_4RhB_4	71	2.904	2.988	18.424	0.067	-0.240	0.001
Mn_4MoB_4	71	2.861	2.902	19.542	0.068	-0.406	1.064
Mn_4TaB_4	71	2.878	2.894	19.978	0.068	-0.470	0.955
Fe_4NbB_4	71	2.863	2.907	19.876	0.068	-0.381	1.298
Co_4LiB_4	71	2.776	2.984	18.980	0.068	-0.297	0.041
Cr_4NbB_4	71	2.937	2.907	20.085	0.069	-0.464	0.000
Cr_4B_5	71	2.917	2.906	17.160	0.070	-0.415	0.003
Co_4CuB_4	71	2.799	3.026	17.758	0.070	-0.295	0.001
Mn_4NbB_4	71	2.885	2.894	20.064	0.071	-0.458	0.945
Cr_4PdB_4	71	2.967	2.907	19.260	0.071	-0.401	0.006
Cr_4MgB_4	71	2.962	2.920	19.743	0.071	-0.397	0.001
Cr_4TaB_4	71	2.932	2.908	19.968	0.072	-0.480	0.001
Fe_4ScB_4	71	2.863	2.937	20.181	0.072	-0.416	1.154
Co_5B_4	71	2.792	3.032	17.541	0.073	-0.292	0.431
Fe_4TaB_4	71	2.857	2.907	19.773	0.073	-0.386	1.241
Co_4CdB_4	71	2.847	3.007	19.419	0.075	-0.290	0.001
Mn_4YB_4	71	2.954	2.938	21.025	0.075	-0.401	0.958
Mn_4CuB_4	71	2.932	2.951	18.281	0.075	-0.369	1.615
Cr_4TiB_4	71	2.937	2.932	19.267	0.075	-0.530	0.002
Mn_4B_5	71	2.888	2.937	16.811	0.078	-0.379	1.069
Fe_4CrB_4	71	2.868	2.917	18.422	0.080	-0.309	1.811
Co_4AuB_4	71	2.860	3.035	18.681	0.080	-0.285	0.003
Cr_4CuB_4	71	2.944	2.910	18.580	0.082	-0.386	0.037
Mn_4VB_4	71	2.863	2.931	18.869	0.083	-0.459	1.144
Co_4FeB_4	71	2.765	3.047	17.871	0.084	-0.290	0.753

Co_4ReB_4	71	2.811	2.985	18.529	0.084	-0.285	0.000
Fe_4YB_4	71	2.906	2.965	20.832	0.085	-0.334	1.243
Fe_4VB_4	71	2.870	2.912	18.813	0.086	-0.374	1.592
Co_4CaB_4	71	2.837	3.014	20.640	0.087	-0.278	0.245
Fe_4GeB_4	71	2.903	2.961	18.490	0.088	-0.247	1.372
Mn_4CdB_4	71	2.915	2.918	20.248	0.088	-0.356	0.926
Mn_4AuB_4	71	2.973	2.972	19.285	0.089	-0.355	1.781
Ni_4FeB_4	71	2.874	2.976	18.178	0.090	-0.214	0.633
Mn_4CrB_4	71	2.897	2.940	18.401	0.090	-0.384	1.619
Co_4TcB_4	71	2.805	2.993	18.540	0.091	-0.285	0.002
Mn_4LiB_4	71	2.902	2.904	18.789	0.092	-0.352	0.881
Mn_4InB_4	71	2.928	2.930	20.097	0.092	-0.352	1.039
Co_4RuB_4	71	2.830	3.002	18.227	0.093	-0.272	0.003
Co_4MnB_4	71	2.768	3.024	18.463	0.094	-0.292	0.960
Ni_4B_5	71	2.962	2.987	16.367	0.096	-0.124	0.000
Cr_4AlB_6	65	2.943	2.947	21.328	0.012	-0.422	0.003
Cr_4BeB_6	65	2.925	2.932	20.320	0.020	-0.391	0.013
Cr_4SiB_6	65	2.924	2.961	20.743	0.043	-0.377	0.018
Mn_4BeB_6	65	2.853	2.935	20.351	0.044	-0.341	0.912
Mn_4AlB_6	65	2.869	2.948	21.493	0.055	-0.362	1.071
Cr_4IrB_6	65	2.930	2.930	21.783	0.060	-0.371	0.008
Cr_4GaB_6	65	2.955	2.955	21.334	0.062	-0.349	0.003
Cr_4ZnB_6	65	2.951	2.943	21.439	0.066	-0.345	0.004
Cr_4PtB_6	65	2.969	2.938	21.766	0.069	-0.370	0.158
Cr_4CuB_6	65	2.947	2.941	21.072	0.079	-0.332	0.008
Cr_4NiB_6	65	2.943	2.943	20.747	0.080	-0.365	0.023
Cr_4MgB_6	65	2.958	2.942	22.329	0.082	-0.339	0.004
Cr_4B_7	65	2.929	2.938	19.646	0.085	-0.339	0.011
Mn_4IrB_6	65	2.939	2.960	21.583	0.089	-0.319	1.973
Mn_4PtB_6	65	2.958	2.965	21.737	0.092	-0.322	2.033
Cr_4PdB_6	65	2.965	2.940	21.726	0.092	-0.348	0.036
Cr_4OsB_6	65	2.918	2.932	21.731	0.093	-0.348	0.004
Fe_4BeB_6	65	2.803	2.970	20.364	0.093	-0.184	1.242
Mn_4SiB_6	65	2.909	2.964	20.680	0.094	-0.307	1.321
Mn_4ZnB_6	65	2.893	2.938	21.635	0.094	-0.291	1.085
Mn_4GaB_6	65	2.884	2.953	21.564	0.097	-0.288	1.153
Cr_4FeB_6	65	2.930	2.950	20.905	0.099	-0.366	0.726
Mn_4MgB_6	65	2.897	2.935	22.512	0.099	-0.303	0.996
Cr_4AuB_6	65	2.961	2.945	22.225	0.100	-0.311	0.011
Cr_5B_3	140	5.431	5.431	9.923	0.000	-0.418	0.000
Fe_5BeB_2	140	5.455	5.455	9.914	0.000	-0.292	1.932
Fe_5SiB_2	140	5.509	5.509	10.299	0.003	-0.359	1.731
Mn_5SiB_2	140	5.559	5.559	10.293	0.003	-0.415	1.583
Cr_5BeB_2	140	5.500	5.500	10.002	0.008	-0.313	0.001
Fe_5B_3	140	5.337	5.337	9.959	0.020	-0.308	1.837
Mn_5GeB_2	140	5.624	5.624	10.504	0.020	-0.303	1.731

Fe_5GeB_2	140	5.553	5.553	10.576	0.024	-0.242	1.825
Ni_5SiB_2	140	5.510	5.510	10.110	0.031	-0.367	0.002
Cr_5PB_2	140	5.537	5.537	10.317	0.033	-0.474	0.022
Fe_5PB_2	140	5.444	5.444	10.303	0.033	-0.392	1.705
Mn_5PB_2	140	5.509	5.509	10.287	0.033	-0.480	1.665
Ni_5B_3	140	5.191	5.191	10.296	0.036	-0.253	0.000
Mn_5B_3	140	5.352	5.352	9.990	0.037	-0.391	1.433
Cr_5AsB_2	140	5.603	5.603	10.619	0.038	-0.292	0.098
Ni_5BeB_2	140	5.443	5.443	9.757	0.039	-0.299	0.000
Mn_5BeB_2	140	5.456	5.456	9.916	0.040	-0.309	1.337
Co_5GeB_2	140	5.545	5.545	10.187	0.040	-0.224	0.462
Co_5SiB_2	140	5.484	5.484	9.942	0.042	-0.337	0.394
Fe_5AsB_2	140	5.536	5.536	10.652	0.044	-0.244	1.807
Co_5BeB_2	140	5.451	5.451	9.487	0.045	-0.238	0.680
Ni_5PB_2	140	5.412	5.412	10.334	0.045	-0.356	0.000
Ni_5AsB_2	140	5.514	5.514	10.609	0.054	-0.246	0.001
Ni_5GeB_2	140	5.559	5.559	10.372	0.055	-0.267	0.001
Ni_5GaB_2	140	5.568	5.568	10.336	0.056	-0.273	0.000
Cr_5SiB_2	140	5.586	5.586	10.359	0.061	-0.384	0.023
Fe_5GaB_2	140	5.583	5.583	10.507	0.062	-0.219	1.885
Ni_5LiB_2	140	5.598	5.598	9.565	0.065	-0.179	0.000
Co_5B_3	140	5.169	5.169	10.115	0.070	-0.238	0.549
Co_5AsB_2	140	5.510	5.510	10.283	0.070	-0.212	0.242
Cr_5GeB_2	140	5.623	5.623	10.571	0.070	-0.259	0.009
Mn_5GaB_2	140	5.626	5.626	10.502	0.074	-0.253	1.616
Fe_5AlB_2	140	5.570	5.570	10.436	0.076	-0.241	1.830
Co_5GaB_2	140	5.566	5.566	10.095	0.076	-0.201	0.620
Ni_5ZnB_2	140	5.611	5.611	10.138	0.078	-0.209	0.001
Co_5PB_2	140	5.279	5.279	10.477	0.080	-0.357	0.409
Cr_5CB_2	140	5.364	5.364	9.960	0.083	-0.232	0.003
Ni_5SnB_2	140	5.361	5.361	12.718	0.088	-0.196	0.001
Cr_5CoB_2	140	5.602	5.602	10.063	0.090	-0.192	0.010
Cr_5NiB_2	140	5.611	5.611	10.084	0.090	-0.192	0.000
Ni_5AlB_2	140	5.581	5.581	10.177	0.096	-0.311	0.001
Fe_5ZnB_2	140	5.605	5.605	10.364	0.098	-0.142	1.996
Ni_5InB_2	140	5.356	5.356	12.785	0.098	-0.174	0.000
Co_5ZnB_2	140	5.590	5.590	9.972	0.099	-0.110	0.699
$Fe_3Al_2B_2$	10	5.685	2.833	8.593	0.000	-0.426	0.523
$Fe_3Pt_2B_2$	10	6.221	2.829	8.657	0.091	-0.216	2.059
$Mn_3Al_2B_2$	10	5.745	2.877	8.524	0.003	-0.410	0.420
$Co_3Be_2B_2$	10	5.264	2.587	8.327	0.004	-0.349	0.050
$Co_3Mg_2B_2$	10	6.309	2.806	8.722	0.006	-0.232	0.013
$Fe_3Be_2B_2$	10	5.239	2.705	8.066	0.006	-0.327	0.402
$Ni_3Li_2B_2$	10	6.234	2.721	8.582	0.011	-0.201	0.000
$Co_3Zn_2B_2$	10	6.007	2.743	8.472	0.029	-0.224	0.012
$Co_3Al_2B_2$	10	5.812	2.781	8.555	0.031	-0.437	0.106
$Ni_3Zn_2B_2$	10	6.009	2.768	8.591	0.037	-0.221	0.000

