Supplementary Information

Combined in- and out-of-plane chemical ordering in super-ordered MAX phases (s-MAX)

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Table S1. PBE potential used for elements considered in this work.

Element	POTCAR	Valence electrons
Sc	Sc_sv	4s 3d 3p 3s
Y	Y_sv	5s 4d 4p 4s
Ti	Ti_pv	4s 3d 3p
Zr	Zr_sv	5s 4d 4p 4s
Hf	Hf_pv	6s 5d 5p
V	V_pv	4s 3d 3p
Nb	Nb_pv	5s 4d 4p
Ta	Ta_pv	6s 5d 5p
Cr	Cr_pv	4s 3d 3p
Mo	Mo_pv	5s 4d 4p
W	W_pv	6s 5d 5p
Mn	Mn_pv	4s 3d 3p
Fe	Fe_pv	4s 3d 3p
Al	Al	3p 3s
C	C	2p 2s

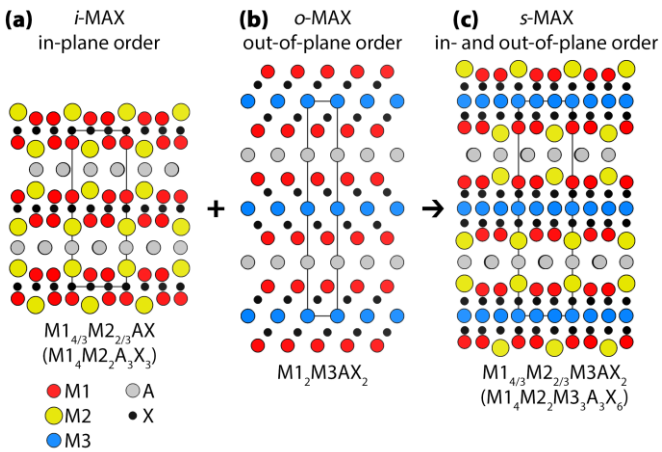

Figure S1. Schematic illustration of (a) in-plane order of two metals, M1 and M2, in a 211 MAX phase, (b) out-of-plane order of two metals, M1 and M3, in a 312 MAX phase, and (c) combined in- and out-of-plane chemical order of three metals, M1, M2 and M3, in a 312 MAX phase.

Table S2. Calculated energy (E) and stability at 2000 K (ΔH_{cp}) for M2 = Y in *s*-MAX, *s*-MAX with disorder, and MAX with disorder for 413 MAX phases along with corresponding energy for their competing phases and identified set of most competing phases. Phases modelled with solid solution disorder have a contribution from configurational entropy evaluated at 2000 K. Competing phases in bold highlight when a MAX phase is part of the set of most competing phases.

M1	M2	M3	Energy (eV/atom)				ΔH_{cp} (meV/atom)			Set of most competing phases
			s-MAX	*s*-MAX disorder	MAX disorder	Competing phases	*s*-MAX	*s*-MAX disorder	MAX disorder	
Sc	Y	Sc	-7.434866	N/A	N/A	-7.592886	158	N/A	N/A	AlY_3C_3 + Sc_3C_4 + Al_2Y + $AlSc_3C$
Sc	Y	Y	-7.371466	N/A	N/A	-7.571161	200	N/A	N/A	AlY_3C_3 + AlY_3C + Y_4C_5 + $AlSc_3C$
Sc	Y	Ti	-8.077566	-8.115098	-8.077288	-8.159419	82	44	82	AlY_3C_3 + Sc_3C_4 + Al_2Y + $AlSc_3C$ + TiC
Sc	Y	Zr	-8.293600	-8.294268	-8.279101	-8.321271	28	27	42	ZrC + AlY_3C_3 + Sc_3C_4 + Al_2Y + $AlSc_3C$
Sc	Y	Hf	-8.709104	-8.702837	-8.676613	-8.741063	32	38	64	AlY_3C_3 + Sc_3C_4 + Al_2Y + $AlSc_3C$ + HfC
Sc	Y	V	-8.217175	-8.297430	-8.236285	-8.317103	100	20	81	**$Al_3Sc_3V_4Y_2C_6$ (312 s-MAX)** + V_6C_5 + Sc_3C_4
Sc	Y	Nb	-8.602831	-8.662783	-8.618902	-8.647334	45	-15	28	Y_2C + **$Al_3Nb_4Sc_3Y_2C_6$ (312 s-MAX with partial disorder)** + **$Al_3Nb_{10}Sc_2C_9$ (disorder M_4AX_3)** + Y_4C_5 + **$AlNb_2Sc_2C_3$ (disorder M_4AX_3)**
Sc	Y	Ta	-9.112934	-9.161713	-9.110761	-9.138535	26	-23	28	**$Al_3Sc_3Ta_4Y_2C_6$ (312 s-MAX with partial disorder)** + **$AlSc_2Ta_2C_3$ (disorder M_4AX_3)** + Y_4C_5 + Y_2C + **$Al3Sc_2Ta_{10}C_9$ (disorder M_4AX_3)**
Sc	Y	Cr	-8.060732	N/A	N/A	-8.312736	252	N/A	N/A	Y_4C_7 + AlY_3C_3 + $CrSc_2C_3$ + $Cr_2Y_2C_3$ + **$Al_3Cr_4Sc_2C_3$ (i-MAX)**
Sc	Y	Mo	-8.463800	N/A	N/A	-8.638239	174	N/A	N/A	Sc_3C_4 + **$Al_3Mo_4Sc_3Y_2C_6$ (312 s-MAX)** + C + Mo_2C
Sc	Y	W	-8.985872	N/A	N/A	-9.163127	177	N/A	N/A	WYC_2 + **$Al_3Sc_3W_4C_6$ (disorder M_4AX_3)** + **$Al_3Sc_3W_4Y_2C_6$ (s-MAX)** + WC
Sc	Y	Mn	-7.877035	N/A	N/A	-8.199559	323	N/A	N/A	Y_4C_7 + $Mn_{13}Y_{10}C_{18}$ + AlY_3C_3 + Sc_3C_4 + **$Al_3Mn_4Sc_2C_3$ (i-MAX)**
Sc	Y	Fe	-7.554108	N/A	N/A	-7.986556	432	N/A	N/A	$AlFe_3C$ + Y_4C_7 + $AlFe_3$ + Al_6Fe_6Sc + $FeSc_3C_4$
Y	Y	Ti	N/A	N/A	-7.988232	-8.135413	N/A	N/A	147	AlY_3C_3 + AlY_3C + Al_2Y + TiC
Y	Y	Zr	N/A	N/A	-8.231576	-8.297264	N/A	N/A	66	AlY_3C_3 + AlY_3C + Al_2Y + ZrC
Y	Y	Hf	N/A	N/A	-8.616919	-8.717057	N/A	N/A	100	AlY_3C_3 + AlY_3C + Al_2Y + HfC
Y	Y	V	N/A	N/A	-8.134106	-8.291619	N/A	N/A	158	V_6C_5 + AlY_3C + AlY_3C_3 + Al_2Y
Y	Y	Nb	N/A	N/A	-8.536906	-8.552239	N/A	N/A	15	**$Al_3Nb_7Y_2C_6$ (s-MAX)** + AlY_3C_3 + AlY_3C
Y	Y	Ta	N/A	N/A	-9.018272	9.025330	N/A	N/A	7	AlY_3C + **$Al_3Ta_{10}Y_2C_9$ (disorder M_4AX_3)** + AlY_3C_3 + Y_4C_5
Ti	Y	Sc	-7.851286	N/A	N/A	-7.970575	119	N/A	N/A	AlY_3C_3 + Sc_3C_4 + Al_2Y + $AlSc_3C$ + TiC
Ti	Y	Y	-7.730338	N/A	N/A	-7.941196	211	N/A	N/A	AlY_3C_3 + AlY_3C + Al_2Y + TiC
Ti	Y	Ti	-8.498346	N/A	-8.446045	-8.498689	0	N/A	53	**$Al_3Ti_7Y_2C_6$ (312 s-MAX)** + TiC
Ti	Y	Zr	-8.662583	-8.662403	-8.606394	-8.661233	1	1	57	**$Al_3Ti_4Y_2Zr_3C_6$ (312 s-MAX disorder)** + ZrC
Ti	Y	Hf	-9.085900	-9.080662	-9.009876	-9.082742	-3	2	73	**$Al_3Hf_3Ti_4Y_2C_6$ (312 s-MAX)** + HfC
Ti	Y	V	-8.586062	-8.681575	-8.578059	-8.682079	103	7	111	**$Al_3Ti_3V_4Y_2C_6$ (312 s-MAX disorder)** + C + V_6C_5 + TiC
Ti	Y	Nb	-8.921938	-8.979750	-8.918915	-8.949152	52	-6	55	**$Al_3Nb_4Ti_3Y_2C_6$ (312 s-MAX disorder)** + $NbTiC_2$ + C + Nb_6C_5
Ti	Y	Ta	-9.428338	-9.470341	-9.403383	-9.464740	36	-6	61	**$Al_3Ta_{10}Y_2C_9$ (disorder M_4AX_3)** + $TaTiC_2$ + **$Al_3Ta_4Ti_3Y_2C_6$ (312 s-MAX with partial disorder)**
Ti	Y	Cr	-8.431953	N/A	N/A	-8.654134	222	N/A	N/A	Cr_3C_2 + **$Al_3Cr_4Ti_3Y_2C_6$ (s-MAX)** + **$Al_3Cr_4Ti_6Y_2C_9$ (s-MAX)** + C
Ti	Y	Mo	-8.816394	N/A	N/A	-8.979824	163	N/A	N/A	**$AlMo_2Ti_2C_3$ (413 o-MAX)** + $MoYC_2$ + **$Al_3Mo_4Y_2C_3$ (i-MAX)** + TiC
Ti	Y	W	-9.328072	N/A	N/A	-9.481675	158	N/A	N/A	**$Al_3Ti_3W_4Y_2C_6$ (312 s-MAX disorder)** + WC + TiC
Ti	Y	Mn	-8.255668	N/A	N/A	-8.533319	278	N/A	N/A	**$Al_3Mn_4Ti_6Y_2C_9$ (s-MAX)** + **$Al_3Mn_4Y_2C_3$ (i-MAX)** + $AlMn_3C$ + C + $Mn_{13}Y_{10}C_{18}$
Ti	Y	Fe	-7.917327	N/A	N/A	-8.325073	408	N/A	N/A	$AlFe_3C$ + Y_4C_7 + AlFe + TiC
Zr	Y	Sc	-7.932774	N/A	N/A	-8.078476	146	N/A	N/A	ZrC + AlY_3C_3 + Sc_3C_4 + Al_2Y + $AlSc_3C$

Zr	Y	Y	-7.864203	N/A	N/A	-8.049097	185	N/A	N/A	AlY_3C_3 + AlY_3C + Al_2Y + ZrC
Zr	Y	Ti	-8.528713	-8.609292	-8.544825	-8.607282	81	0	64	**$Al_3Ti_4Y_2Zr_3C_6$ (312 s-MAX disorder)** + TiC + ZrC
Zr	Y	Zr	-8.760315	N/A	-8.767119	-8.765354	5	N/A	-2	$Zr_{10}C_9$ + AlY_2 + Al_2Y
Zr	Y	Hf	-9.170243	-9.209975	-9.159406	-9.200794	31	-9	41	**$Al_3Hf_4Y_2Zr_6C_9$ (413 s-MAX with partial disorder)** + **Al3Hf4Y2Zr3C6 (312 s-MAX with partial disorder)** + HfC
Zr	Y	V	-8.589325	-8.700685	-8.644363	-8.783945	195	83	140	**$Al_3V_4Y_2C_3$ (i-MAX)** + AlY_3C + ZrC + V_6C_5 + Al_2Y
Zr	Y	Nb	-8.980346	-9.069724	-9.036945	-9.067452	87	-2	31	$NbZrC_2$ + **$Al_3Nb_{10}Y_2C_9$ (disorder M_4AX_3)** + **$Al_3Nb_4Y_2Zr_3C_6$ (312 s-MAX with partial disorder)**
Zr	Y	Ta	-9.482677	-9.550962	-9.513788	-9.552592	70	2	39	**$Al_3Ta_4Y_2Zr_3C_6$ (312 s-MAX with partial disorder)** + $TaZrC_2$ + **$Al_3Ta_{10}Y_2C_9$ (disorder M_4AX_3)**
Zr	Y	Cr	-8.444864	N/A	N/A	-8.752256	307	N/A	N/A	**$Al_3Cr_4Y_2C_3$ (i-MAX)** + Cr_3C_2 + C + ZrC
Zr	Y	Mo	-8.839338	N/A	N/A	-9.082046	243	N/A	N/A	ZrC + **$Al_3Mo_4Y_2C_3$ (i-MAX)** + C + Mo_2C
Zr	Y	W	-9.349815	N/A	N/A	-9.581603	232	N/A	N/A	ZrC + WC + **$Al_3W_4Y_2Zr_3C_6$ (312 s-MAX)**
Zr	Y	Mn	-8.264128	N/A	N/A	-8.637357	373	N/A	N/A	**$Al_3Mn_4Zr_2C_3$ (i-MAX)** + **$Al_3Mn_4Y_2C_3$ (i-MAX)** + C + $Mn_{13}Y_{10}C_{18}$ + ZrC
Zr	Y	Fe	-7.945398	N/A	N/A	-8.432974	488	N/A	N/A	$AlFe_3C$ + Y_4C_7 + AlFe + ZrC
Hf	Y	Sc	-8.193235	N/A	N/A	-8.358337	165	N/A	N/A	AlY_3C_3 + Sc_3C_4 + Al_2Y + $AlSc_3C$ + HfC
Hf	Y	Y	-8.116882	N/A	N/A	-8.890163	90	-3	73	**$Al_3Hf_6Ti_4Y_2C_9$ (413 s-MAX)** + Al3Ti7Y_2C6 + TiC
Hf	Y	Ti	-8.800167	-8.893363	-8.817142	-9.062127	42	-13	35	**$Al_3Hf_6Y_2Zr_4C_9$ (413 s-MAX with partial disorder)** + **$Al_3Hf_3Y_2Zr_4C_6$ (312 s-MAX with partial disorder)** + AlY_3C + Al_2Y + $Zr_{10}C_9$
Hf	Y	Zr	-9.020327	-9.075342	-9.027332	-9.044537	37	-18	30	ZrC + **$Al_3Hf_3Y_2Zr4C_6$ (312 s-MAX disorder)** + HfC
Hf	Y	Hf	-9.433600	N/A	-9.422662	-9.435935	2	N/A	13	**$AlHf_4C_3$ (M_4AX_3)** + AlY_2 + Al_2Y + HfC
Hf	Y	V	-8.861987	-8.985538	-8.914218	-9.063806	202	78	150	**$Al_3V_4Y_2C_3$ (i-MAX)** + AlY_3C + V_6C_5 + Al_2Y + HfC
Hf	Y	Nb	-9.241965	-9.341373	-9.299155	-9.338387	96	-3	39	**$Al_3Hf_3Nb_4Y_2C_6$ (312 s-MAX with partial disorder)** + **$Al_3Nb_{10}Y_2C_9$ (disorder M_4AX_3)** + HfC
Hf	Y	Ta	-9.742197	-9.823812	-9.776825	-9.823761	82	0	47	**$Al_3Hf_3Ta_4Y_2C_6$ (312 s-MAX with partial disorder)** + $HfTaC_2$ + **Al3Ta10Y_2C_9 (disorder M_4AX_3)**
Hf	Y	Cr	-8.715080	N/A	N/A	-9.032117	317	N/A	N/A	**$Al_3Cr_4Y_2C_3$ (i-MAX)** + C + Cr_3C_2 + HfC
Hf	Y	Mo	-9.101227	N/A	N/A	-9.361908	261	N/A	N/A	Mo_2C + C + **$Al_3Mo_4Y_2C_3$ (i-MAX)** + HfC
Hf	Y	W	-9.609511	N/A	N/A	-9.860091	251	N/A	N/A	**$Al_3W_4Y_2C_3$ (i-MAX)** + WC + HfC
Hf	Y	Mn	-8.532970	N/A	N/A	-8.915838	383	N/A	N/A	**$Al_3Mn_4Y_2C_3$ (i-MAX)** + $AlMn_3C$ + C + $Mn_{13}Y_{10}C_{18}$ + HfC
Hf	Y	Fe	-8.211844	N/A	N/A	-8.712835	501	N/A	N/A	$AlFe_3C$ + Y_4C_7 + AlFe + HfC
V	Y	Sc	-8.023168	N/A	N/A	-8.076785	54	N/A	N/A	**$Al_3Sc_3V_4Y_2C_6$ (312 s-MAX)** + Sc_3C_4 + Sc_4C_3
V	Y	Y	-7.862737	N/A	N/A	-8.045334	183	N/A	N/A	V_6C_5 + AlY_3C + AlY_3C_3 + Al_2Y
V	Y	Ti	-8.632490	-8.638360	-8.535389	-8.631136	9	3	106	**$Al_3Ti_3V_4Y_2C_6$ (312 s-MAX disorder)** + TiC
V	Y	Zr	-8.759575	-8.709068	-8.663779	-8.779145	20	70	115	**$Al_3V_4Y_2C_3$ (i-MAX)** + ZrC
V	Y	Hf	-9.181749	-9.127591	-9.065509	-9.198937	17	71	133	**$Al_3V_4Y_2C_3$ (i-MAX)** + HfC
V	Y	V	-8.717176	N/A	-8.666226	-8.783293	66	N/A	117	V_6C_5 + Al_3YC_3 + AlY_3C_3 + Al_2Y
V	Y	Nb	-9.030229	-9.023428	-8.970583	-9.048898	19	25	78	**$Al_3Nb_3V_4Y_2C_6$ (s-MAX)** + C + **$Al_3Nb_{10}Y_2C_9$ (disorder M_4AX_3)** + V_6C_5
V	Y	Ta	-9.535590	-9.514704	-9.453046	-9.533991	-2	19	81	TaC + **$Al_3Ta_3V_4Y_2C_6$ (312 s-MAX)**
V	Y	Cr	-8.572404	N/A	N/A	-8.739447	167	N/A	N/A	Cr_3C_2 + **$Al_3Cr_4Y_2C_3$ (i-MAX)** + C + V_6C_5
V	Y	Mo	-8.941122	N/A	N/A	-9.069237	128	N/A	N/A	Mo_2C + V_6C_5 + C + **$Al_3Mo_4Y2C_3$ (i-MAX)**
V	Y	W	-9.445767	N/A	N/A	-9.567421	122	N/A	N/A	**$Al_3W_4Y_2C_3$ (i-MAX)** + WC + C + V_6C_5
V	Y	Mn	-8.403655	N/A	N/A	-8.623167	220	N/A	N/A	**$Al_3Mn_4Y_2C_3$ (i-MAX)** + V_6C_5 + $AlMn_3C$ + $Mn_{13}Y_{10}C_{18}$ + C
V	Y	Fe	-8.076536	N/A	N/A	-8.420165	344	N/A	N/A	Y_4C_7 + $AlFe_3C$ + V_6C_5 + C + AlFe
Nb	Y	Sc	-8.220423	N/A	N/A	-8.312319	92	N/A	N/A	**$Al_3Nb_3Sc_4Y_2C_6$ (312 s-MAX with partial disorder)** + Y_4C_5 + **$AlNb_2Sc_2C_3$ (disorder M_4AX_3)** + Sc_3C_4 + Sc_4C_3
Nb	Y	Y	-8.105550	N/A	N/A	-8.217249	112	N/A	N/A	**$Al_3Nb_7Y_2C_6$ (312 s-MAX)** + AlY_3C_3 + AlY_3C + Nb_6C_5
Nb	Y	Ti	-8.785927	-8.844034	-8.768548	-8.812442	54	-5	71	**$Al_3Nb_4Ti_3Y_2C_6$ (312 s-MAX disorder)** + TiC
Nb	Y	Zr	-8.971718	-8.986185	-8.951064	-8.972077	15	1	36	**$Al_3Nb_4Y_2Zr_3C_6$ (312 s-MAX disorder)** + ZrC
Nb	Y	Hf	-9.384247	-9.391638	-9.344324	-9.384674	13	5	52	**$Al_3Hf_3Nb_4Y_2C_6$ (312 s-MAX)** + HfC
Nb	Y	V	-8.830672	-8.924987	-8.858827	-8.962664	132	38	104	**Al3Nb3V4Y_2C6 (s-MAX)** + C + **$Al_3Nb_{10}Y_2C_9$ (disorder M_4AX_3)** + V_6C_5

Nb	Y	Nb	-9.203695	N/A	-9.221367	-9.215434	12	N/A	-6	**$Al_3Nb_7Y_2C_6$ (312 s-MAX)** + C + Nb_6C_5
Nb	Y	Ta	-9.706597	-9.733591	-9.697171	-9.725609	19	-8	28	**$Al_3Nb_4Ta_3Y_2C_6$ (312 s-MAX disorder)** + TaC
Nb	Y	Cr	-8.689448	N/A	N/A	-8.924927	235	N/A	N/A	Cr_3C_2 + **$Al_3Cr_4Nb_3Y_2C_6$ (312 s-MAX)** + C + Nb_6C_5
Nb	Y	Mo	-9.065601	N/A	N/A	-9.247077	181	N/A	N/A	**$Al_3Mo_4Nb_6Y_2C_9$ (s-MAX)** + **$Al_3Mo_4Y_2C_3$ (i-MAX) + C + Mo_2C**
Nb	Y	W	-9.565763	N/A	N/A	-9.741260	175	N/A	N/A	**$Al_3W4Y_2C_3$ (i-MAX)** + **$Al_3Nb_{10}Y_2C_9$ (disorder M_4AX_3)** + WC
Nb	Y	Mn	-8.515343	N/A	N/A	-8.801330	286	N/A	N/A	**$Al_3Mn_4Nb_6Y_2C_9$ (s-MAX)** + **$Al_3Mn_4Y_2C_3$ (i-MAX)** + $AlMn_3C$ + C + $Mn_{13}Y_{10}C_{18}$
Nb	Y	Fe	-8.192085	N/A	N/A	-8.590248	398	N/A	N/A	AlFe + $AlFe_3C$ + Y_4C_7 + C + Nb_6C_5
Ta	Y	Sc	-8.548336	N/A	N/A	-8.645800	97	N/A	N/A	**$Al_3Sc_4Ta_3Y_2C_6$ (disorder M_3AX_2)** + **$AlSc_2Ta_2C_3$ (disorder M_4AX_3)** + Y_4C_5 + Sc_3C_4 + Sc_4C_3
Ta	Y	Y	-8.428205	N/A	N/A	-8.531868	104	N/A	N/A	AlY_3C + **Al3Ta10Y2C9 (disorder M4AX3)** + AlY_3C_3 + Y_4C_5
Ta	Y	Ti	-9.102829	-9.177053	-9.096252	-9.154629	65	-9	72	$TaTiC_2$ + **$Al_3Ta_3Ti_4Y_2C_6$ (312 s-MAX disorder)** + TiC
Ta	Y	Zr	-9.283585	-9.310213	-9.272020	-9.283950	23	-3	25	$TaZrC_2$ + **$Al_3Ta_3Zr_4Y_2C_6$ (312 s-MAX disorder)** + TiC
Ta	Y	Hf	-9.696521	-9.716521	-9.665621	-9.696429	18	-2	49	**$Al_3Hf_3Ta_4Y_2C_6$ (312 s-MAX disorder)** + HfC
Ta	Y	V	-9.139318	-9.255151	-9.182430	-9.289921	151	35	107	C + TaC + **$Al_3Ta_3V_4Y_2C_6$ (31_2 s-MAX)** + V_6C_5
Ta	Y	Nb	-9.504032	-9.573411	-9.539094	-9.539873	61	-9	26	AlY_3C_3 + **$AlNb_2Ta_2C_3$ (disorder M_4AX_3)** + Y_4C_5 + **$Al_3Nb_4Ta_3Y_2C_6$ (312 s-MAX)** + Nb_6C_5
Ta	Y	Ta	-10.004879	N/A	-10.012254	-10.000050	-5	N/A	-12	**$Al_3Ta_7Y_2C_6$ (312 s-MAX)** + TaC
Ta	Y	Cr	-8.999218	N/A	N/A	-9.256067	257	N/A	N/A	**$Al_3Cr_4Ta_3Y_2C_6$ (312 s-MAX)** + **$Al_3Cr_4Ta_6Y_2C_9$ (413 s-MAX)** + C + Cr_3C_2
Ta	Y	Mo	-9.364882	N/A	N/A	-9.579381	214	N/A	N/A	**$Al_3Mo_4Ta_6Y_2C_9$ (312 s-MAX)** + **$Al_3Mo_4Y_2C_3$ (i-MAX)** + C + Mo_2C
Ta	Y	W	-9.860668	N/A	N/A	-10.071456	211	N/A	N/A	**Al_3W4Y_2C3 (i-MAX)** + **Al3Ta6W4Y2C9 (413 s-MAX)** + WC
Ta	Y	Mn	-8.824557	N/A	N/A	-9.136872	312	N/A	N/A	**$Al_3Mn_4Ta_6Y_2C_9$ (413 s-MAX)** + $AlMn_3C$ + $Mn_{13}Y_{10}C_{18}$ + **$Al_3Mn_4Y_2C_3$ (i-MAX)** + C
Ta	Y	Fe	-8.499285	N/A	N/A	-8.920712	421	N/A	N/A	$AlFe_3C$ + $Fe_{17}Y_2C_3$ + Y_4C_7 + **$Al_3Fe_4Ta_6Y_2C_9$ (413 s-MAX)** + C
Cr	Y	Sc	-8.008351	N/A	N/A	-8.083576	75	N/A	N/A	**$Al_3Cr_4Sc_3Y_2C_6$ (312 s-MAX)** + $CrSc_2C_3$ + $Cr_2Y_2C_3$ + Al_2Y + $AlSc_3C$
Cr	Y	Y	-7.846272	N/A	N/A	-8.050025	204	N/A	N/A	$Cr_2Y_2C_3$ + AlY_3C_3 + Al_2Y
Cr	Y	Ti	-8.631338	-8.561460	-8.465639	-8.626793	-5	65	161	**$Al_3Cr_4Ti_3Y_2C_6$ (312 s-MAX)** + TiC
Cr	Y	Zr	-8.744629	-8.623996	-8.586699	-8.780380	36	156	194	**$Al_3Cr_4Y_2C_3$ (i-MAX)** + ZrC
Cr	Y	Hf	-9.167705	-9.042304	-8.985440	-9.200173	32	158	215	**$Al_3Cr_4Y_2C_3$ (i-MAX)** + HfC
Cr	Y	V	-8.729483	-8.707547	-8.614576	-8.761167	32	54	147	**$Al_3Cr_4Y_2C_3$ (i-MAX)** + C + V_6C_5
Cr	Y	Nb	-9.031522	-8.950986	-8.891556	-9.031690	0	81	140	**$Al_3Cr_4Nb_3Y_2C_6$ (312 s-MAX)** + C + Nb_6C_5
Cr	Y	Ta	-9.534004	-9.440730	-9.379961	-9.515785	-18	75	136	**$Al_3Cr_4Ta_3Y_2C_6$ (312 s-MAX)** + TaC
Cr	Y	Cr	-8.584375	N/A	N/A	-8.696006	112	N/A	N/A	**$Al_3Cr_4Y_2C_3$ (i-MAX)** + C + Cr_3C_2
Cr	Y	Mo	-8.942537	N/A	N/A	-9.025796	83	N/A	N/A	C + Cr_3C_2 + **$Al_3Mo_4Y_2C_3$ (i-MAX)** + Mo_2C
Cr	Y	W	-9.442294	N/A	N/A	-9.541819	100	N/A	N/A	**$Al_3Cr_4Y_2C_3$ (i-MAX)** + WC
Cr	Y	Mn	-8.410031	N/A	N/A	-8.590807	181	N/A	N/A	**$Al_3Cr_2Mn_4C_3$ (disorder M_2AX)** + **$Al_3Cr_4Mn_2C_3$ (disorder M_2AX)** + $Mn_{13}Y_{10}C_{18}$ + C + Cr_3C_2
Cr	Y	Fe	-8.092598	N/A	N/A	-8.386801	294	N/A	N/A	$AlFe_3C$ + $Cr_2Y_2C_3$ + C + Cr_3C_2 + AlFe
Mo	Y	Sc	-8.267087	N/A	N/A	-8.320038	53	N/A	N/A	Sc_3C_4 + **$Al_3Mo_4Sc_3Y_2C_6$ (312 s-MAX)** + Sc_4C_3
Mo	Y	Y	-8.133481	N/A	N/A	-8.245524	112	N/A	N/A	**$Al_3Mo_4Y_2C_3$ (i-MAX)** + Y_2C + Y_4C_5
Mo	Y	Ti	-8.847640	-8.830929	-8.762989	-8.848715	1	18	86	**$Al_3Mo_4Y_2C_3$ (i-MAX)** + TiC
Mo	Y	Zr	-9.002024	-8.939672	-8.912426	-9.010567	9	71	98	ZrC + **$Al_3Mo_4Y_2C_3$ (i-MAX)**
Mo	Y	Hf	-9.417594	-9.348925	-9.308156	-9.430359	13	81	122	**$Al_3Mo_4Y_2C_3$ (i-MAX)** + HfC
Mo	Y	V	-8.912917	-8.934031	-8.857698	-8.991353	78	57	134	V_6C_5 + C + **$Al_3Mo_4Y_2C_3$ (i-MAX**)
Mo	Y	Nb	-9.258114	-9.219243	-9.181885	-9.249548	-9	30	68	**$Al_3Mo_4Nb_3Y_2C_6$ (s-MAX)** + C + Nb_6C_5
Mo	Y	Ta	-9.756570	-9.699642	-9.653827	-9.729702	-27	30	76	**$Al_3Mo_4Ta_3Y_2C_6$ (s-MAX)** + TaC
Mo	Y	Cr	-8.761336	N/A	N/A	-8.926192	165	N/A	N/A	C + Cr_3C_2 + **$Al_3Mo_4Y_2C_3$ (i-MAX)**
Mo	Y	Mo	-9.121273	N/A	N/A	-9.225005	104	N/A	N/A	**$Al_3Mo_4Y_2C_3$ (i-MAX)** + C + Mo_2C
Mo	Y	W	-9.614620	N/A	N/A	-9.772005	157	N/A	N/A	**$Al_3Mo_4Y_2C_3$ (i-MAX)** + WC