$Mn_3Re_2B_2$	10	6.114	2.775	8.533	0.038	-0.279	0.024
$Fe_3Re_2B_2$	10	6.119	2.737	8.574	0.043	-0.214	0.617
$Mn_3Be_2B_2$	10	5.268	2.826	7.835	0.043	-0.346	0.003
$Cr_3Re_2B_2$	10	5.894	2.920	8.735	0.046	-0.268	0.005
$Ni_3Pt_2B_2$	10	6.056	2.903	8.580	0.048	-0.213	0.002
$Cr_3Tc_2B_2$	10	5.848	2.918	8.702	0.053	-0.264	0.017
$Ni_3Be_2B_2$	10	5.386	2.660	8.271	0.057	-0.283	0.000
Fe_5B_2	10	5.558	2.861	8.483	0.059	-0.210	3.349
$Ni_3Cu_2B_2$	10	5.779	2.804	8.395	0.065	-0.140	0.000
$Co_3Y_2B_2$	10	6.735	3.047	9.550	0.067	-0.279	0.020
$Cr_3Al_2B_2$	10	5.916	2.957	8.384	0.067	-0.305	0.007
$Mn_3Tc_2B_2$	10	6.055	2.780	8.508	0.069	-0.268	0.029
$Fe_3Ir_2B_2$	10	6.082	2.827	8.507	0.071	-0.178	1.851
$Cr_3Os_2B_2$	10	5.976	2.883	8.588	0.071	-0.243	0.004
$Fe_3Tc_2B_2$	10	6.078	2.734	8.532	0.071	-0.211	0.616
Cr_5B_2	10	5.553	2.883	8.553	0.076	-0.245	0.006
$Cr_3Ru_2B_2$	10	5.951	2.880	8.532	0.078	-0.236	0.002
$Fe_3Mo_2B_2$	10	6.285	2.700	8.604	0.078	-0.208	0.046
$Fe_3Zn_2B_2$	10	6.030	2.803	8.425	0.079	-0.167	1.130
$Ni_3Mg_2B_2$	10	6.276	2.870	8.855	0.079	-0.254	0.001
$Ni_3Pd_2B_2$	10	6.002	2.902	8.572	0.083	-0.193	0.000
$Fe_3W_2B_2$	10	6.276	2.703	8.640	0.083	-0.197	0.066
$Fe_3Rh_2B_2$	10	6.023	2.848	8.521	0.084	-0.184	2.233
$Fe_3Co_2B_2$	10	5.589	2.824	8.345	0.084	-0.186	2.794
$Cr_3Mn_2B_2$	10	5.594	2.848	8.356	0.085	-0.249	0.011
$Ni_3Al_2B_2$	10	5.848	2.817	8.626	0.085	-0.370	0.001
$Cr_3Ir_2B_2$	10	6.216	2.816	8.544	0.088	-0.303	0.046
$Mn_3Ir_2B_2$	10	6.090	2.843	8.545	0.089	-0.263	1.391
$Co_3Pt_2B_2$	10	6.134	2.815	8.587	0.091	-0.176	0.663
$Mn_3Co_2B_2$	10	5.534	2.935	8.434	0.091	-0.227	3.310
$Co_3Tc_2B_2$	10	6.087	2.690	8.602	0.092	-0.172	0.281
$Mn_3Os_2B_2$	10	6.077	2.758	8.549	0.095	-0.221	0.211
$Cr_3W_2B_2$	10	5.891	2.969	8.866	0.096	-0.218	0.009
$Cr_3Mo_2B_2$	10	5.861	2.968	8.869	0.096	-0.219	0.007
$Mn_3Si_2B_2$	10	5.398	2.818	8.550	0.096	-0.366	0.016
$Co_3Rh_2B_2$	10	5.987	2.786	8.542	0.097	-0.139	1.060
$Co_3Fe_2B_2$	10	5.629	2.705	8.674	0.098	-0.160	2.565
$Mn_3Rh_2B_2$	10	6.029	2.914	8.477	0.098	-0.242	2.156
$Co_3Re_2B_2$	10	6.106	2.724	8.587	0.098	-0.159	0.032
Co_5B_2	10	5.633	2.629	8.641	0.099	-0.136	1.905
$Co_4Be_3B_2$	123	7.586	7.586	2.586	0.000	-0.395	0.001
$Fe_4Al_3B_2$	123	8.083	8.083	2.791	0.000	-0.411	0.001
$Ni_4Li_3B_2$	123	8.049	8.049	2.734	0.000	-0.203	0.000
$Fe_4Be_3B_2$	123	7.487	7.487	2.697	0.028	-0.287	0.530
Fe_7B_2	123	7.917	7.917	2.875	0.037	-0.171	3.606
$Co_4Zn_3B_2$	123	8.273	8.273	2.679	0.042	-0.162	0.003
$Ni_4Be_3B_2$	123	7.643	7.643	2.649	0.049	-0.320	0.001

$Mn_4V_3B_2$	123	8.067	8.067	2.850	0.063	-0.384	0.198
$Co_4Al_3B_2$	123	8.181	8.181	2.736	0.063	-0.437	0.420
$Mn_4Cr_3B_2$	123	7.948	7.948	2.786	0.072	-0.197	0.250
$Ni_4Zn_3B_2$	123	8.398	8.398	2.687	0.074	-0.187	0.000
$Co_4Fe_3B_2$	123	8.118	8.118	2.640	0.075	-0.145	2.677
$Co_4Mg_3B_2$	123	8.486	8.486	2.791	0.075	-0.112	0.001
$Mn_4Al_3B_2$	123	8.250	8.250	2.823	0.075	-0.306	1.181
Co_7B_2	123	8.146	8.146	2.571	0.075	-0.107	2.106
$Ni_4Cu_3B_2$	123	8.282	8.282	2.614	0.085	-0.111	0.000
Cr_7B_2	123	7.963	7.963	2.890	0.086	-0.163	0.020
$Ni_4Pt_3B_2$	123	8.479	8.479	2.838	0.087	-0.138	0.002
$Fe_4Co_3B_2$	123	7.855	7.855	2.851	0.088	-0.136	3.111
Mn_7B_2	123	7.937	7.937	2.764	0.089	-0.180	1.288
Ni_7B_2	123	7.482	7.482	3.099	0.091	-0.146	0.007

Here, we found that there are two kind of AFM structures (interlayer and intralayer) existing in 212-type MAB phase, as shown in the following Figure.

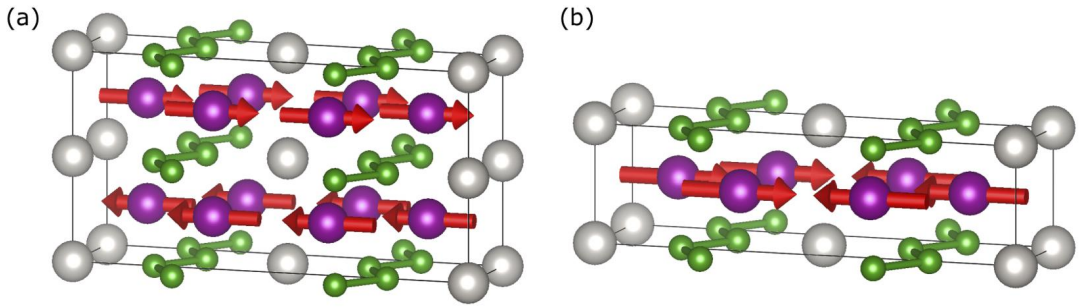


Figure S0: Antiferromagnetic structure of 212-type MAB (a) intralyer: the antiferromagnetic direction exists in two layers; (b) interlayer: the antiferromagnetic direction exsts in single layer. The red arrow presents magnetic direction.

Table S2: The magnetic ground state of stable 212-MAB phases, the stable state of compound is highlighted by blue color.