Mo	Y	Mn	-8.577507	N/A	N/A	-8.790865	213	N/A	N/A	$AlMn_3C$ + **$Al_3Mo_4Y_2C_3$ (i-MAX)** + $Mn_{13}Y_{10}C_{18}$ + C + Mo_2C
Mo	Y	Fe	-8.268426	N/A	N/A	-8.589291	321	N/A	N/A	$Fe_{17}Y_2C_3$ + **$Al_3Mo_4Y_2C_3$ (i-MAX)** + C + Mo_2C + $AlFe_3C$
W	Y	Sc	-8.611707	N/A	N/A	-8.659096	47	N/A	N/A	Sc_3C_4 + **$Al_3Sc_3W_4Y_2C_6$ (312 s-MAX)** + Sc_4C_3
W	Y	Y	-8.476886	N/A	N/A	-8.579640	103	N/A	N/A	WYC_2 + AlY_3C_3 + **$Al_3W_4Y_5C_6$ (312 s-MAX)** + AlY_3C
W	Y	Ti	-9.172895	-9.177765	-9.109187	-9.173912	6	1	70	**$Al_3Ti_3W_4Y_2C_6$ (312 s-MAX disorder)** + TiC
W	Y	Zr	-9.325239	-9.281503	-9.255444	-9.327790	3	46	72	ZrC + **$Al_3W_4Y_2Zr_3C_6$ (s-MAX)**
W	Y	Hf	-9.740491	-9.689766	-9.649798	-9.746209	6	56	96	**$Al_3W_4Y_2C_3$ (i-MAX)** + HfC
W	Y	V	-9.226428	-9.271411	-9.191794	-9.307203	81	36	115	**$Al_3W_4Y_2C_3$ (i-MAX)** + C + V_6C_5
W	Y	Nb	-9.567571	-9.547637	-9.508514	-9.567962	0	20	59	**$Al_3W_4Y_2C_3$ (i-MAX)** + **$Al_3Nb_{10}Y_2C_9$ (disorder M_4AX_3)** + WC
W	Y	Ta	-10.063256	-10.021972	-9.973958	-10.042495	-21	21	69	**$Al_3W_4Y_2C_3$ (i-MAX)**+ **$Al_3Ta_{10}Y_2C_9$ (disorder M_4AX_3)** + WC
W	Y	Cr	-9.075305	N/A	N/A	-9.259881	185	N/A	N/A	Cr_3C_2 + C + **$Al_3Cr_4Y_2C_3$ (i-MAX)** + WC
W	Y	Mo	-9.422339	N/A	N/A	-9.589672	167	N/A	N/A	**$Al_3Mo_4Y_2C_3$ (i-MAX)** + C + WC + Mo_2C
W	Y	W	-9.908329	N/A	N/A	-10.087855	180	N/A	N/A	**$Al_3W_4Y_2C_3$ (i-MAX)** + WC
W	Y	Mn	-8.889779	N/A	N/A	-9.143602	254	N/A	N/A	**$Al_3Mn_4Y_2C_3$ (i-MAX)** + $AlMn_3C$ + $Mn_{13}Y_{10}C_{18}$ + C + WC
W	Y	Fe	-8.579042	N/A	N/A	-8.945738	367	N/A	N/A	$AlFe_3C$ + WYC_2 + C + WC + AlFe
Mn	Y	Sc	-7.933694	N/A	N/A	-7.997827	64	N/A	N/A	$Mn_{13}Y_{10}C_{18}$ + AlY_3C_3 + Sc_3C_4 + $AlSc_3C$ + **$Al_3Mn_4Sc_2C_3$ (i-MAX)**
Mn	Y	Y	-7.783324	N/A	N/A	-7.973601	190	N/A	N/A	AlY_3C_3 + $Mn_{13}Y_{10}C_{18}$ + AlY_3C + Al_2Y
Mn	Y	Ti	-8.550963	-8.438665	-8.348873	-8.543098	-8	104	194	**$Al_3Mn_4Y_2C_3$ (i-MAX)** + TiC
Mn	Y	Zr	-8.656546	-8.507528	-8.475255	-8.704950	48	197	230	**$Al_3Mn_4Y_2C_3$ (i-MAX)** + ZrC
Mn	Y	Hf	-9.079433	-8.923722	-8.875184	-9.124742	45	201	250	**$Al_3Mn_4Y_2C_3$ (i-MAX)** + HfC
Mn	Y	V	-8.653978	-8.595123	-8.502284	-8.685736	32	91	183	**$Al_3Mn_4Y_2C_3$ (i-MAX)** + V_6C_5 + C
Mn	Y	Nb	-8.952981	-8.828920	-8.777597	-8.943234	-10	114	166	**$Al_3Mn_4Nb_3Y_2C_6$ (312 s-MAX)** + C + Nb_6C_5
Mn	Y	Ta	-9.456294	-9.319016	-9.263338	-9.427129	-29	108	164	**$Al_3Mn_4Ta_3Y_2C_6$ (312 s-MAX)** + TaC
Mn	Y	Cr	-8.501350	N/A	N/A	-8.628203	127	N/A	N/A	**$Al_3Cr_4Mn_2C_3$ (disorder M_2AX)** + **$Al_3Cr_4Y_2C_3$ (i-MAX)** + $Mn_{13}Y_{10}C_{18}$ + C + Cr_3C_2
Mn	Y	Mo	-8.838313	N/A	N/A	-8.935578	97	N/A	N/A	$AlMn_3C$ + **$Al_3Mo_4Y_2C_3$ (i-MAX)** + $Mn_{13}Y_{10}C_{18}$ + C + Mo_2C
Mn	Y	W	-9.331862	N/A	N/A	-9.466388	135	N/A	N/A	**$Al_3Mn_4Y_2C_3$ (i-MAX)** + WC
Mn	Y	Mn	-8.315838	N/A	N/A	-8.498029	182	N/A	N/A	**$Al_3Mn_4Y_2C_3$ (i-MAX)** + $Mn_{13}Y_{10}C_{18}$ + C + $AlMn_3C$
Mn	Y	Fe	-7.991697	N/A	N/A	-8.314707	323	N/A	N/A	$AlFe_3C$ + $AlMn_3C$ + $Mn_{13}Y_{10}C_{18}$ + C + AlFe
Fe	Y	Sc	-7.788676	N/A	N/A	-7.885714	97	N/A	N/A	Al_6Fe_6Sc + $FeSc_3C_4$ + AlY_3C_3 + AlY_3C + $AlSc_3C$
Fe	Y	Y	-7.660560	N/A	N/A	-7.822435	162	N/A	N/A	Y_3C_4 + $AlFe_3$ + AlY_3C_3
Fe	Y	Ti	-8.390390	-8.226878	-8.160438	-8.404209	14	177	244	Y_4C_7 + AlY_3C_3 + Al_8Fe_4Y + $AlFe_3$ + TiC
Fe	Y	Zr	-8.508687	-8.303875	-8.282462	-8.566060	57	262	284	Y_4C_7 + AlY_3C_3 + Al_8Fe_4Y + $AlFe_3$ + ZrC
Fe	Y	Hf	-8.929831	-8.706665	-8.675001	-8.985852	56	279	311	Y_4C_7 + AlY_3C_3 + Al_8Fe_4Y + $AlFe_3$ + HfC
Fe	Y	V	-8.487544	-8.395325	-8.318037	-8.548185	61	153	230	Y_4C_7 + $AlFe_3C$ + V_6C_5 + AlFe
Fe	Y	Nb	-8.795202	-8.624187	-8.577727	-8.803310	8	179	226	AlFe + $AlFe_3C$ + Y_4C_7 + Nb_6C_5
Fe	Y	Ta	-9.300378	-9.112400	-9.062425	-9.279071	-21	167	217	Al_8Fe_4Y + Y_4C_7 + $AlFe_3$ + $AlFe_2Ta$ + TaC
Fe	Y	Cr	-8.334966	N/A	N/A	-8.493101	158	N/A	N/A	$AlFe_3C$ + $Cr_2Y_2C_3$ + C + Cr_3C_2 + AlFe
Fe	Y	Mo	-8.668229	N/A	N/A	-8.801196	133	N/A	N/A	$Fe_{17}Y_2C_3$ + **$Al_3Mo_4Y_2C_3$ (i-MAX)** + C + Mo_2C + $AlFe_3C$
Fe	Y	W	-9.158035	N/A	N/A	-9.333975	176	N/A	N/A	$AlFe_3C$ + WYC_2 + C + WC + AlFe
Fe	Y	Mn	-8.157096	N/A	N/A	-8.376729	220	N/A	N/A	$AlFe_3C$ + $AlMn_3C$ + $Mn_{13}Y_{10}C_{18}$ + C + AlFe
Fe	Y	Fe	-7.826330	N/A	N/A	-8.161381	335	N/A	N/A	$Fe_{17}Y_2C_3$ + Y_4C_7 + $AlFe_3C$ + C

Table S3. Calculated energy (E) and stability at 2000 K (ΔH_{cp}) for M2 = Sc in *s*-MAX, *s*-MAX with disorder, and MAX with disorder for 413 MAX phases along with corresponding energy for their competing phases and identified set of most competing phases. Phases modelled with solid solution disorder have a contribution from configurational entropy evaluated at 2000 K. Competing phases in bold highlight when a MAX phase is part of the set of most competing phases.

M1	M2	M3	Energy (eV/atom)				ΔH_{cp} (meV/atom)			Set of most competing phases
			s-MAX	*s*-MAX disorder	MAX disorder	Competing phases	*s*-MAX	*s*-MAX disorder	MAX disorder	
Sc	Sc	Ti	N/A	N/A	-8.130469	N/A	N/A	N/A	28	Al_3ScC_3 + $AlSc_3C$ + TiC
Sc	Sc	Zr	N/A	N/A	-8.302433	N/A	N/A	N/A	18	Al_3ScC_3 + $AlSc_3C$ + ZrC
Sc	Sc	Hf	N/A	N/A	-8.710607	N/A	N/A	N/A	30	Al_3ScC_3 + $AlSc_3C$ + HfC
Sc	Sc	V	N/A	N/A	-8.309669	N/A	N/A	N/A	7	Sc_3C_4 + **$Al_3Sc_2V_7C_6$** + V_6C_5 + $AlSc_3C$
Sc	Sc	Nb	N/A	N/A	-8.673278	N/A	N/A	N/A	-31	**$Al_3Nb_{10}Sc_2C_9$** + Sc_3C_4 + **$Al_3Nb_4Sc_5C_6$** + Sc_4C_3
Sc	Sc	Ta	N/A	N/A	-9.171859	N/A	N/A	N/A	-44	**$Al_3Sc_2Ta_{10}C_9$** + Sc_3C_4 + Sc_4C_3 + **$Al_3Sc_5Ta_4C_6$**
Y	Sc	Sc	-7.365386	N/A	N/A	-7.589384	224	N/A	N/A	AlY_3C_3 + Sc_3C_4 + Sc_4C_3 + $AlSc_3C$
Y	Sc	Y	-7.328947	N/A	N/A	-7.558053	229	N/A	N/A	AlY_3C_3 + AlY_3C + Y_4C_5 + $AlSc_3C$
Y	Sc	Ti	-7.982399	-7.969359	-8.024876	-8.148521	166	179	124	AlY_3C_3 + AlY_3C + Al_2Y + $AlSc_3C$ + TiC
Y	Sc	Zr	-8.232805	-8.207055	-8.252041	-8.310373	78	103	58	ZrC + AlY_3C_3 + Al_2Y + AlY_3C + $AlSc_3C$
Y	Sc	Hf	-8.643278	-8.599599	-8.643231	-8.730165	87	131	87	AlY_3C_3 + AlY_3C + Al_2Y + $AlSc_3C$ + HfC
Y	Sc	V	-8.100171	-8.114145	-8.175186	-8.308660	208	195	133	**$Al_3Sc_3V_4Y_2C_6$** + V_6C_5 + AlY_3C_3 + AlY_3C + Al_2Y
Y	Sc	Nb	-8.517018	-8.517159	-8.564777	-8.617265	100	100	52	AlY_3C + **$Al_3Nb_6Sc_4Y_2C_9$** + AlY_3C_3 + **$Al_3Nb_{10}Sc_2C_9$** + Y_4C_5
Y	Sc	Ta	-9.021710	-9.007849	-9.050584	-9.103524	82	96	53	AlY_3C_3 + **$Al_3Sc_4Ta_6Y_2C_9$** + AlY_3C + Y_4C_5 + **$Al_3Sc_2Ta_{10}C_9$**
Y	Sc	Cr	-7.947882	N/A	N/A	-8.297372	349	N/A	N/A	Y_4C_7 + AlY_3C_3 + $CrSc_2C_3$ + $Cr_2Y_2C_3$ + **$Al_3Cr_4Sc_2C_3$**
Y	Sc	Mo	-8.358438	N/A	N/A	-8.623452	265	N/A	N/A	**$Al_3Mo_4Sc_3Y_2C_6$** + **$Al_3Mo_4Y_2C_3$** + $MoYC_2$
Y	Sc	W	-8.880748	N/A	N/A	-9.141503	261	N/A	N/A	WYC_2 + **$Al_3Sc_3W_4Y_2C_6$** + **$Al_3W_4Y_2C_3$**
Y	Sc	Mn	-7.771014	N/A	N/A	-8.193482	422	N/A	N/A	Y_4C_7 + $Mn_{13}Y_{10}C_{18}$ + AlY_3C_3 + Sc_3C_4 + **$Al_3Mn_4Sc_2C_3$**
Y	Sc	Fe	-7.456765	N/A	N/A	-7.965976	509	N/A	N/A	Y_3C_4 + Y_4C_7 + $AlFe_3$ + Al_6Fe_6Sc + $FeSc_3C_4$
Ti	Sc	Sc	-7.841289	N/A	N/A	-7.970180	129	N/A	N/A	Sc_3C_4 + Al_3ScC_3 + $AlSc_3C$ + TiC
Ti	Sc	Y	-7.693000	N/A	N/A	-7.954305	261	N/A	N/A	AlY_3C_3 + AlY_3C + Al_2Y + $AlSc_3C$ + TiC
Ti	Sc	Ti	-8.502966	N/A	-8.534432	-8.520244	17	N/A	-14	**$Al_3Sc_2Ti_7C_6$** + TiC
Ti	Sc	Zr	-8.639927	-8.648219	-8.659016	-8.693110	53	45	34	**$Al_3Sc_2Zr_{10}C_9$** + **$Al_3Sc_2Ti_{10}C_9$**
Ti	Sc	Hf	-9.067886	-9.070799	-9.073137	-9.096218	28	25	23	**$Al_3Sc_2Ti_{10}C_9$** + **$Al_3Hf_{10}Sc_2C_9$**
Ti	Sc	V	-8.603169	-8.698170	-8.689776	-8.701929	99	4	12	Sc_3C_4 + **$Al_3Sc_2Ti_3V_4C_6$** + Al_3ScC_3 + V_6C_5 + TiC
Ti	Sc	Nb	-8.915776	-8.979887	-9.001604	-9.003095	87	23	1	**$Al_3Nb_4Sc_2Ti_6C_9$** + **$Al_3Nb_{10}Sc_2C_9$**
Ti	Sc	Ta	-9.425534	-9.473389	-9.492910	-9.492154	67	19	-1	**$Al_3Sc_2Ta_4Ti_6C_9$** + **$Al_3Sc_2Ta_{10}C_9$**
Ti	Sc	Cr	-8.447597	N/A	N/A	-8.671307	224	N/A	N/A	**$Al_3Cr_4Sc_2Ti_3C_6$** + **$Al_3Cr_4Sc_2Ti_6C_9$** + C + Cr_3C_2
Ti	Sc	Mo	-8.827430	N/A	N/A	-8.997056	170	N/A	N/A	**$AlMo_2Ti_2C_3$** + C + Mo_2C + **$Al_3Mo_4Sc_5C_6$** + TiC
Ti	Sc	W	-9.337211	N/A	N/A	-9.506156	169	N/A	N/A	**$Al_3Sc_2Ti_6W_4C_9$** + **$Al_3Sc_2Ti_3W_4C_6$** + WC
Ti	Sc	Mn	-8.267174	N/A	N/A	-8.551910	285	N/A	N/A	Mn_7C_3 + C + **$Al_3Mn_4Sc_2C_3$** + TiC
Ti	Sc	Fe	-7.927386	N/A	N/A	-8.345799	418	N/A	N/A	$AlFe_3C$ + Al_6Fe_6Sc + C + $FeSc_3C_4$ + TiC
Zr	Sc	Sc	-7.924151	N/A	N/A	-8.078081	154	N/A	N/A	Sc_3C_4 + Al_3ScC_3 + $AlSc_3C$ + ZrC
Zr	Sc	Y	-7.815289	N/A	N/A	-8.062206	247	N/A	N/A	ZrC + AlY_3C_3 + Al_2Y + AlY_3C + $AlSc_3C$
Zr	Sc	Ti	-8.529873	-8.599797	-8.605310	-8.640217	110	40	35	**$Al_3Sc_2Zr_{10}C_9$** + **$Al_3Sc_2Ti_{10}C_9$**

Zr	Sc	Zr	-8.738645	N/A	-8.798895	-8.783282	45	N/A	-16	**$Al_3Sc_2Zr_7C_6$** + ZrC
Zr	Sc	Hf	-9.152616	-9.192561	-9.200017	-9.202004	49	9	2	**$Al_3Sc_2Zr_{10}C_9$** + **$Al_3Hf_{10}Sc_2C_9$**
Zr	Sc	V	-8.603676	-8.697709	-8.719337	-8.801693	198	104	82	**$Al_3Sc_2V_7C_6$** + ZrC + **$Al_3Sc_2Zr_{10}C_9$**
Zr	Sc	Nb	-8.975378	-9.059580	-9.095316	-9.102764	127	43	7	ZrC + **$Al_3Nb_4Sc_2Zr_6C_9$** + **$Al_3Nb_7Sc_2C_6$**
Zr	Sc	Ta	-9.475027	-9.543834	-9.578195	-9.585947	111	42	8	**$Al_3Sc_2Ta_4Zr_6C_9$** + **$Al_3Sc_2Ta_{10}C_9$**
Zr	Sc	Cr	-8.454540	N/A	N/A	-8.774157	320	N/A	N/A	C + **$Al_3Cr_4Sc_2C_3$** + Cr_3C_2 + ZrC
Zr	Sc	Mo	-8.852146	N/A	N/A	-9.080932	229	N/A	N/A	ZrC + **$Al_3Mo_4Sc_2C_3$** + C + Mo_2C
Zr	Sc	W	-9.363303	N/A	N/A	-9.581404	218	N/A	N/A	**$Al_3Sc_2W_4C_3$** + ZrC + WC
Zr	Sc	Mn	-8.268885	N/A	N/A	-8.659811	391	N/A	N/A	Mn_7C_3 + C + **$Al_3Mn_4Sc_2C_3$** + ZrC
Zr	Sc	Fe	-7.955722	N/A	N/A	-8.453700	498	N/A	N/A	Al_6Fe_6Sc + $AlFe_3C$ + C + $FeSc_3C_4$ + ZrC
Hf	Sc	Sc	-8.189173	N/A	N/A	-8.357942	169	N/A	N/A	Sc_3C_4 + Al_3ScC_3 + $AlSc_3C$ + HfC
Hf	Sc	Y	-8.088819	N/A	N/A	-8.342067	253	N/A	N/A	AlY_3C_3 + AlY_3C + Al_2Y + $AlSc_3C$ + HfC
Hf	Sc	Ti	-8.803875	-8.887298	-8.885716	-8.908956	105	22	23	**$Al_3Sc_2Ti_{10}C_9$** + **$Al_3Hf_{10}Sc_2C_9$**
Hf	Sc	Zr	-9.000064	-9.056848	-9.065245	-9.067634	68	11	2	**$Al_3Sc_2Zr_{10}C_9$** + **$Al_3Hf_{10}Sc_2C_9$**
Hf	Sc	Hf	-9.417145	N/A	-9.470742	-9.456605	39	N/A	-14	**$Al_3Hf_7Sc_2C_6$** + HfC
Hf	Sc	V	-8.878334	-8.986978	-9.000065	-9.078815	200	92	79	**$Al_3Sc_2V_4C_3$** + **$Al_3Sc_2V_7C_6$** + HfC
Hf	Sc	Nb	-9.237806	-9.334325	-9.364810	-9.378297	140	44	13	**$Al_3Hf_{10}Sc_2C_9$** + **$Al_3Nb_7Sc_2C_6$** + HfC
Hf	Sc	Ta	-9.735205	-9.820013	-9.848718	-9.855133	120	35	6	**$Al_3Hf_6Sc_2Ta_4C_9$** + **$Al_3Sc_2Ta_{10}C_9$**
Hf	Sc	Cr	-8.727473	N/A	N/A	-9.054019	327	N/A	N/A	**$Al_3Cr_4Sc_2C_3$** + C + Cr_3C_2 + HfC
Hf	Sc	Mo	-9.115648	N/A	N/A	-9.360794	245	N/A	N/A	**$Al_3Mo_4Sc_2C_3$** + C + Mo_2C + HfC
Hf	Sc	W	-9.624561	N/A	N/A	-9.861266	237	N/A	N/A	**$Al_3Sc_2W_4C_3$** + WC + HfC
Hf	Sc	Mn	-8.540835	N/A	N/A	-8.939673	399	N/A	N/A	Mn_7C_3 + C + **$Al_3Mn_4Sc_2C_3$** + HfC
Hf	Sc	Fe	-8.224457	N/A	N/A	-8.733562	509	N/A	N/A	$AlFe_3C$ + Al_6Fe_6Sc + C + $FeSc_3C_4$ + HfC
V	Sc	Sc	-8.008068	N/A	N/A	-8.076981	69	N/A	N/A	**$AlSc_2VC_2$** + Sc_3C_4 + **$Al_3Sc_2V_7C_6$** + $AlSc_3C$
V	Sc	Y	-7.825516	N/A	N/A	-8.059917	234	N/A	N/A	**$Al_3Sc_3V_4Y_2C_6$** + V_6C_5 + AlY_3C_3 + AlY_3C + $AlSc_3C$
V	Sc	Ti	-8.644974	-8.650518	-8.640908	-8.654369	9	4	13	**$Al_3Sc_2Ti_3V_4C_6$** + TiC
V	Sc	Zr	-8.743064	-8.698088	-8.726897	-8.800760	58	103	74	**$Al_3Sc_2V_7C_6$** + ZrC + **$Al_3Sc_2Zr_{10}C_9$**
V	Sc	Hf	-9.170925	-9.121460	-9.140284	-9.212335	41	91	72	**$Al_3Sc_2V_4C_3$** + HfC
V	Sc	V	-8.745051	N/A	-8.795788	-8.793111	48	N/A	-3	Sc_3C_4 + **$Al_3Sc_2V_7C_6$** + Al_3ScC_3 + V_6C_5
V	Sc	Nb	-9.037499	-9.033391	-9.066985	-9.099395	62	66	32	**$Al_3Sc_2V_{10}C_9$** + **$Al_3Nb_{10}Sc_2C_9$**
V	Sc	Ta	-9.544519	-9.527567	-9.556722	-9.580586	36	53	24	**$Al_3Sc_2V_{10}C_9$** + **$Al_3Sc_2Ta_{10}C_9$**
V	Sc	Cr	-8.591272	N/A	N/A	-8.764204	173	N/A	N/A	Cr_3C_2 + **$Al_3Cr_4Sc_2V_3C_6$** + C + V_6C_5
V	Sc	Mo	-8.957421	N/A	N/A	-9.068123	111	N/A	N/A	V_6C_5 + **$Al_3Mo_4Sc_2C_3$** + C + Mo_2C
V	Sc	W	-9.461475	N/A	N/A	-9.579155	118	N/A	N/A	Al_3ScC_3 + **$Al_3V_4W_2C_3$** + **$Al_3Sc_5W_4C_6$** + WC + V_6C_5
V	Sc	Mn	-8.422101	N/A	N/A	-8.647002	225	N/A	N/A	V_6C_5 + Mn_7C_3 + C + **$Al_3Mn_4Sc_2C_3$**
V	Sc	Fe	-8.092177	N/A	N/A	-8.440891	349	N/A	N/A	$AlFe_3C$ + Al_6Fe_6Sc + C + $FeSc_3C_4$ + V_6C_5
Nb	Sc	Sc	-8.203353	N/A	N/A	-8.316238	113	N/A	N/A	**$AlNb_2Sc_2C_3$** + Sc_3C_4 + **$AlNbSc_2C_2$** + Sc_4C_3
Nb	Sc	Y	-8.069761	N/A	N/A	-8.274998	205	N/A	N/A	AlY_3C + **$Al_3Nb_6Sc_4Y_2C_9$** + AlY_3C_3 + **$Al_3Nb_{10}Sc_2C_9$** + Y_4C_5
Nb	Sc	Ti	-8.793135	-8.844265	-8.853743	-8.845880	53	2	-8	**$Al_3Sc_2Ti_{10}C_9$** + **$Al_3Nb_6Sc_2Ti_4C_9$**
Nb	Sc	Zr	-8.953801	-8.970888	-9.002305	-9.001237	47	30	-1	ZrC + **$Al_3Sc_2Zr_{10}C_9$** + **$Al_3Nb_7Sc_2C_6$**
Nb	Sc	Hf	-9.372226	-9.380248	-9.405433	-9.409112	37	29	4	**$Al_3Hf_{10}Sc_2C_9$** + **$Al_3Nb_7Sc_2C_6$** + HfC
Nb	Sc	V	-8.850353	-8.939836	-8.964364	-8.998193	148	58	34	**$Al_3Sc_2V_{10}C_9$** + **$Al_3Nb_{10}Sc_2C_9$**
Nb	Sc	Nb	-9.206708	N/A	-9.301800	-9.270949	64	N/A	-31	**$Al_3Nb_7Sc_2C_6$** + C + Nb_6C_5
Nb	Sc	Ta	-9.711573	-9.739090	-9.783995	-9.783966	72	45	0	**$Al_3Nb_6Sc_2Ta_4C_9$** + **$Al_3Sc_2Ta_{10}C_9$**