Compounds	AFM-1(interlayer)	AFM-2 (intralayer)	FM	NM
Co_2AlB_2	-65.88683765	-65.88739406	-65.89295922	-65.88713772
Fe_2BeB_2	-70.64633821	-70.819765	-70.70739773	-70.62268063
Mn_2BeB_2	-74.58037508	-74.580124	-74.58040138	-74.58040414
Fe_2AlB_2	-71.13230669	-71.09418939	-71.22404215	-70.89307686
Mn_2AlB_2	-74.8532619	-74.98085613	-74.88387864	-74.84775026
Cr_2AlB_2	-76.85518352	-76.86093353	-76.85519078	-76.86519042
Cr_2SiB_2	-79.71707885	-79.7170405	-79.71708159	-79.71708801
Cr_2BeB_2	-76.13809946	-76.13763057	-76.13897144	-76.13825155
Cr_2ReB_2	-93.44839084	-93.44947192	-93.4483936	-93.4484053
Fe_2MgB_2	-65.35932093	-65.487255	-65.40892677	-65.22253462
Co_2BeB_2	-65.46095924	-65.46052103	-65.46096941	-65.46096508
Cr_2TcB_2	-89.32741701	-89.32863	-89.32741413	-89.32742021
Mn_2IrB_2	-84.04569417	-83.71480308	-83.93695103	-83.29687721

Fe_2ZnB_2	-64.29285113	-64.3351	-64.4243543	-64.06986852
Cr_2IrB_2	-86.19893738	-86.19928	-86.19893654	-86.19894242
Ni_2LiB_2	-54.27823214	-54.277735	-54.27824987	-54.27825027
Ni_2PtB_2	-62.98827476	-62.98661738	-62.98827225	-62.98825967
Cr_2FeB_2	-84.74945681	-84.74946883	-84.77690838	-84.2112152
Fe_2IrB_2	-79.92897498	-79.74748988	-79.79422707	-79.42577378
Ni_2CuB_2	-57.44034817	-57.43990365	-57.44036768	-57.44036423
Ni_2ZnB_2	-52.56202703	-52.56513507	-52.56201213	-52.56202985
Cr_3B_2	-87.43351322	-87.43396514	-87.43798357	-87.43751847
Fe_2PtB_2	-74.70423426	-74.62013806	-74.59938047	-74.22282814
Cr_2WB_2	-94.30228641	-94.29669283	-94.30228909	-94.30228437
Co_2MgB_2	-60.52900881	-60.52999946	-60.52899462	-60.52898785
Cr_2MoB_2	-90.20335062	-90.19891642	-90.20335146	-90.20335561
Mn_2CoB_2	-79.69489999	-79.35527983	-80.1317531	-78.96686236
Mn_2FeB_2	-81.85999957	-81.93613345	-82.61290818	-81.17754211
Mn_2RhB_2	-80.76741383	-80.42217598	-80.70689175	-80.09631274
Fe_3B_2	-78.20603462	-77.97281357	-78.85399875	-77.44795282
Cr_2RuB_2	-86.69911492	-86.70007	-86.69911455	-86.69911566
Cr_2OsB_2	-90.66864023	-90.668995	-90.66864015	-90.66865212
Mn_2PtB_2	-78.79303215	-78.45515068	-78.58993224	-77.82327552
Fe_2GaB_2	-67.88642365	-67.75845476	-67.92364477	-67.62770421
Ni_2BeB_2	-58.26200763	-58.26036285	-58.26200875	-58.2619976
Ni_2PdB_2	-61.07432402	-61.0729872	-61.07429402	-61.0742564
Mn_2SiB_2	-77.09190803	-77.26047303	-77.09190222	-77.09192171
Mn_2ReB_2	-90.6081387	-90.7066324	-90.74289642	-90.60827896
Cr_2RhB_2	-82.79945631	-82.799195	-82.79944198	-82.79945691
Cr_2VB_2	-87.46225672	-87.46198938	-87.46225834	-87.46226062
Ni_2AuB_2	-56.23165208	-56.22294795	-56.2316556	-56.23166659
Cr_2CoB_2	-82.01197093	-82.01197657	-82.16236059	-81.79494385
Cr_2NiB_2	-79.102105	-79.10211	-79.10212617	-79.10191962
Co_2PtB_2	-69.63778263	-69.65924301	-69.63859647	-69.63785776
Cr_2MnB_2	-86.38774777	-86.389125	-86.28089684	-86.28099021
Fe_2ReB_2	-86.89963676	-86.69655193	-86.90407834	-86.44485698
Fe_2NiB_2	-73.2030513	-73.05261169	-73.10598643	-72.71702075
Mn_2ScB_2	-79.49799809	-79.47839842	-79.51282108	-79.48712127
Cr_2PtB_2	-80.49575377	-80.496715	-80.49590885	-80.49575249
Fe_2RhB_2	-76.83798018	-76.64636958	-76.77048282	-76.27060534
Mn_2RuB_2	-84.07773177	-84.02944525	-84.24640701	-83.72690734
Mn_2NiB_2	-77.03817855	-76.59623733	-76.85380813	-76.52395167
Mn_2WB_2	-92.01502458	-92.015225	-92.01504492	-92.01504981
Mn_2TcB_2	-86.50318745	-86.60635618	-86.64415689	-86.50455953

Here, we list three representative Mn-based M_2AB_2 phases: Mn_2AlB_2 (reported), Mn_2PtB_2 (calculated large MAE) and Mn_2BeB_2 (stable on the convex hull) as an example. Table S3 summarizes the lattice parameters, total energies and magnetization of Mn_2AlB_2, Mn_2PtB_2 and Mn_2BeB_2 with different magnetic configurations. The calculated lattice parameters and on-site atomic

magnetic moment of Mn agree well with experiments. The relaxed lattice parameters of M_2AB_2 not only vary with element A but also depend on the spin configuration. For Mn_2AlB_2, b and c increase when the spin configuration changes from NM→FM→AFM, which is agree with Ke's calculated results[9]. And the E_{tot} of Mn_2AlB_2 with AFM is lowest, which indicates the magnetic ground state of it is AFM. This result matched with above mentioned studies. For Mn_2PtB_2, the magnetic ground state is confirmed as AFM. For Mn_2BeB_2, the magnetic ground state is NM which can be proved by total energy and magnetization results (0.008 μB per Mn in FM).

Table S3: Lattice parameters (Å), total energy E_{tot} (eV/at.) and on-site atomic magnetic moment of Mn, M_{Mn} (μB) in Mn_2AB_2 with A = Al, Pt and Be.

Compounds	Magnetism	a	b	c	E_{tot}	M_{Mn}
Mn_2AlB_2	AFM	2.893	11.113	2.835	-7.498	0.765
	FM	2.894	11.080	2.831	-7.488	0.410
	NM	2.895	11.066	2.822	-7.484	0
CAL[9]	AFM	2.887	11.109	2.830		0.750
	FM	2.892	11.056	2.826		0.420
	NM	2.890	11.050	2.817		0
EXP[10]	AFM	2.923	11.072	2.898		0.712
EXP[11]	AFM	2.930	11.019	2.898		0.690
EXP[12]	FM	2.936	11.120	2.912		0.410
Mn_2PtB_2	AFM	3.008	11.106	3.066	-7.879	2.664
	FM	2.982	11.160	3.025	-7.848	2.310
	NM	2.877	11.506	2.915	-7.778	0
Mn_2BeB_2	AFM	2.843	9.972	2.818	-7.457	0.002
	FM	2.846	9.969	2.815	-7.457	0.008
	NM	2.844	9.965	2.813	-7.458	0

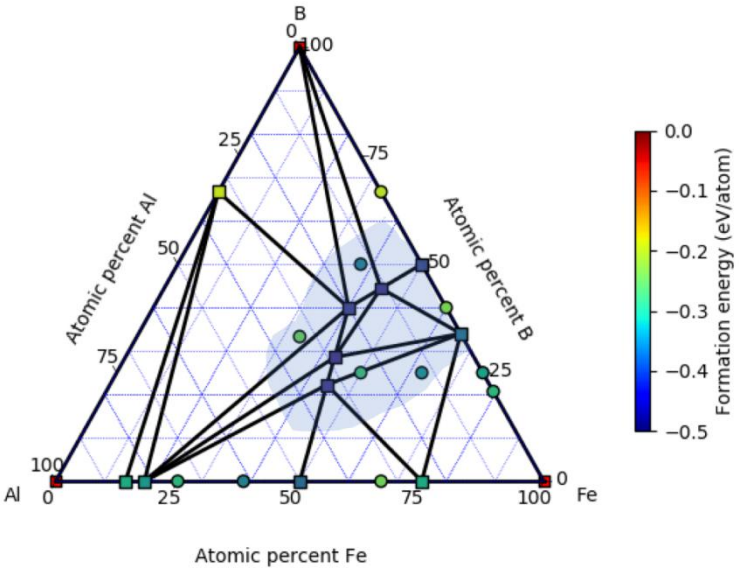


Figure S1: Calculated phase diagram of the Fe-Al-B system based on formation energies calculated with VASP. The color scale gives the formation energies in eV per atom. Black lines connect the convex hull. Square means stable compounds and circle means unstable compounds. Dark shadow indicates the high potential stable area.

It is well known that the melting temperature of boron (2573K) is much higher than those of the most other constituent elements considered, thus it is challenging to obtain binary and ternary borides via direct chemical reactions between pure elements. Taking the Fe-Al-B system as an example, the phase diagram is shown in Fig. S1, where the relative stability of all the known and predicted phases is visualized based on the calculated ΔE_f and ΔE_h . Interestingly, it results in a composition range within 50 at. % < Al at. % < 100 at. %, 10 at. % < B at. % < 60 at. %, and 30 at. % < Fe at. % < 70 at.% collecting the stable phases, as highlighted by the shaded region in Fig. S1. We suspect that there might exist more stable structures in the composition range, entailing further exploration. Moreover, it can be seen in Fig.S1, there are some stable compounds that are experimentally synthesized and present predicted appearing in the dark shadow area. We can suspect that more unreported stable compounds might be in the area, and people who are interested can explore them in the future. Furthermore, based on the phase diagram, we would propose two possible chemical reactions to synthesize the predicted Fe_4AlB_4 as follows:

$$Fe_2AlB_2 + 2FeB \rightarrow Fe_4AlB_4$$

$$Al + 4FeB \rightarrow Fe_4AlB_4$$

It is worthy pointing out that such suggestions are based on our calculations at 0 K, where more dedicated assessment of ternary phase diagrams based on the CALPHAD method will give us more insights, saved for future investigations.