Nb	Sc	Cr	-8.699975	N/A	N/A	-8.951465	251	N/A	N/A	C + **$Al_3Cr_4Sc_2C_3$** + Cr_3C_2 + **$Al_3Nb_{10}Sc_2C_9$**
Nb	Sc	Mo	-9.071983	N/A	N/A	-9.255055	183	N/A	N/A	**$Al_3Mo_4Sc_2C_3$** + **$Al_3Nb_{10}Sc_2C_9$** + Mo_2C + C
Nb	Sc	W	-9.571512	N/A	N/A	-9.774138	203	N/A	N/A	**$Al_3Nb_{10}Sc_2C_9$** + **$Al_3Sc_2W_4C_3$** + WC
Nb	Sc	Mn	-8.521170	N/A	N/A	-8.826779	306	N/A	N/A	**$Al_3Nb_{10}Sc_2C_9$** + Mn_7C_3 + C + **$Al_3Mn_4Sc_2C_3$**
Nb	Sc	Fe	-8.195131	N/A	N/A	-8.630017	435	N/A	N/A	**$Al_3Nb_{10}Sc_2C_9$** + $AlFe_3C$ + $FeSc_3C_4$ + C + Fe
Ta	Sc	Sc	-8.533132	N/A	N/A	-8.647643	115	N/A	N/A	Sc_3C_4 + **$AlSc_2TaC_2$** + $AlSc_3C$ + **$AlSc_2Ta_2C_3$**
Ta	Sc	Y	-8.393658	N/A	N/A	-8.603394	210	N/A	N/A	AlY_3C_3 + **$Al_3Sc_4Ta_6Y_2C_9$** + AlY_3C + Y_4C_5 + **$Al_3Sc_2Ta_{10}C_9$**
Ta	Sc	Ti	-9.111317	-9.178925	-9.186339	-9.173494	62	-5	-13	**$Al_3Sc_2Ta_3Ti_4C_6$** + **$Al_3Sc_2Ta_6Ti_4C_9$** + TiC
Ta	Sc	Zr	-9.266708	-9.296219	-9.327028	-9.320851	54	25	-6	**$Al_3Sc_2Zr_{10}C_9$** + **$Al_3Sc_2Ta_{10}C_9$**
Ta	Sc	Hf	-9.685138	-9.706499	-9.730807	-9.726651	42	20	-4	**$Al_3Hf_3Sc_2Ta_4C_6$** + HfC
Ta	Sc	V	-9.162379	-9.272585	-9.293475	-9.318987	157	46	26	**$Al_3Sc_2V_{10}C_9$** + **$Al_3Sc_2Ta_{10}C_9$**
Ta	Sc	Nb	-9.509728	-9.578150	-9.624056	-9.623263	114	45	-1	**$Al_3Nb_4Sc_2Ta_6C_9$** + **$Al_3Nb_{10}Sc_2C_9$**
Ta	Sc	Ta	-10.010016	N/A	-10.103785	-10.057719	48	N/A	-46	**$Al_3Sc_2Ta_7C_6$** + TaC
Ta	Sc	Cr	-9.011281	N/A	N/A	-9.272259	261	N/A	N/A	Cr_3C_2 + **$Al_3Cr_4Sc_2C_3$** + C + **$Al_3Sc_2Ta_{10}C_9$**
Ta	Sc	Mo	-9.376012	N/A	N/A	-9.578604	203	N/A	N/A	**$Al_3Mo_4Sc_2C_3$** + **$Al_3Mo_4Sc_2Ta_6C_9$** + C + Mo_2C
Ta	Sc	W	-9.869880	N/A	N/A	-10.094932	225	N/A	N/A	**$Al_3Sc_2W_4C_3$** + WC + **$Al_3Sc_2Ta_{10}C_9$**
Ta	Sc	Mn	-8.833607	N/A	N/A	-9.153513	320	N/A	N/A	**$Al_3Mn_4Sc_2Ta_6C_9$** + C + Mn_7C_3 + **$Al_3Mn_4Sc_2C_3$**
Ta	Sc	Fe	-8.505270	N/A	N/A	-8.950811	446	N/A	N/A	$AlFe_3C$ + **$Al_3Sc_2Ta_{10}C_9$** + Fe + C + $FeSc_3C_4$
Cr	Sc	Sc	-7.998431	N/A	N/A	-8.087152	89	N/A	N/A	$CrSc_2C_3$ + **$Al_3Cr_4Sc_2C_3$** + Al_3ScC_3 + $AlSc_3C$
Cr	Sc	Y	-7.812645	N/A	N/A	-8.061285	249	N/A	N/A	AlY_3C_3 + $CrSc_2C_3$ + $Cr_2Y_2C_3$ + Al_2Y + $AlSc_3C$
Cr	Sc	Ti	-8.647034	-8.575762	-8.569880	-8.644705	-2	69	75	**$Al_3Cr_4Sc_2Ti_3C_6$** + TiC
Cr	Sc	Zr	-8.731232	-8.612132	-8.646231	-8.802282	71	190	156	**$Al_3Cr_4Sc_2C_3$** + ZrC
Cr	Sc	Hf	-9.159880	-9.035767	-9.056991	-9.222074	62	186	165	**$Al_3Cr_4Sc_2C_3$** + HfC
Cr	Sc	V	-8.765365	-8.739429	-8.733892	-8.785924	21	46	52	**$Al_3Cr_4Sc_2V_3C_6$** + C + V_6C_5
Cr	Sc	Nb	-9.040332	-8.956817	-8.983734	-9.068243	28	111	85	C + **$Al_3Cr_4Sc_2C_3$** + Cr_3C_2 + **$Al_3Nb_{10}Sc_2C_9$**
Cr	Sc	Ta	-9.544656	-9.451546	-9.472929	-9.549434	5	98	77	Cr_3C_2 + **$Al_3Cr_4Sc_2C_3$** + C + **$Al_3Sc_2Ta_{10}C_9$**
Cr	Sc	Cr	-8.617383	N/A	N/A	-8.717908	101	N/A	N/A	**$Al_3Cr_4Sc_2C_3$** + Cr_3C_2 + C
Cr	Sc	Mo	-8.966372	N/A	N/A	-9.024682	58	N/A	N/A	Mo_2C + **$Al_3Mo_4Sc_2C_3$** + C + Cr_3C_2
Cr	Sc	W	-9.465741	N/A	N/A	-9.563721	98	N/A	N/A	WC + **$Al_3Cr_4Sc_2C_3$**
Cr	Sc	Mn	-8.436497	N/A	N/A	-8.603561	167	N/A	N/A	Mn_7C_3 + C + Cr_3C_2 + **$Al_3Mn_4Sc_2C_3$**
Cr	Sc	Fe	-8.114465	N/A	N/A	-8.402138	288	N/A	N/A	Cr_3C_2 + Al_6Fe_6Sc + C + $AlFe_3C$ + $CrScC_2$
Mo	Sc	Sc	-8.250587	N/A	N/A	-8.320725	70	N/A	N/A	**$Al_3Mo_4Sc_5C_6$** + Sc_3C_4 + Sc_4C_3
Mo	Sc	Y	-8.093127	N/A	N/A	-8.284426	191	N/A	N/A	**$Al_3Mo_4Sc_3Y_2C_6$** + **$Al_3Mo_4Y_2C_3$** + Y_2C + Y_4C_5
Mo	Sc	Ti	-8.855784	-8.840201	-8.860351	-8.854983	-1	15	-5	**$Al_3Mo_4Sc_2Ti_3C_6$** + TiC
Mo	Sc	Zr	-8.982245	-8.928851	-8.972061	-9.009453	27	81	37	ZrC + **$Al_3Mo_4Sc_2C_3$**
Mo	Sc	Hf	-9.404282	-9.342884	-9.378440	-9.429245	25	86	51	**$Al_3Mo_4Sc_2C_3$** + HfC
Mo	Sc	V	-8.937284	-8.954780	-8.973368	-8.990239	53	35	17	V_6C_5 + **$Al_3Mo_4Sc_2C_3$** + C
Mo	Sc	Nb	-9.256036	-9.220689	-9.267701	-9.270636	15	50	3	**$Al_3Mo_4Sc_2C_3$** + **$Al_3Nb_{10}Sc_2C_9$** + Mo_2C + C
Mo	Sc	Ta	-9.755960	-9.703979	-9.745162	-9.751828	-4	48	7	**$Al_3Mo_4Sc_2C_3$** + **$Al_3Sc_2Ta_{10}C_9$** + C + Mo_2C
Mo	Sc	Cr	-8.773427	N/A	N/A	-8.925078	152	N/A	N/A	**$Al_3Mo_4Sc_2C_3$** + C + Cr_3C_2
Mo	Sc	Mo	-9.129466	N/A	N/A	-9.223891	94	N/A	N/A	**$Al_3Mo_4Sc_2C_3$** + C + Mo_2C
Mo	Sc	W	-9.621814	N/A	N/A	-9.770891	149	N/A	N/A	**$Al_3Mo_4Sc_2C_3$** + WC
Mo	Sc	Mn	-8.589596	N/A	N/A	-8.802770	213	N/A	N/A	Mn_7C_3 + Mo_2C + C + **$Al_3Mn_4Sc_2C_3$**
Mo	Sc	Fe	-8.275299	N/A	N/A	-8.603612	328	N/A	N/A	$AlFe_3C$ + **$Al_3Mo_4Sc_5C_6$** + C + $FeSc_3C_4$ + Mo_2C