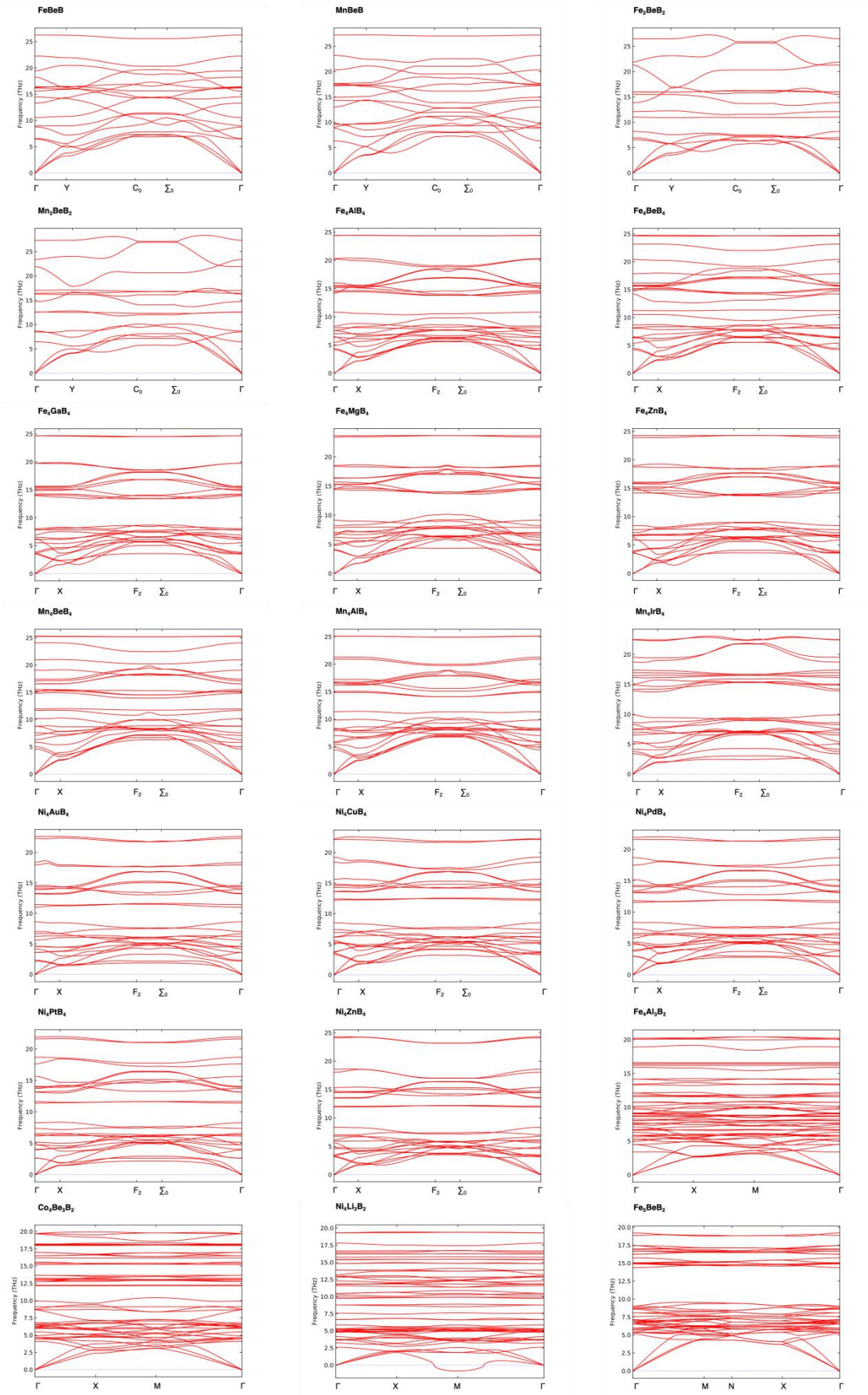


Figure S2: Phonon bands of unreported MAB and Non-MAB phases.

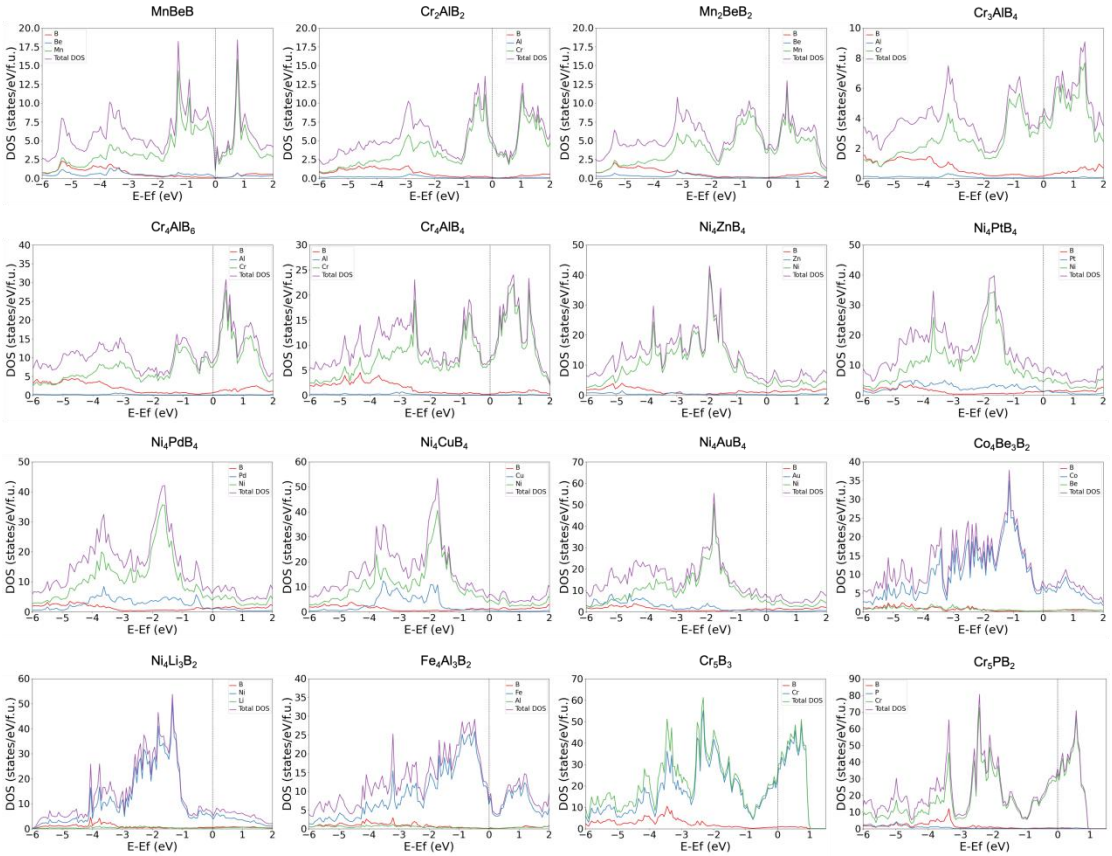


Figure S3: Density of states of predicted non-magnetic MAB phases.

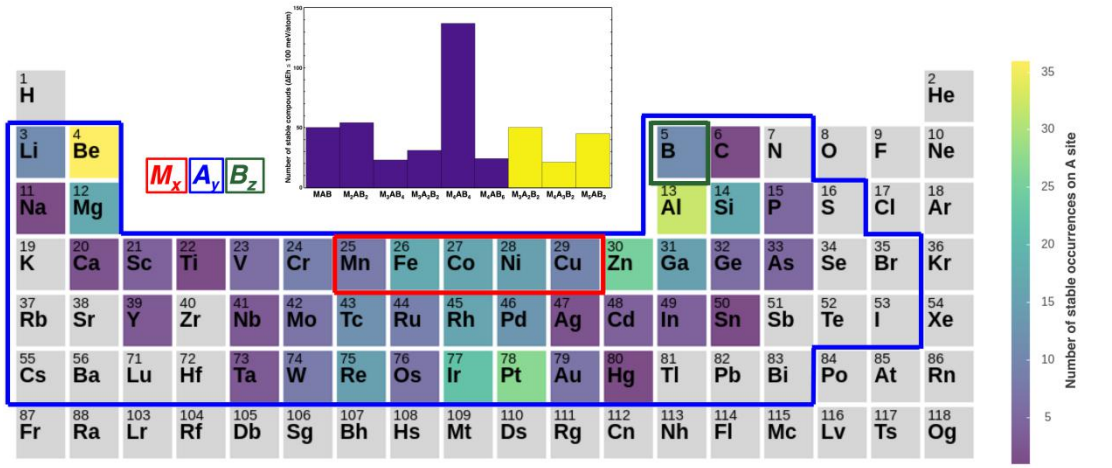


Figure S4: Elements are color-coded as a function of the number of stable compounds with the respective element on the **A** sites. (Above) Histogram representation of number of stable compounds of different systems calculated in this work, purple bar means MAB phases and yellow bar means Non-MAB phases.

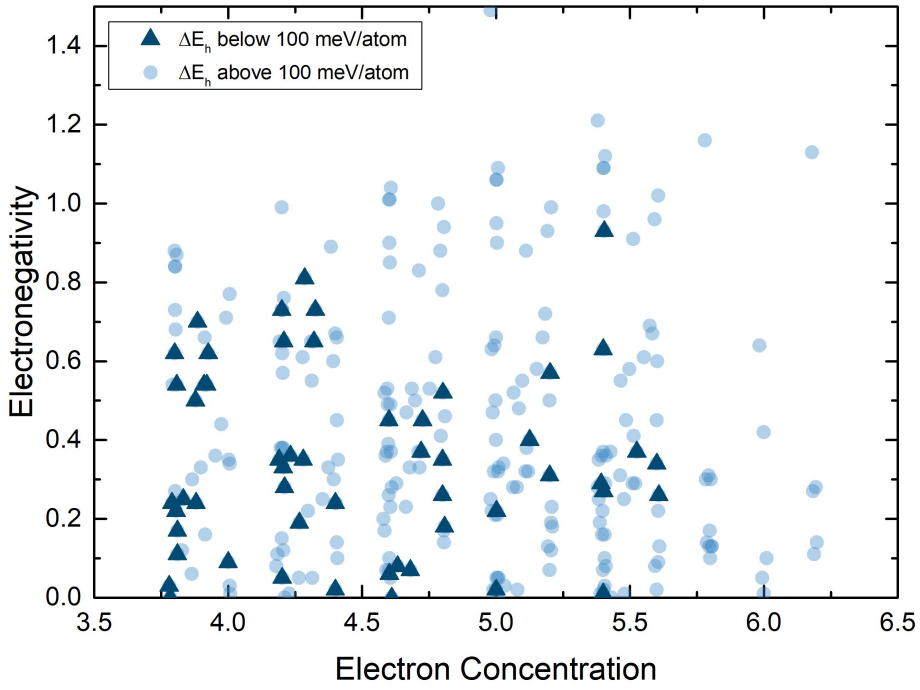


Figure S5: The stability map of 212-MAB phases according to the feature factors electronegativity and electron concentration (circle symbols represent unstable phases in the present work; triangle symbols represent possible stable phases with convex hull distance below 100 meV/atom in the present).

Table S4: The valence/itinerant electron values adopted in this work.

Elements(M)	Valence Electrons	Elements(A)	Itinerant Electrons	Elements(B)	Valence Electrons
Cr	6	Li	1.02	B	3
Co	9	Na	1.01		
Ni	10	K	1.01		
Fe	8	Rb	1.01		
Mn	7	Cs	1.04		
B	3	Be	2		
Sc	3	Mg	2.01		
Ti	4	Ca	1.56		
Zr	4	Sr	1.96		
Hf	4	Ba	2.03		
V	5	Sc	1.33		
Mo	6	Y	1.87		
W	6	Ti	1.14		
Tc	7	Zr	1.49		
Ru	8	Hf	1.76		
Rh	9	V	0.9		
		Nb	1.32		
		Ta	1.57		

Cr	0.92
Mo	1.39
W	1.43
Mn	1.05
Tc	0.95
Re	1.4
Fe	1.05
Ru	1.04
Os	1.55
Co	1.03
Rh	1
Ir	1.6
Ni	1.16
Pd	0.96
Pt	1.63
Cu	1
Ag	1.01
Au	1
Zn	2.04
Cd	2.03
Hg	2.03
B	2.98
Al	3.01
Ga	3
In	3.03
Tl	3.03
C	3.92
Si	4
Ge	4.05
Sn	3.97
Pb	4
N	4.9
P	4.97
As	4.92
Sb	4.99
Bi	4.94

Table S5: The atomic radius values adopted in this work.

Elements(M)	Atomic Radius	Elements(A)	Atomic Radius	Elements(B)	Atomic Radius
Cr	1.3	Li	1.3	B	0.84
Co	1.18	Na	1.6		
Ni	1.17	K	2		
Fe	1.24	Rb	2.15		
Mn	1.29	Cs	2.38		
Sc	1.59	Be	0.99		
Ti	1.48	Mg	1.4		
Zr	1.64	Ca	1.74		
Hf	1.64	Sr	1.9		
V	1.44	Ba	2.06		
Mo	1.46	Sc	2.15		
W	1.5	Y	1.76		
Tc	1.38	Ti	2.11		
Ru	1.36	Zr	1.64		
Rh	1.34	Hf	1.64		
		V	1.44		
		Nb	1.56		
		Ta	1.58		
		Cr	1.3		
		Mo	1.46		
		W	1.5		
		Mn	1.29		
		Tc	1.38		
		Re	1.41		
		Fe	1.24		
		Ru	1.36		
		Os	1.36		
		Co	1.18		
		Rh	1.34		
		Ir	1.32		
		Ni	1.17		
		Pd	1.3		
		Pt	1.3		
		Cu	1.22		
		Ag	1.36		
		Au	1.3		
		Zn	1.2		

Cd	1.4
Hg	1.32
B	0.84
Al	1.24
Ga	1.23
In	1.42
Tl	1.44
C	0.75
Si	1.14
Ge	1.2
Sn	1.4
Pb	1.45
N	0.71
P	1.09
As	1.2
Sb	1.4
Bi	1.5

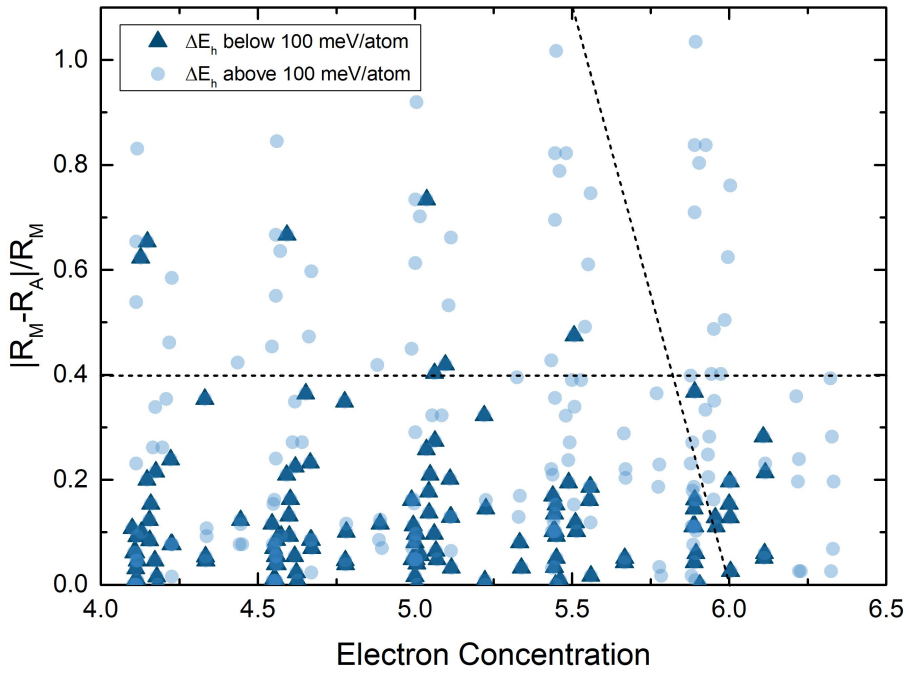


Figure S6: The stability map of 414-MAB phases (circle symbols represent unstable phases in the present work; triangle symbols represent possible stable phases with convex hull distance below 100 meV/atom in the present).

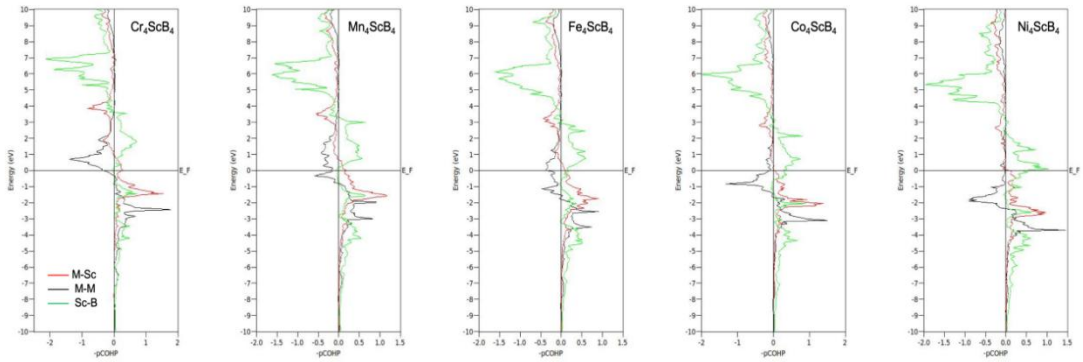


Figure S7: COHP of M_4ScB_4 (where M are Cr, Mn, Fe, Co and Ni).

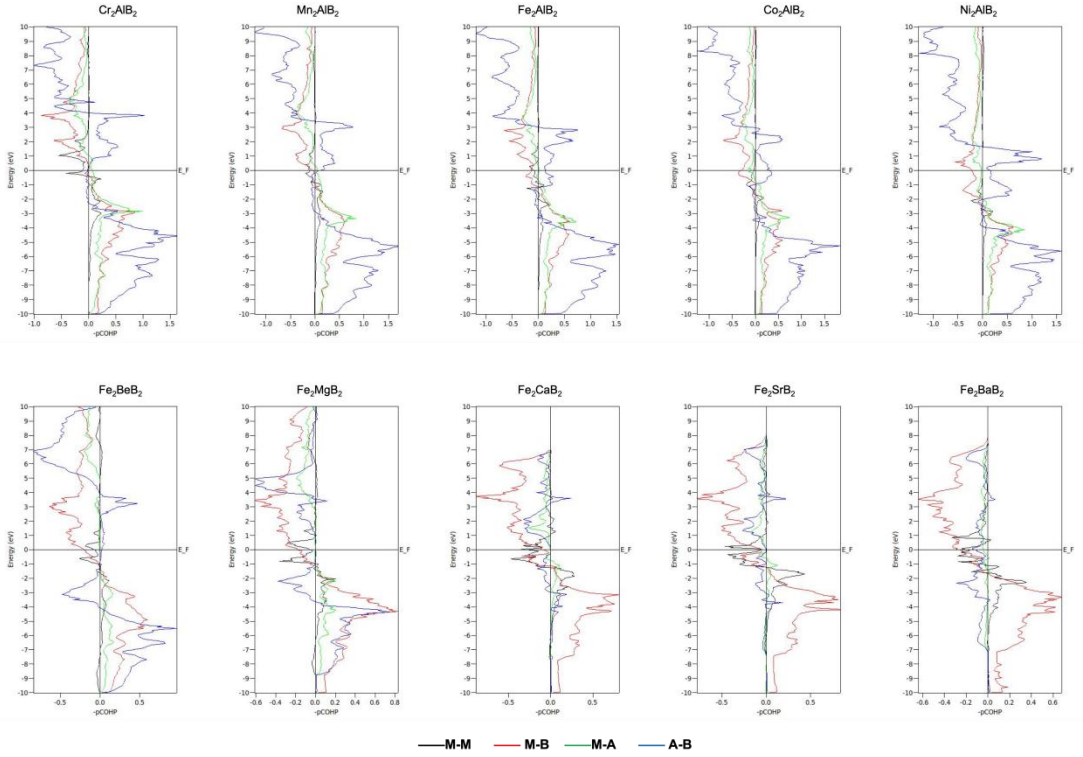


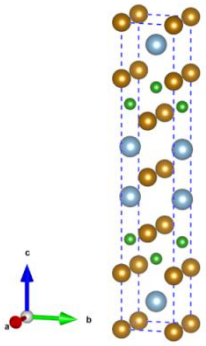
Figure S8: COHP of (upper) M_2AlB_2 (where M are Cr, Mn, Fe, Co and Ni) and (bottom) Fe_2AB_2 (where A are Be, Mg, Ca, Sr and Ba).

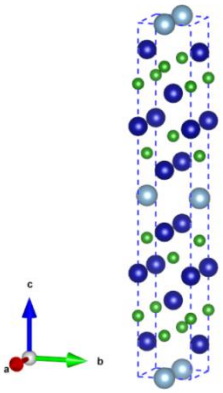
Table S6: The novel MAB and Non-MAB phases with $|K_{i-j}| > 1$ MJ/m^3.