W	Sc	Sc	-8.598376	N/A	N/A	-8.664898	67	N/A	N/A	Sc_3C_4 + **$Al_3Sc_5W_4C_6$** + Sc_4C_3
W	Sc	Y	-8.440500	N/A	N/A	-8.626896	186	N/A	N/A	AlY_3C_3 + WYC_2 + **$Al_3Sc_3W_4Y_2C_6$** + AlY_3C + Y_4C_5
W	Sc	Ti	-9.184518	-9.188560	-9.211041	-9.192068	8	4	-19	**$Al_3Sc_2Ti_3W_4C_6$** + TiC
W	Sc	Zr	-9.308233	-9.273176	-9.318450	-9.327591	19	54	9	**$Al_3Sc_2W_4C_3$** + ZrC
W	Sc	Hf	-9.730481	-9.686098	-9.723876	-9.747384	17	61	24	**$Al_3Sc_2W_4C_3$** + HfC
W	Sc	V	-9.254990	-9.293158	-9.310941	-9.320239	65	27	9	Al_3ScC_3 + **$Al_3V_4W_2C_3$** + **$Al_3Sc_5W_4C_6$** + WC + V_6C_5
W	Sc	Nb	-9.568692	-9.550138	-9.596753	-9.616692	48	67	20	**$Al_3Nb_{10}Sc_2C_9$** + **$Al_3Sc_2W_4C_3$** + WC
W	Sc	Ta	-10.065846	-10.027311	-10.067809	-10.097883	32	71	30	**$Al_3Sc_2W_4C_3$** + WC + **$Al_3Sc_2Ta_{10}C_9$**
W	Sc	Cr	-9.090076	N/A	N/A	-9.281783	192	N/A	N/A	Cr_3C_2 + C + WC + **$Al_3Cr_4Sc_2C_3$**
W	Sc	Mo	-9.432676	N/A	N/A	-9.588558	156	N/A	N/A	C + **$Al_3Mo_4Sc_2C_3$** + WC + Mo_2C
W	Sc	W	-9.917963	N/A	N/A	-10.089030	171	N/A	N/A	**$Al_3Sc_2W_4C_3$** + WC
W	Sc	Mn	-8.904911	N/A	N/A	-9.167437	263	N/A	N/A	Mn_7C_3 + C + WC + **$Al_3Mn_4Sc_2C_3$**
W	Sc	Fe	-8.587750	N/A	N/A	-8.961326	374	N/A	N/A	Al_6Fe_6Sc + C + $AlFe_3C$ + $FeSc_3C_4$ + WC
Mn	Sc	Sc	-7.927239	N/A	N/A	-8.001948	75	N/A	N/A	Sc_3C_4 + **$Al_3Mn_4Sc_2C_3$** + Sc_4C_3
Mn	Sc	Y	-7.757085	N/A	N/A	-7.988108	231	N/A	N/A	AlY_3C + $Mn_{13}Y_{10}C_{18}$ + AlY_3C_3 + $AlSc_3C$ + **$Al_3Mn_4Sc_2C_3$**
Mn	Sc	Ti	-8.572314	-8.451449	-8.447143	-8.572816	1	121	126	**$Al_3Mn_4Sc_2C_3$** + TiC
Mn	Sc	Zr	-8.652260	-8.492593	-8.532617	-8.734668	82	242	202	**$Al_3Mn_4Sc_2C_3$** + ZrC
Mn	Sc	Hf	-9.080152	-8.917492	-8.944527	-9.154460	74	237	210	**$Al_3Mn_4Sc_2C_3$** + HfC
Mn	Sc	V	-8.697353	-8.621910	-8.610691	-8.715454	18	94	105	V_6C_5 + C + **$Al_3Mn_4Sc_2C_3$**
Mn	Sc	Nb	-8.970087	-8.832731	-8.864893	-8.985119	15	152	120	**$Al_3Nb_{10}Sc_2C_9$** + Mn_7C_3 + C + **$Al_3Mn_4Sc_2C_3$**
Mn	Sc	Ta	-9.475221	-9.326305	-9.351706	-9.466310	-9	140	115	C + **$Al_3Sc_2Ta_{10}C_9$** + Mn_7C_3 + **$Al_3Mn_4Sc_2C_3$**
Mn	Sc	Cr	-8.540426	N/A	N/A	-8.650293	110	N/A	N/A	C + Cr_3C_2 + **$Al_3Mn_4Sc_2C_3$**
Mn	Sc	Mo	-8.868289	N/A	N/A	-8.949106	81	N/A	N/A	Mo_2C + C + **$Al_3Mn_4Sc_2C_3$**
Mn	Sc	W	-9.360783	N/A	N/A	-9.496106	135	N/A	N/A	WC + **$Al_3Mn_4Sc_2C_3$**
Mn	Sc	Mn	-8.349995	N/A	N/A	-8.510098	160	N/A	N/A	**$Al_3Mn_4Sc_2C_3$** + C + Mn_7C_3
Mn	Sc	Fe	-8.017351	N/A	N/A	-8.313362	296	N/A	N/A	$AlFe_3C$ + **$Al_3Mn_4Sc_2C_3$** + C + $FeSc_3C_4$ + Mn_7C_3
Fe	Sc	Sc	-7.792756	N/A	N/A	-7.894206	101	N/A	N/A	Al_6Fe_6Sc + Al_8Fe_4Sc + $FeSc_3C_4$ + $AlSc_3C$
Fe	Sc	Y	-7.646698	N/A	N/A	-7.845462	199	N/A	N/A	$AlFe_3$ + Al_6Fe_6Sc + $FeSc_3C_4$ + AlY_3C_3 + Y_4C_5
Fe	Sc	Ti	-8.417082	-8.240216	-8.240061	-8.427170	10	187	187	$AlFe_3C$ + Al_6Fe_6Sc + C + $FeSc_3C_4$ + TiC
Fe	Sc	Zr	-8.511387	-8.291442	-8.339770	-8.589022	78	298	249	Al_6Fe_6Sc + $AlFe_3C$ + C + $FeSc_3C_4$ + ZrC
Fe	Sc	Hf	-8.936821	-8.699272	-8.731137	-9.008814	72	310	278	$AlFe_3C$ + Al_6Fe_6Sc + C + $FeSc_3C_4$ + HfC
Fe	Sc	V	-8.531344	-8.422114	-8.408402	-8.569808	38	148	161	$AlFe_3C$ + Al_6Fe_6Sc + C + $FeSc_3C_4$ + V_6C_5
Fe	Sc	Nb	-8.819571	-8.625931	-8.651382	-8.853945	34	228	203	**$Al_3Nb_{10}Sc_2C_9$** + $AlFe_3C$ + $FeSc_3C_4$ + C + Fe
Fe	Sc	Ta	-9.325782	-9.119208	-9.137913	-9.335136	9	216	197	$AlFe_3C$ + **$Al_3Sc_2Ta_{10}C_9$** + Fe + C + $FeSc_3C_4$
Fe	Sc	Cr	-8.375897	N/A	N/A	-8.508888	133	N/A	N/A	Cr_3C_2 + Al_6Fe_6Sc + C + $AlFe_3C$ + $CrScC_2$
Fe	Sc	Mo	-8.701017	N/A	N/A	-8.812457	111	N/A	N/A	**$AlMo_2ScC_2$** + $AlFe_3C$ + **$Al_3Mo_4Sc_5C_6$** + C + Mo_2C
Fe	Sc	W	-9.190135	N/A	N/A	-9.350460	160	N/A	N/A	Al_6Fe_6Sc + C + $AlFe_3C$ + $FeSc_3C_4$ + WC
Fe	Sc	Mn	-8.195341	N/A	N/A	-8.378941	184	N/A	N/A	$AlFe_3C$ + **$Al_3Mn_4Sc_2C_3$** + C + $FeSc_3C_4$ + Mn_7C_3
Fe	Sc	Fe	-7.857263	N/A	N/A	-8.182162	325	N/A	N/A	$AlFe_3C$ + Fe + $FeSc_3C_4$ + C

Table S4. Structural information for stable 413 *s*-MAX phases in Figure 3a. The space group symmetry is $P6_3/mcm$ (#193).

s-MAX phase	*a* (Å)	*c* (Å)	Wyckoff positions
$Cr_4Sc_2Ta_6Al_3C_9$	5.36118	23.21780	Cr1 8h (0.33333, 0.66667, 0.34703) Sc1 4e (0.00000, 0.00000, 0.82546) Ta1 12k (0.67223, 0.00000, -0.05816) Al1 6g (0.48933, 0.00000, 0.25000) C1 4d (0.33333, 0.66667, 0.00000) C2 2b (0.00000, 0.00000, 0.00000) C3 12k (0.65965, 0.00000, 0.38513)
$Cr_4Sc_2Ti_6Al_3C_9$	5.28647	22.79810	Cr1 8h (0.33333, 0.66667, 0.84961) Sc1 4e (0.00000, 0.00000, 0.82735) Ti1 12k (0.33106, 0.00000, -0.05308) Al1 6g (0.51043, 0.00000, 0.25000) C1 4d (0.33333, 0.66667, 0.00000) C2 2b (0.00000, 0.00000, 0.00000) C3 12k (0.34639, 0.00000, 0.38758)
$Fe_4Sc_2Ta_6Al_3C_9$	5.38285	22.39540	Fe1 8h (0.33333, 0.66667, 0.34730) Sc1 4e (0.00000, 0.00000, 0.82312) Ta1 12k (0.67036, 0.00000, -0.06036) Al1 6g (0.49514, 0.00000, 0.25000) C1 4d (0.33333, 0.66667, 0.00000) C2 2b (0.00000, 0.00000, 0.00000) C3 12k (0.66248, 0.00000, 0.38132)
$Mn_4Sc_2Ta_6Al_3C_9$	5.36220	22.77920	Mn1 8h (0.33333, 0.66667, 0.34682) Sc1 4e (0.00000, 0.00000, 0.82458) Ta1 12k (0.67163, 0.00000, -0.05952) Al1 6g (0.49094, 0.00000, 0.25000) C1 4d (0.33333, 0.66667, 0.00000) C2 2b (0.00000, 0.00000, 0.00000) C3 12k (0.66079, 0.00000, 0.38321)
$Mo_4Sc_2Nb_6Al_3C_9$	5.45648	24.08740	Mo1 8h (0.33333, 0.66667, 0.15305) Sc1 4e (0.00000, 0.00000, 0.66998) Nb1 12k (0.67275, 0.00000, 0.05592) Al1 6g (0.52070, 0.00000, 0.25000) C1 4d (0.33333, 0.66667, 0.00000) C2 2b (0.00000, 0.00000, 0.00000) C3 12k (0.66695, 0.00000, 0.61070)
$Mo_4Sc_2Ta_6Al_3C_9$	5.44239	24.00560	Mo1 8h (0.33333, 0.66667, 0.15289) Sc1 4e (0.00000, 0.00000, 0.66972) Ta1 12k (0.67282, 0.00000, 0.05594) Al1 6g (0.52009, 0.00000, 0.25000) C1 4d (0.33333, 0.66667, 0.00000) C2 2b (0.00000, 0.00000, 0.00000) C3 12k (0.66841, 0.00000, 0.60923)
$Mo_4Sc_2Ti_6Al_3C_9$	5.37472	23.55790	Mo1 8h (0.33333, 0.66667, 0.15078) Sc1 4e (0.00000, 0.00000, 0.66832) Ti1 12k (0.66881, 0.00000, 0.05110) Al1 6g (0.51966, 0.00000, 0.25000) C1 4d (0.33333, 0.66667, 0.00000) C2 2b (0.00000, 0.00000, 0.00000) C3 12k (0.66207, 0.00000, 0.60696)
$Ta_4Sc_2Ta_6Al_3C_9$	5.47424	24.39320	Ta1 8h (0.33333, 0.66667, 0.15497) Sc1 4e (0.00000, 0.00000, 0.66194) Ta2 12k (0.67134, 0.00000, 0.05445) Al1 6g (0.62752, 0.00000, 0.25000) C1 4d (0.33333, 0.66667, 0.00000) C2 2b (0.00000, 0.00000, 0.00000) C3 12k (0.66420, 0.00000, 0.60697)

$Ti_4Sc_2Ti_6Al_3C_9$	5.39517	23.78740	Ti1 8h (0.33333, 0.66667, 0.35089) Sc1 4e (0.00000, 0.00000, 0.83570) Ti2 12k (0.66832, 0.00000, -0.05073) Al1 6g (0.47512, 0.00000, 0.25000) C1 4d (0.33333, 0.66667, 0.00000) C2 2b (0.00000, 0.00000, 0.00000) C3 12k (0.66248, 0.00000, 0.39374)
$V_4Sc_2Ta_6Al_3C_9$	5.38606	23.65430	V1 8h (0.33333, 0.66667, 0.34610) Sc1 4e (0.00000, 0.00000, 0.82933) Ta1 12k (0.67189, 0.00000, -0.05676) Al1 6g (0.48211, 0.00000, 0.25000) C1 4d (0.33333, 0.66667, 0.00000) C2 2b (0.00000, 0.00000, 0.00000) C3 12k (0.66141, 0.00000, 0.38805)
$W_4Sc_2Ta_6Al_3C_9$	5.43799	24.04390	W1 8h (0.33333, 0.66667, 0.34685) Sc1 4e (0.00000, 0.00000, 0.33006) Ta1 12k (0.32659, 0.00000, 0.44413) Al1 6g (0.47526, 0.00000, 0.25000) C1 4d (0.33333, 0.66667, 0.00000) C2 2b (0.00000, 0.00000, 0.00000) C3 12k (0.33197, 0.00000, 0.89061)

Table S5. Structural information for stable 413 *s*-MAX phases in Figure 3b. The space group symmetry is $P6_3/mcm$ (#193).