Compounds	Space Group	MAE (MJ/m^3)			Magnetic moment	Magnetic density	Crystal Structure
		$K_{001-100}$	$K_{001-010}$	$k_{010-100}$	(μB/f.u)	(emu/cm^3)	
CoCrB	63	-1.884	-1.884	0.000	5.514	462.330	
Fe_2B	63	2.230	1.865	0.365	16.310	1352.627	
FeIrB	63	-2.627	-1.258	-1.369	5.805	436.918	
FeNiB	63	0.834	-0.654	1.488	7.909	672.329	
FePtB	63	-3.421	7.225	-10.646	7.550	542.026	
FeRhB	63	2.528	0.309	2.220	7.409	561.255	
FeZnB	63	0.300	-1.997	2.297	4.602	351.641	
CoMnB	63	1.292	1.743	-0.451	14.160	1174.969	
MnIrB	63	4.135	8.049	-3.914	7.967	584.998	
MnNiB	63	1.245	1.767	-0.521	9.792	811.435	
MnPdB	63	0.790	1.592	-0.802	9.739	688.735	
MnPtB	63	9.126	11.969	-2.843	9.763	683.691	
MnRhB	63	2.863	4.016	-1.153	8.943	661.411	
Co_2PtB_2	65	-2.412	-3.102	0.690	1.228	119.739	
Fe_2AlB_2	65	-1.110	0.031	-1.141	5.319	538.463	
Fe_2BeB_2	65	-1.917	-0.047	-1.869	3.043	355.462	
Fe_3B_2	65	0.245	1.666	-1.421	11.596	1209.796	
Fe_2GaB_2	65	-1.122	0.096	-1.218	5.439	541.505	
Fe_2IrB_2	65	5.056	7.245	-2.190	6.736	661.715	
Fe_2MgB_2	65	-2.438	0.470	-2.908	3.640	340.502	
Fe_2NiB_2	65	-2.443	0.010	-2.453	6.147	652.780	
Fe_2PtB_2	65	-3.924	1.211	-5.135	6.392	611.442	
Fe_2ReB_2	65	-4.958	-8.999	4.042	5.541	548.443	
Fe_2RhB_2	65	0.619	1.838	-1.219	7.597	748.423	
Fe_2ZnB_2	65	-1.919	0.636	-2.555	4.183	419.456	
Mn_2CoB_2	65	1.981	1.756	0.225	10.868	1124.732	
Mn_2FeB_2	65	1.446	1.565	-0.119	11.320	1165.646	
Mn_2IrB_2	65	1.803	-2.559	4.362	8.270	789.006	
Mn_2NiB_2	65	1.407	0.101	1.305	8.382	869.483	
Mn_2PtB_2	65	20.271	20.271	0.000	9.414	869.433	
Mn_2ReB_2	65	-8.247	-2.133	-6.114	6.589	635.442	
Mn_2RhB_2	65	1.609	1.609	0.000	8.678	833.085	
Mn_2TcB_2	65	-1.424	-0.811	-0.613	6.417	622.289	
Fe_3BeB_4	47	-1.672	0	1.672	3.594	532.907	
Fe_3IrB_4	47	1.021	-5.786	-6.807	4.307	575.519	
Fe_3MgB_4	47	-1.054	-0.099	0.954	3.778	481.034	
Fe_3PtB_4	47	-1.921	7.214	9.134	4.350	570.827	
Fe_3ZnB_4	47	-1.324	-0.056	1.269	4.093	550.002	
Mn_3IrB_4	47	0.965	-3.888	-4.853	6.657	860.514	
Mn_3PtB_4	47	-3.324	-8.892	-5.568	6.773	857.270	
Mn_4AlB_6	65	-1.123	-1.123	0.000	8.566	436.975	
Mn_4GaB_6	65	-1.004	0.010	-1.014	9.221	465.665	
Mn_4IrB_6	65	3.816	3.768	0.047	15.786	779.608	
Mn_4PtB_6	65	6.258	4.738	1.519	16.260	790.929	
Mn_4ZnB_6	65	-0.892	0.149	-1.041	8.680	437.764	

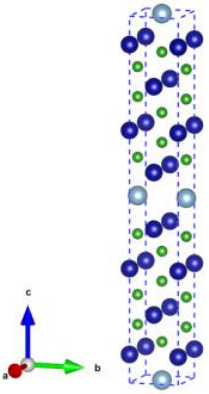
$Co_3Pt_2B_2$	65	-2.429	-1.745	-0.685	2.864	180.640

$Co_3Pt_2B_2$	65	-2.429	-1.745	-0.685	2.864	180.640
$Fe_3Al_2B_2$	65	-1.420	0.066	-1.487	4.410	295.705
$Fe_3Be_2B_2$	65	-2.012	-2.012	0.000	5.274	421.961
$Fe_3Co_2B_2$	65	-0.159	1.158	-1.317	18.609	1291.798
Fe_5B_2	65	0.774	1.528	-0.754	21.114	1448.993
$Fe_3Ir_2B_2$	65	8.212	6.782	1.430	12.651	792.503
$Fe_3Rh_2B_2$	65	0.131	1.027	-0.896	13.009	845.070
$Fe_3Zn_2B_2$	65	-3.001	-1.361	-1.640	8.907	571.752
$Mn_3Al_2B_2$	65	-0.197	0.950	-1.148	5.771	372.455
$Mn_3Co_2B_2$	65	1.788	1.666	0.122	19.929	1348.995
$Mn_3Ir_2B_2$	65	-10.171	-7.582	-2.589	16.385	992.463
$Mn_3Pt_2B_2$	65	6.415	4.767	1.648	16.765	972.699
Mn_4PtB_4	71	11.948	-1.550	13.498	16.588	919.450
Fe_4OsB_4	71	4.573	-3.677	8.251	11.281	664.139
Fe_4IrB_4	71	7.789	4.471	3.318	12.238	714.201
Fe_4ReB_4	71	-7.417	-1.875	-5.543	11.486	672.519
Fe_4TaB_4	71	1.785	6.706	-4.921	9.930	560.842
Co_4IrB_4	71	-6.061	-3.840	-2.221	0.129	7.657
Mn_4IrB_4	71	-5.757	-3.647	-2.109	16.027	905.022
Mn_4ReB_4	71	0.411	4.484	-4.073	13.815	785.087
Mn_4OsB_4	71	-3.608	-0.049	-3.560	14.938	850.492
Fe_4AuB_4	71	0.570	3.051	-2.481	11.687	654.290
Fe_4WB_4	71	2.543	2.647	-0.103	11.096	641.107
Fe_4AgB_4	71	0.927	2.465	-1.538	11.353	633.953
Fe_4PdB_4	71	0.098	2.453	-2.355	12.053	695.196
Fe_4TcB_4	71	-0.746	1.474	-2.220	11.881	695.087
Fe_4ZnB_4	71	0.311	2.213	-1.902	10.608	624.239
Fe_4CuB_4	71	0.375	2.059	-1.684	11.498	690.269
Fe_4NbB_4	71	0.528	2.038	-1.511	10.379	581.800
Fe_4CdB_4	71	1.125	2.030	-0.905	11.340	619.058
Fe_4RuB_4	71	1.976	1.591	0.385	12.221	717.097
Fe_4B_5	71	-0.741	1.231	-1.973	8.371	556.735
Fe_4MgB_4	71	1.086	1.942	-0.856	11.129	623.970
Fe_4MoB_4	71	0.857	1.809	-0.952	11.036	637.712
Co_4FeB_4	71	1.379	-0.420	1.799	6.020	370.788
Fe_4NiB_4	71	0.243	1.776	-1.533	11.622	711.144
Fe_4LiB_4	71	0.710	1.774	-1.064	11.077	645.627
Mn_4CoB_4	71	1.568	-0.188	1.756	17.969	1062.915
Mn_4AuB_4	71	1.749	0.153	1.596	14.244	775.212
Fe_4VB_4	71	-0.111	1.511	-1.622	12.732	750.986
Fe_4CrB_4	71	0.151	1.591	-1.439	14.488	871.794
Fe_4RhB_4	71	1.582	1.526	0.056	12.909	752.215
Co_4MnB_4	71	1.562	0.209	1.353	7.677	460.624

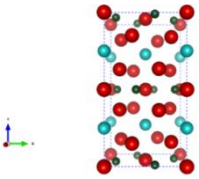




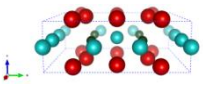
Fe_4InB_4	71	0.156	1.560	-1.404	10.395	569.677
Fe_5B_4	71	1.017	1.497	-0.480	17.079	1032.848
Mn_4FeB_4	71	1.491	0.226	1.265	17.898	1059.765
Mn_4PdB_4	71	1.202	-0.237	1.439	16.137	897.1075
Fe_4BeB_4	71	-0.182	1.253	-1.435	8.133	523.344
Fe_4MnB_4	71	0.982	1.326	-0.344	17.299	1036.999
Fe_4GaB_4	71	0.170	1.235	-1.065	10.306	607.816
Fe_4CoB_4	71	0.792	1.209	-0.416	15.379	934.922
Fe_4GeB_4	71	0.029	1.182	-1.153	10.975	640.336
Fe_4AlB_4	71	0.063	1.153	-1.090	10.166	604.617
Mn_4VB_4	71	0.513	-0.616	1.130	9.149	535.797
Mn_5B_4	71	1.090	0.352	0.738	17.017	999.941
Mn_4RhB_4	71	0.335	-0.685	1.019	16.572	935.596
Fe_4YB_4	71	0.575	1.014	-0.438	9.945	513.817



Co_5BeB_2	140	1.810	1.810	0	13.608	447.646
Co_5ZnB_2	140	1.689	1.689	0	13.972	415.771
Fe_5ZnB_2	140	1.889	1.889	0	39.919	1136.984



$Co_3Fe_2B_2$	10	1.072	0.000	-1.072	15.387	1080.426
$Co_3Pt_2B_2$	10	4.492	1.922	-2.570	3.979	249.501
$Fe_3Ir_2B_2$	10	3.395	7.741	4.346	11.105	706.387
$Fe_3Pt_2B_2$	10	4.931	2.545	-2.386	12.353	755.315
$Fe_3Rh_2B_2$	10	-0.115	1.043	1.157	13.396	852.345
$Fe_3Zn_2B_2$	10	-1.503	-0.368	1.135	6.781	443.081
$Mn_3Co_2B_2$	10	1.210	0.628	-0.582	19.858	1342.777
$Mn_3Ir_2B_2$	10	5.313	0.000	-5.313	8.346	525.648
$Mn_3Rh_2B_2$	10	-0.846	-1.380	-0.533	12.938	807.529



$Co_4Fe_3B_2$	123	1.156	1.156	0.000	21.417	1141.436

Table S7: The novel MAB and Non-MAB phases with uniaxial MAE.

Compounds	Space Group		MAE (MJ/m^3)		
			$K_{001-100}$	$K_{001-010}$	$k_{010-100}$
CoCrB	63	Out-of-plane	-1.884	-1.884	0.000
FeIrB	63	Out-of-plane	-2.627	-1.258	-1.369
MnPtB	63	In-plane	9.126	11.969	-2.843
MnRhB	63	In-plane	2.863	4.016	-1.153
Fe_2B	63	In-plane	2.230	1.865	0.365
CoMnB	63	In-plane	1.292	1.743	-0.451

MnNiB	63	In-plane	1.245	1.767	-0.521
Co_2PtB_2	65	Out-of-plane	-2.412	-3.102	0.690
Fe_2ReB_2	65	Out-of-plane	-4.958	-8.999	4.042
Mn_2CoB_2	65	In-plane	1.981	1.756	0.225
Mn_2RhB_2	65	In-plane	1.609	1.609	0.000
Mn_2FeB_2	65	In-plane	1.446	1.565	-0.119
Cr_2CoB_2	65	In-plane	0.697	0.697	0.000
Cr_2FeB_2	65	In-plane	0.446	0.446	0.000
$Ni_3Pt_2B_2$	65	Out-of-plane	-0.467	-0.467	0.000
$Fe_3Be_2B_2$	65	Out-of-plane	-2.012	-2.012	0.000
$Co_3Pt_2B_2$	65	Out-of-plane	-2.429	-1.745	-0.685
$Fe_3Zn_2B_2$	65	Out-of-plane	-3.001	-1.361	-1.640
$Mn_3Ir_2B_2$	65	Out-of-plane	-10.171	-7.582	-2.589
$Fe_3Ir_2B_2$	65	In-plane	8.212	6.782	1.430
$Mn_3Pt_2B_2$	65	In-plane	6.415	4.767	1.648
$Mn_3Co_2B_2$	65	In-plane	1.788	1.666	0.122
Fe_3MgB_4	47	Out-of-plane	-1.054	-0.099	0.954
Fe_4PtB_4	71	Out-of-plane	-0.442	-0.557	0.115
Ni_4CoB_4	71	Out-of-plane	-0.502	-0.801	0.299
Fe_4ReB_4	71	Out-of-plane	-7.417	-5.543	-1.875
Mn_4PtB_4	71	In-plane	11.948	13.498	-1.550
Mn_4AuB_4	71	In-plane	1.749	1.596	0.153
Mn_4CoB_4	71	In-plane	1.568	1.756	-0.188
Co_4MnB_4	71	In-plane	1.562	1.353	0.209
Mn_4FeB_4	71	In-plane	1.491	1.265	0.226
Co_4FeB_4	71	In-plane	1.379	1.799	-0.420
Mn_4PdB_4	71	In-plane	1.202	1.439	-0.237
Mn_4PB_4	71	In-plane	0.975	0.924	0.051
Co_4CrB_4	71	In-plane	0.890	1.015	-0.125
Mn_4GeB_4	71	In-plane	0.788	0.742	0.046
Mn_4NiB_4	71	In-plane	0.769	0.928	-0.159
Mn_4TiB_4	71	In-plane	0.731	0.590	0.141
Mn_4SiB_4	71	In-plane	0.679	0.694	-0.015
Mn_4AlB_4	71	In-plane	0.556	0.500	0.055
Mn_4NbB_4	71	In-plane	0.482	0.491	-0.009
Mn_4GaB_4	71	In-plane	0.461	0.609	-0.148
Mn_4HgB_4	71	In-plane	0.429	0.510	-0.081
Mn_4ZrB_4	71	In-plane	0.415	0.256	0.158
Mn_4MgB_6	65	Out-of-plane	-0.768	-0.768	0.000
Mn_4AlB_6	65	Out-of-plane	-1.123	-1.123	0.000
Fe_4BeB_6	65	Out-of-plane	-0.745	-0.745	0.000
Mn_4IrB_6	65	In-plane	3.816	3.768	0.047
Mn_4PtB_6	65	In-plane	6.258	4.738	1.519
Fe_5PB_2	140	Out-of-plane	-0.634	-0.634	0.000
Co_5AsB_2	140	In-plane	0.486	0.486	0.000
Fe_5AlB_2	140	In-plane	0.475	0.475	0.000
Mn_5BeB_2	140	In-plane	0.559	0.559	0.000
Co_5PB_2	140	In-plane	0.665	0.665	0.000

Co_5GaB_2	140	In-plane	0.642	0.642	0.000
Co_5B_3	140	In-plane	0.762	0.762	0.000
Co_5GeB_2	140	In-plane	0.755	0.755	0.000
Mn_5GaB_2	140	In-plane	0.783	0.783	0.000
Fe_5BeB_2	140	In-plane	0.898	0.898	0.000
Co_5BeB_2	140	In-plane	1.810	1.810	0.000
Co_5ZnB_2	140	In-plane	1.689	1.689	0.000
Fe_5ZnB_2	140	In-plane	1.889	1.889	0.000
$Fe_3Tc_2B_2$	10	Out-of-plane	-0.581	0.162	0.742
Co_5B_2	10	Out-of-plane	-0.595	-0.684	-0.089
$Mn_3Rh_2B_2$	10	Out-of-plane	-0.846	-1.380	-0.533
$Fe_3Al_2B_2$	10	Out-of-plane	-0.971	0.025	0.996
$Fe_3Zn_2B_2$	10	Out-of-plane	-1.503	-0.368	1.135
$Fe_3Pt_2B_2$	10	In-plane	4.931	2.545	-2.386
$Co_3Pt_2B_2$	10	In-plane	4.492	1.922	-2.570
$Fe_3Ir_2B_2$	10	In-plane	3.395	7.741	4.346
$Mn_3Co_2B_2$	10	In-plane	1.210	0.628	-0.582
Fe_5B_2	10	In-plane	0.408	0.482	0.074
Fe_7B_2	123	Out-of-plane	-0.681	-0.681	0.000
$Co_4Fe_3B_2$	123	In-plane	1.156	1.156	0.000

Table S8: The MAE and E_{SOC} for the FeXB (where X are Ni, Pd, and Pt).

		FeNiB	**FePdB**	**FePtB**
	[100]-[001]	-0.028	0.002	0.579
MAE (meV/f.u.)	[100]-[010]	-0.128	0.181	2.106
	[001]-[010]	-0.100	0.179	1.526
	[100]	-10.660	-10.443	-6.934
E_{SOC} (Fe) (meV/atom)	[001]	-10.391	-10.230	-6.787
	[010]	-10.167	-10.026	-7.424
	[100]-[001]	-0.269	-0.213	-0.147
ΔE_{SOC} (Fe) (meV/atom)	[100]-[010]	-0.492	-0.417	0.490
	[001]-[010]	-0.223	-0.204	0.637
	[100]	-18.892	-338.919	-4223.153
E_{SOC} (X) (meV/atom)	[001]	-18.918	-339.122	-4224.317
	[010]	-18.799	-339.621	-4225.756
	[100]-[001]	0.026	0.203	1.164
ΔE_{SOC} (X) (meV/atom)	[100]-[010]	-0.093	0.702	2.603
	[001]-[010]	-0.119	0.499	1.439
	[100]	-29.569	-349.380	-4230.111
E_{SOC} (FeXB) (meV/f.u.)	[001]	-29.326	-349.369	-4231.125
	[010]	-28.983	-349.665	-4233.204
	[100]-[001]	-0.243	-0.011	1.014
ΔE_{SOC} (FeXB) (meV/f.u.)	[100]-[010]	-0.586	0.284	3.092
	[001]-[010]	-0.343	0.296	2.078

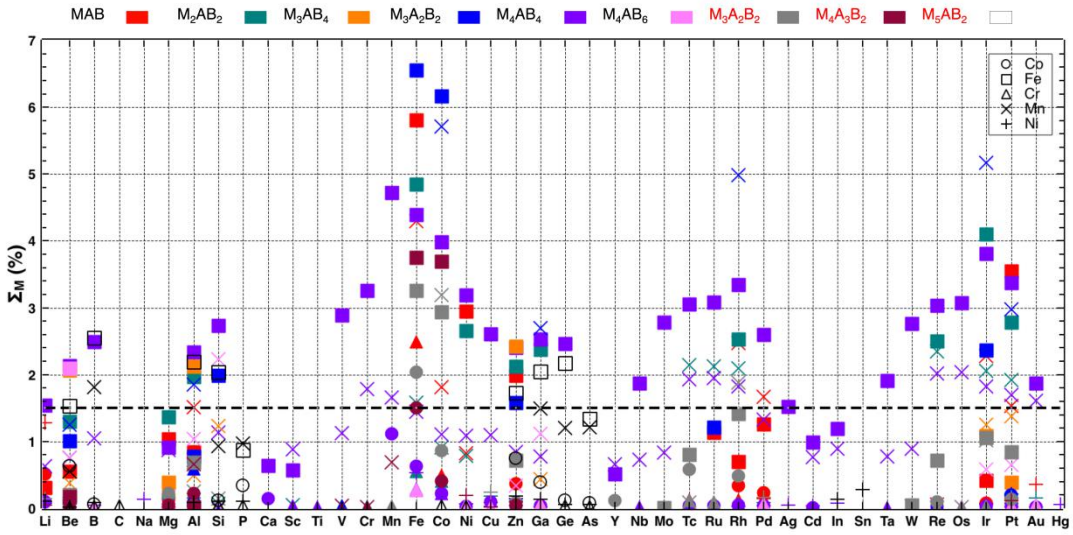


Figure S9: The calculated Σ_M for all 434 compounds with convex hull tolerance of ΔE_h meV/atom. Different structures were presented with different color in the square above the figure. Magnetic elements were shown in different symbols. The black bold dash line indicates Σ_M = 1.5 %; candidates above this line are predicted to show large ΔS_M values.