s-MAX phase	*a* (Å)	*c* (Å)	Wyckoff positions
$Cr_4Y_2Ta_6Al_3C_9$	5.40528	23.64300	Cr1 8h (0.33333, 0.66667, 0.14999) Y1 4e (0.00000, 0.00000, 0.67655) Ta1 12k (0.67317, 0.00000, 0.05685) Al1 6g (0.50415, 0.00000, 0.25000) C1 4d (0.33333, 0.66667, 0.00000) C2 2b (0.00000, 0.00000, 0.00000) C3 12k (0.65394, 0.00000, 0.61199)
$Cr_4Y_2Ti_6Al_3C_9$	5.34229	23.23110	Cr1 8h (0.33333, 0.66667, 0.64745) Y1 4e (0.00000, 0.00000, 0.67478) Ti1 12k (0.66911, 0.00000, 0.55179) Al1 6g (0.49586, 0.00000, 0.25000) C1 4d (0.33333, 0.66667, 0.00000) C2 2b (0.00000, 0.00000, 0.00000) C3 12k (0.64603, 0.00000, 0.10989)
$Fe_4Y_2Ta_6Al_3C_9$	5.42269	22.97520	Fe1 8h (0.33333, 0.66667, 0.14922) Y1 4e (0.00000, 0.00000, 0.67789) Ta1 12k (0.67136, 0.00000, 0.05867) Al1 6g (0.50332, 0.00000, 0.25000) C1 4d (0.33333, 0.66667, 0.00000) C2 2b (0.00000, 0.00000, 0.00000) C3 12k (0.65668, 0.00000, 0.61464)
$Mn_4Y_2Nb_6Al_3C_9$	5.41947	23.31100	Mn1 8h (0.33333, 0.66667, 0.65054) Y1 4e (0.00000, 0.00000, 0.67738) Nb1 12k (0.67263, 0.00000, 0.55800) Al1 6g (0.49543, 0.00000, 0.25000) C1 4d (0.33333, 0.66667, 0.00000) C2 2b (0.00000, 0.00000, 0.00000) C3 12k (0.65142, 0.00000, 0.11525)
$Mn_4Y_2Ta_6Al_3C_9$	5.40765	23.22590	Mn1 8h (0.33333, 0.66667, 0.65022) Y1 4e (0.00000, 0.00000, 0.17722) Ta1 12k (0.67274, 0.00000, 0.55813) Al1 6g (0.49557, 0.00000, 0.25000) C1 4d (0.33333, 0.66667, 0.00000) C2 2b (0.00000, 0.00000, 0.00000) C3 12k (0.65485, 0.00000, 0.11362)
$Mn_4Y_2Ti_6Al_3C_9$	5.32595	22.86680	Mn1 8h (0.33333, 0.66667, 0.35195) Y1 4e (0.00000, 0.00000, 0.32426) Ti1 12k (0.33088, 0.00000, 0.44704) Al1 6g (0.49678, 0.00000, 0.25000) C1 4d (0.33333, 0.66667, 0.00000) C2 2b (0.00000, 0.00000, 0.00000) C3 12k (0.35641, 0.00000, 0.88844)
$Mo_4Y_2Nb_6Al_3C_9$	5.50401	24.33560	Mo1 8h (0.33333, 0.66667, 0.15086) Y1 4e (0.00000, 0.00000, 0.67416) Nb1 12k (0.67403, 0.00000, 0.05510) Al1 6g (0.50631, 0.00000, 0.25000) C1 4d (0.33333, 0.66667, 0.00000) C2 2b (0.00000, 0.00000, 0.00000) C3 12k (0.66076, 0.00000, 0.60867)
$Mo_4Y_2Ta_6Al_3C_9$	5.48786	24.26010	Mo1 8h (0.33333, 0.66667, 0.15076) Y1 4e (0.00000, 0.00000, 0.67390) Ta1 12k (0.67414, 0.00000, 0.05518) Al1 6g (0.50616, 0.00000, 0.25000) C1 4d (0.33333, 0.66667, 0.00000) C2 2b (0.00000, 0.00000, 0.00000) C3 12k (0.66294, 0.00000, 0.60720)

$Sc_4Y_2Ta_6Al_3C_9$	5.61798	24.96750	Sc1 8h (0.33333, 0.66667, 0.35119) Y1 4e (0.00000, 0.00000, 0.83306) Ta1 12k (0.67114, 0.00000, -0.04988) Al1 6g (0.49065, 0.00000, 0.25000) C1 4d (0.33333, 0.66667, 0.00000) C2 2b (0.00000, 0.00000, 0.00000) C3 12k (0.66780, 0.00000, 0.39896)
$Ta_4Y_2Ta_6Al_3C_9$	5.52494	24.61530	Ta1 8h (0.33333, 0.66667, 0.84793) Y1 4e (0.00000, 0.00000, 0.32885) Ta1 12k (0.67418, 0.00000, 0.44620) Al1 6g (0.50913, 0.00000, 0.25000) C1 4d (0.33333, 0.66667, 0.00000) C2 2b (0.00000, 0.00000, 0.00000) C3 12k (0.66188, 0.00000, 0.89489)
$Ti_4Y_2Hf_6Al_3C_9$	5.64643	24.72880	Ti1 8h (0.33333, 0.66667, 0.34843) Y1 4e (0.00000, 0.00000, 0.32677) Hf1 12k (0.33192, 0.00000, 0.44672) Al1 6g (0.48986, 0.00000, 0.25000) C1 4d (0.33333, 0.66667, 0.00000) C2 2b (0.00000, 0.00000, 0.00000) C3 12k (0.34588, 0.00000, 0.88916)
$V_4Y_2Ta_6Al_3C_9$	5.43355	24.00550	V1 8h (0.33333, 0.66667, 0.34909) Y1 4e (0.00000, 0.00000, 0.82564) Ta1 12k (0.67298, 0.00000, -0.05556) Al1 6g (0.49390, 0.00000, 0.25000) C1 4d (0.33333, 0.66667, 0.00000) C2 2b (0.00000, 0.00000, 0.00000) C3 12k (0.65616, 0.00000, 0.39045)
$W_4Y_2Nb_6Al_3C_9$	5.50399	24.32730	W1 8h (0.33333, 0.66667, 0.34869) Y1 4e (0.00000, 0.00000, 0.82553) Nb1 12k (0.67469, 0.00000, -0.05517) Al1 6g (0.49235, 0.00000, 0.25000) C1 4d (0.33333, 0.66667, 0.00000) C2 2b (0.00000, 0.00000, 0.00000) C3 12k (0.66048, 0.00000, 0.39101)
$W_4Y_2Ta_6Al_3C_9$	5.48705	24.25110	W1 8h (0.33333, 0.66667, 0.34882) Y1 4e (0.00000, 0.00000, 0.32577) Ta1 12k (0.32508, 0.00000, 0.44478) Al1 6g (0.49283, 0.00000, 0.25000) C1 4d (0.33333, 0.66667, 0.00000) C2 2b (0.00000, 0.00000, 0.00000) C3 12k (0.33751, 0.00000, 0.89249)

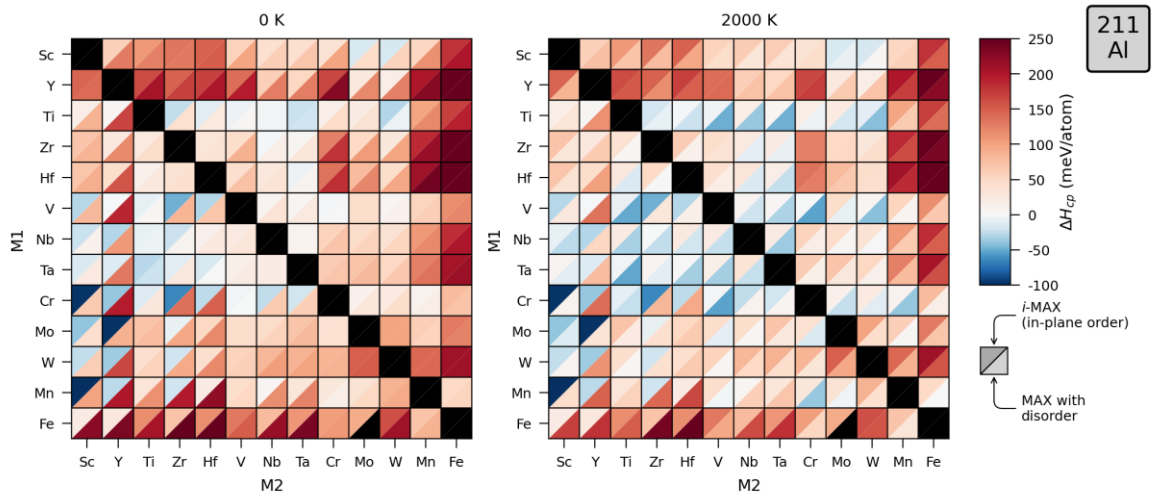

Figure S2. Stability heatmap for order (*i*-MAX) and disorder in 211 MAX phases at (a) 0 K and (b) 2000 K upon mixing metals M1 and M2 in a 2:1 ratio.

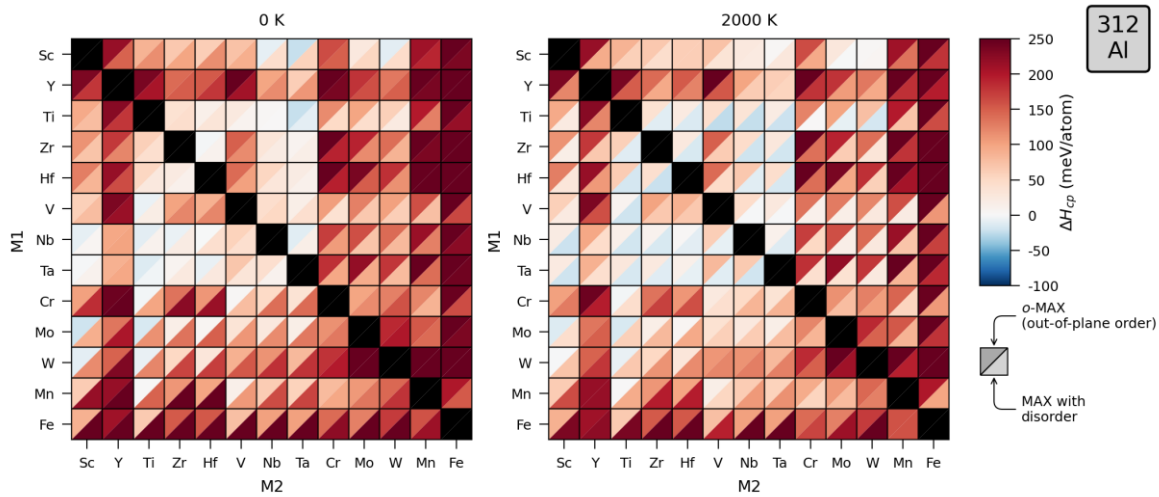

Figure S3. Stability heatmap for order (*o*-MAX) and disorder in 312 MAX phases at (a) 0 K and (b) 2000 K upon mixing metals M1 and M2 in a 2:1 ratio.

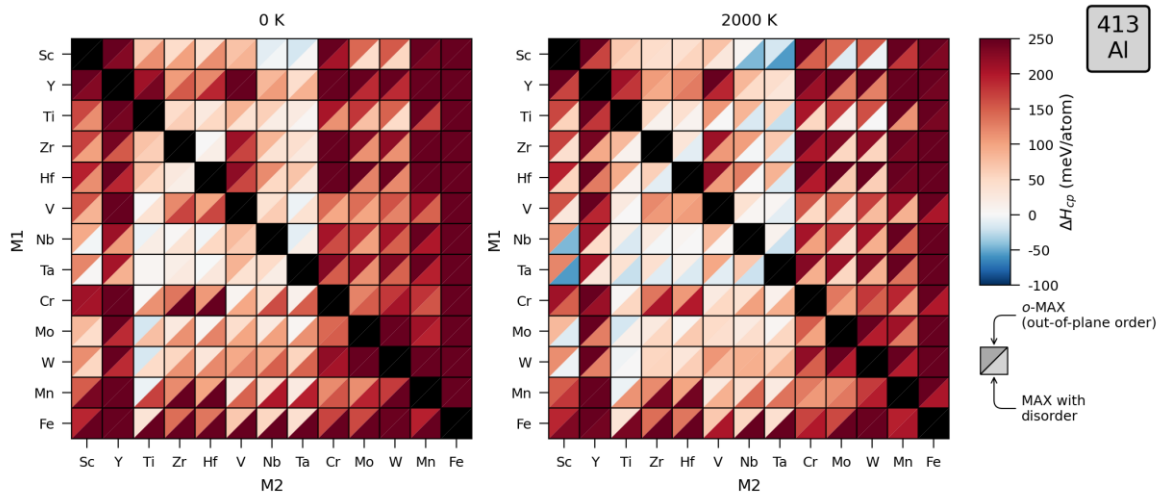

Figure S4. Stability heatmap for order (*o*-MAX) and disorder in 413 MAX phases at (a) 0 K and (b) 2000 K upon mixing metals M1 and M2 in a 1:1 ratio.

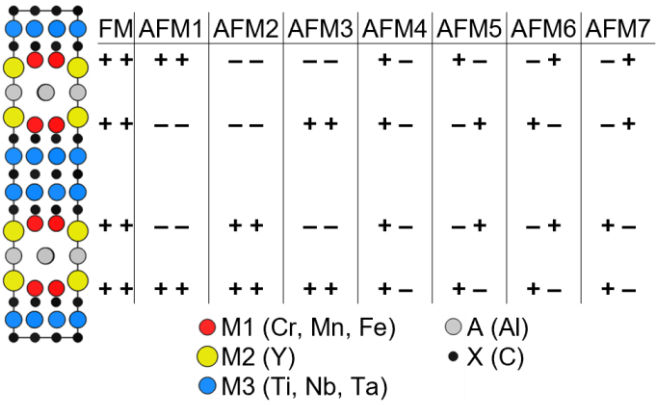

Figure S5. Seven ordered collinear magnetic spin configurations considered for 413 s-MAX phases with an initial magnetic moment assigned to the magnetic element occupying the M1 site (red).

Table S6. Relative energies for different AFM spin configurations as compared to FM for selected 413 *s*-MAX phases with M2 = Y. $\Delta E_{FM} < 0$ indicates that AFM is lower in energy than FM.