Table S9: The novel MAB and Non-MAB phases with larger magnetic deformation Σ_M (>1.5%).

Compounds	Space group	Σ_M (%)	Magnetic density (emu/cm^3)	Convexhull (meV/atom)	Formation energy (eV/atom)
CrFeB	63	2.494	739.926	40.600	-0.310
Fe_2B	63	5.811	1352.627	68.300	-0.244
FeNiB	63	2.946	672.329	96.500	-0.209
FePtB	63	3.548	542.026	62.500	-0.242
FeZnB	63	1.984	351.641	44.600	-0.206
MnAlB	63	1.514	301.458	66.300	-0.329
CoMnB	63	1.815	1174.969	83.700	-0.255
FeMnB	63	4.300	1277.649	56.900	-0.301
MnIrB	63	2.277	584.998	61.800	-0.271
MnPdB	63	1.669	688.735	90.200	-0.296
MnPtB	63	1.531	683.691	73.000	-0.340
MnRhB	63	2.469	661.411	89.400	-0.273
Fe_2AlB_2	65	1.964	538.463	0.000	-0.400
Fe_3B_2	65	4.844	1209.796	73.500	-0.265
Fe_2GaB_2	65	2.376	541.505	77.700	-0.237
Fe_2IrB_2	65	4.105	661.715	64.900	-0.236
Fe_2NiB_2	65	2.656	652.780	90.300	-0.244
Fe_2PtB_2	65	2.780	611.442	67.000	-0.267
Fe_2ReB_2	65	2.502	548.443	88.400	-0.232
Fe_2RhB_2	65	2.527	748.423	94.600	-0.248
Fe_2ZnB_2	65	2.122	419.456	53.500	-0.248
Mn_2FeB_2	65	1.577	1165.646	70.900	-0.344

Mn_2IrB_2	65	2.060	789.006	45.900	-0.354
Mn_2PtB_2	65	1.920	869.433	77.100	-0.384
Mn_2ReB_2	65	2.346	635.442	80.700	-0.319
Mn_2RhB_2	65	2.093	833.085	71.100	-0.346
Mn_2RuB_2	65	2.123	700.555	95.800	-0.304
Mn_2TcB_2	65	2.146	622.289	99.151	-0.320
Fe_3AlB_4	47	2.119	513.407	0.000	-0.445
Fe_3BeB_4	47	2.068	532.907	46.900	-0.240
Fe_3ZnB_4	47	2.423	550.002	87.600	-0.194
Fe_4BeB_6	65	2.096	543.420	92.700	-0.184
Mn_4SiB_6	65	2.227	549.679	93.600	-0.307
Fe_5AlB_2	140	2.196	1048.528	75.700	-0.241
Fe_5B_3	140	2.550	1201.186	20.300	-0.308
Fe_5BeB_2	140	1.535	1214.282	0.000	-0.292
Fe_5GaB_2	140	2.041	1067.626	61.900	-0.219
Fe_5GeB_2	140	2.169	1037.702	24.000	-0.242
Fe_5SiB_2	140	2.033	1027.393	0.000	-0.359
Fe_5ZnB_2	140	1.730	1136.984	97.500	-0.142
Mn_5B_3	140	1.813	929.282	36.600	-0.391
$Co_3Fe_2B_2$	10	2.038	1080.426	97.677	-0.160
$Fe_3Co_2B_2$	10	2.935	1180.767	84.000	-0.186
Fe_5B_2	10	3.257	1379.485	58.500	-0.210
$Mn_3Co_2B_2$	10	3.189	1342.777	90.900	-0.227
$Mn_3Rh_2B_2$	10	1.877	807.529	97.979	-0.242
$Fe_3Co_2B_2$	65	6.170	1291.798	88.400	-0.182
Fe_5B_2	65	6.557	1448.993	56.600	-0.211
$Fe_3Ir_2B_2$	65	2.370	792.503	74.300	-0.174
$Fe_3Si_2B_2$	65	1.984	353.213	91.300	-0.315
$Fe_3Zn_2B_2$	65	1.584	571.752	90.300	-0.156
$Mn_3Al_2B_2$	65	1.855	372.455	6.800	-0.406
$Mn_3Co_2B_2$	65	5.712	1348.995	70.000	-0.248
$Mn_3Ga_2B_2$	65	2.694	417.894	95.000	-0.249
$Mn_3Ir_2B_2$	65	5.165	992.463	49.800	-0.302
$Mn_3Pt_2B_2$	65	2.980	972.699	86.800	-0.351
$Mn_3Rh_2B_2$	65	4.987	1081.082	51.900	-0.299
$Co_4Fe_3B_2$	123	1.505	1141.436	74.500	-0.145
$Fe_4Co_3B_2$	123	3.693	1311.878	88.300	-0.136
Fe_7B_2	123	3.748	1484.725	37.100	-0.171
Fe_4AgB_4	71	1.522	633.953	65.711	-0.269
Fe_4AlB_4	71	2.337	604.617	0.000	-0.417

Fe_4AuB_4	71	1.867	654.290	47.398	-0.288
Fe_4B_5	71	2.496	556.735	65.690	-0.269
Fe_4BeB_4	71	2.137	523.344	0.000	-0.377
Fe_4CoB_4	71	3.988	934.922	28.064	-0.335
Fe_4CrB_4	71	3.255	871.794	79.505	-0.309
Fe_4CuB_4	71	2.607	690.269	31.145	-0.304
Fe_5B_4	71	4.396	1032.848	1.192	-0.354
Fe_4GaB_4	71	2.529	607.816	0.000	-0.343
Fe_4GeB_4	71	2.465	640.336	87.855	-0.247
Fe_4IrB_4	71	3.811	714.201	2.704	-0.332
Fe_4LiB_4	71	1.538	645.627	29.081	-0.306
Fe_4MnB_4	71	4.724	1037.000	32.256	-0.351
Fe_4MoB_4	71	2.787	637.712	51.919	-0.331
Fe_4NbB_4	71	1.866	581.800	67.980	-0.381
Fe_4NiB_4	71	3.193	711.144	7.499	-0.346
Fe_4OsB_4	71	3.073	664.139	41.614	-0.293
Fe_4PdB_4	71	2.601	695.196	25.071	-0.327
Fe_4PtB_4	71	3.375	717.540	8.625	-0.344
Fe_4ReB_4	71	3.035	672.519	25.576	-0.322
Fe_4RhB_4	71	3.345	752.215	20.018	-0.338
Fe_4RuB_4	71	3.088	717.097	38.379	-0.304
Fe_4SiB_4	71	2.735	614.661	24.593	-0.342
Fe_4TaB_4	71	1.913	560.842	73.161	-0.386
Fe_4TcB_4	71	3.051	695.087	36.102	-0.322
Fe_4VB_4	71	2.888	750.986	86.301	-0.374
Fe_4WB_4	71	2.767	641.107	56.825	-0.323
Fe_4ZnB_4	71	2.404	624.239	0.000	-0.348
Mn_4AuB_4	71	1.609	775.212	89.408	-0.355
Mn_4CrB_4	71	1.784	766.225	90.249	-0.384
Mn_4IrB_4	71	1.824	905.022	5.220	-0.439
Mn_5B_4	71	1.655	999.941	51.481	-0.417
Mn_4OsB_4	71	2.039	850.492	40.142	-0.404
Mn_4PtB_4	71	1.699	919.450	34.329	-0.437
Mn_4ReB_4	71	2.019	785.087	28.278	-0.416
Mn_4RhB_4	71	1.826	935.596	19.359	-0.435
Mn_4RuB_4	71	1.949	864.614	38.705	-0.405
Mn_4TcB_4	71	1.932	781.253	45.509	-0.411

Table S10: Comparing the current MAB results with previous predicted results from Ref. 13.

Compounds	Space Group	Lattice Constant (Å)			Convex Hull (eV/atom)	Source
		a	b	c		
CrAlB	63	2.969	3.004	13.881	0.011	This work
		2.969	3.003	13.889	0.008	Ref. 13
MnAlB	63	2.988	2.953	13.908	0.066	This work
		2.989	2.955	13.859	0.065	Ref. 13
Cr_2AlB_2	65	2.932	2.924	11.051	0	This work
		2.934	2.924	11.051	0	Ref. 13
Mn_2AlB_2	65	2.831	2.894	11.080	0	This work
		2.831	2.896	11.074	0	Ref. 13
Fe_2AlB_2	65	2.851	2.916	11.019	0	This work
		2.853	2.917	11.024	0	Ref. 13
$Cr_3Al_2B_2$	65	2.950	2.936	17.311	0.046	This work
		2.951	2.936	17.313	0.038	Ref. 13
$Mn_3Al_2B_2$	65	2.832	2.853	17.788	0.007	This work
		2.833	2.851	17.863	0.004	Ref. 13
$Fe_3Al_2B_2$	65	2.872	2.912	16.537	0.033	This work
		2.875	2.913	16.536	0	Ref. 13
$Ni_3Al_2B_2$	65	2.831	2.961	16.872	0.087	This work
		2.840	2.962	16.926	0.084	Ref. 13
Cr_3AlB_4	47	2.939	2.939	8.091	0	This work
		2.939	2.939	8.088	0	Ref. 13
Mn_3AlB_4	47	2.937	2.834	8.164	0.038	This work
		2.937	2.835	8.153	0.036	Ref. 13
Fe_3AlB_4	47	2.961	2.818	8.149	0.065	This work
		2.960	2.819	8.144	0.063	Ref. 13
Cr_4AlB_6	65	2.943	2.947	21.328	0.012	This work
		2.944	2.947	21.325	0.008	Ref. 13

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