M1	M2	M3	ΔE_{FM} (meV/atom)							
			FM	AFM1	AFM2	AFM3	AFM4	AFM5	AFM6	AFM7
Cr	Y	Nb	0.0	**-0.3**	**-0.3**	-0.1	0.1	0.1	0.1	0.1
Cr	Y	Ta	0.0†	**-0.2†**	**-0.2***	0.0	0.2	0.2	0.2	0.2
Cr	Y	Ti	0.0*	**-1.4†**	0.5	**-1.4†**	2.7	2.7	2.7	2.7
Fe	Y	Nb	**0.0**	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Fe	Y	Ta	**0.0†**	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Fe	Y	Ti	0.0	0.2	0.2	0.0	2.0	**-0.4**	0.2	**-0.4**
Mn	Y	Nb	0.0†	-0.2	-0.2	-0.2	**-0.3†**	-0.2	**-0.3†**	-0.2
Mn	Y	Ta	0.0*	-0.2*	-0.2†	0.0	0.0	0.0	**-0.3***	0.0
Mn	Y	Ti	0.0*	0.0	0.0	-0.1	-0.1	**-1.4†**	-0.8*	-0.1

Spin configuration(s) of lowest energy
†Dynamically stable
*Dynamically unstable

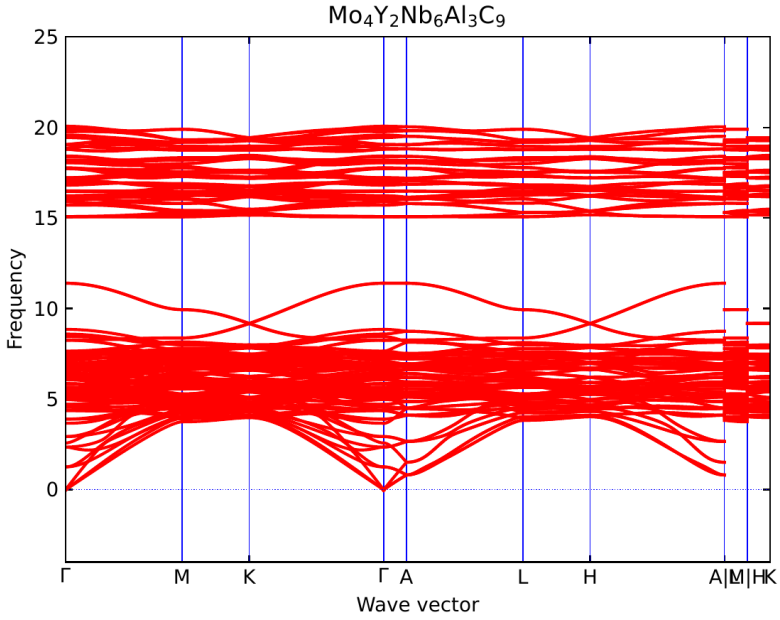

Figure S6. Phonon dispersion spectra for *s*-MAX phase $Mo_4Y_2Nb_6Al_3C_9$.

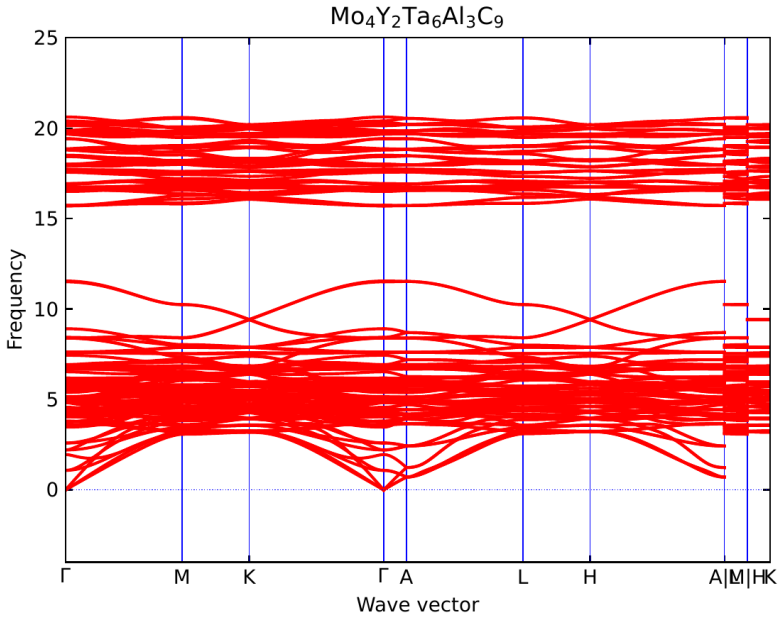

Figure S7. Phonon dispersion spectra for *s*-MAX phase $Mo_4Y_2Ta_6Al_3C_9$.

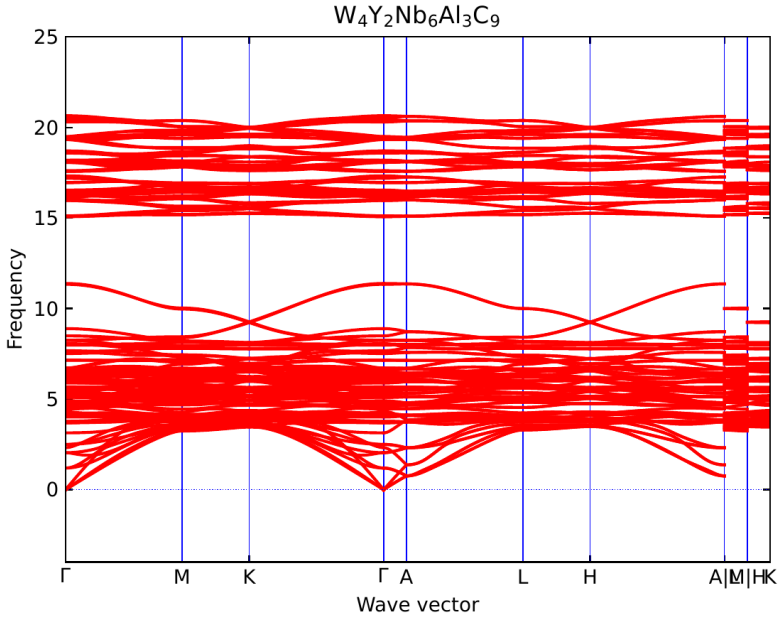

Figure S8. Phonon dispersion spectra for *s*-MAX phase $W_4Y_2Nb_6Al_3C_9$.

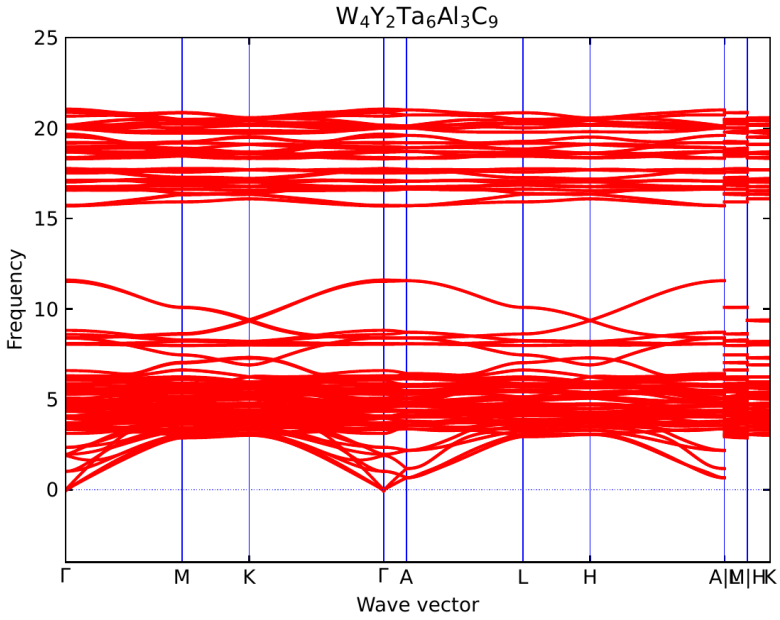

Figure S9. Phonon dispersion spectra for *s*-MAX phase $W_4Y_2Ta_6Al_3C_9$.

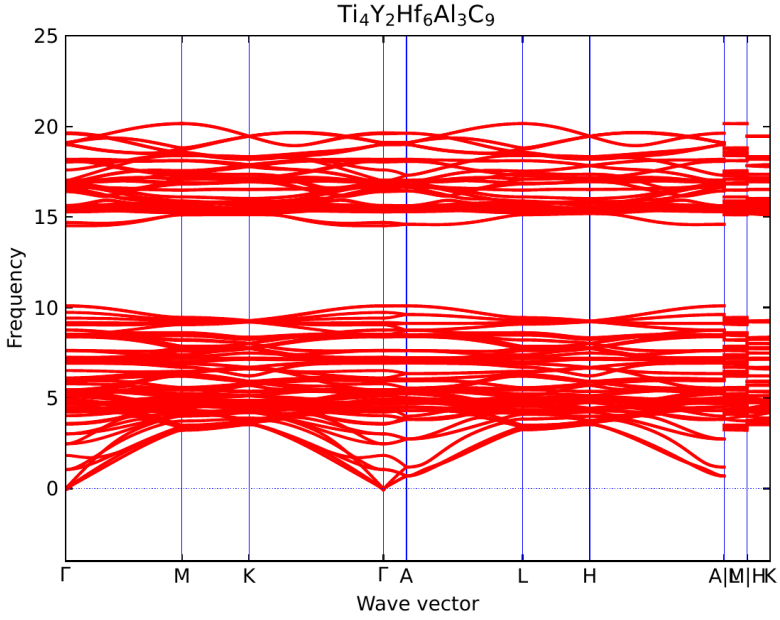

Figure S10. Phonon dispersion spectra for *s*-MAX phase $Ti_4Y_2Hf_6Al_3C_9$.

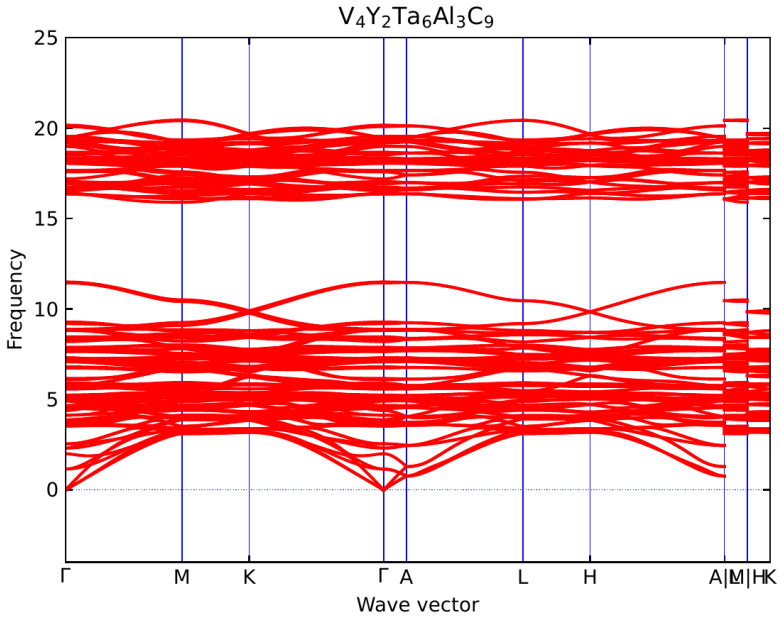

Figure S11. Phonon dispersion spectra for *s*-MAX phase $V_4Y_2Ta_6Al_3C_9$.

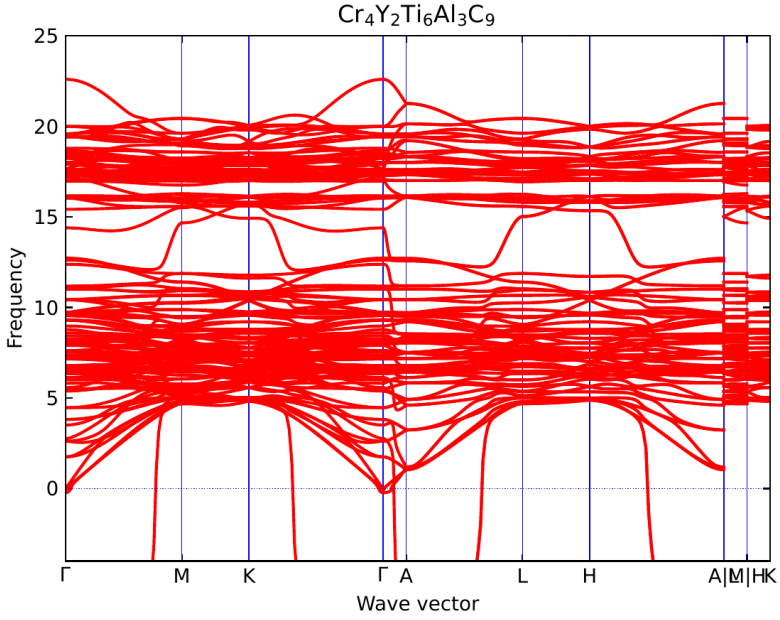

Figure S12. Phonon dispersion spectra for *s*-MAX phase $Cr_4Y_2Ti_6Al_3C_9$ with FM spin configuration. Presence of imaginary frequencies indicate dynamical unstable structure.

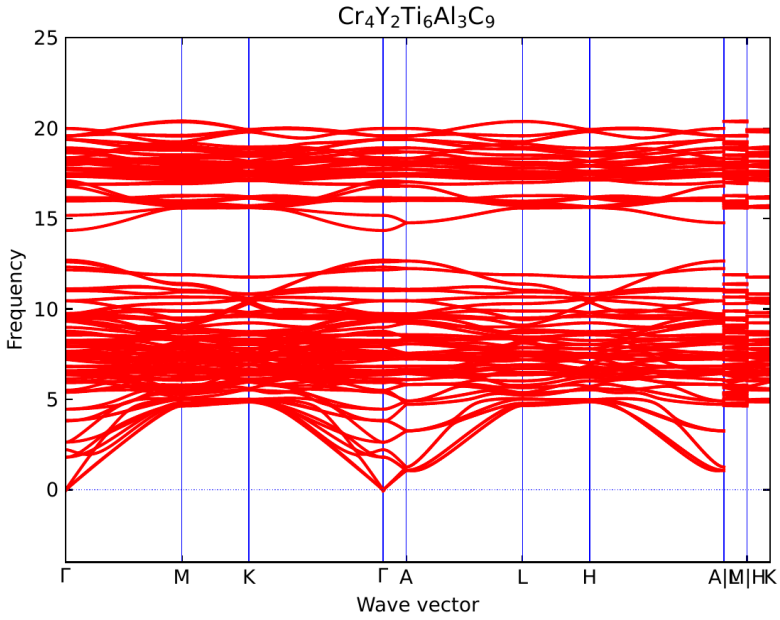

Figure S13. Phonon dispersion spectra for *s*-MAX phase $Cr_4Y_2Ti_6Al_3C_9$ with AFM1 spin configuration.

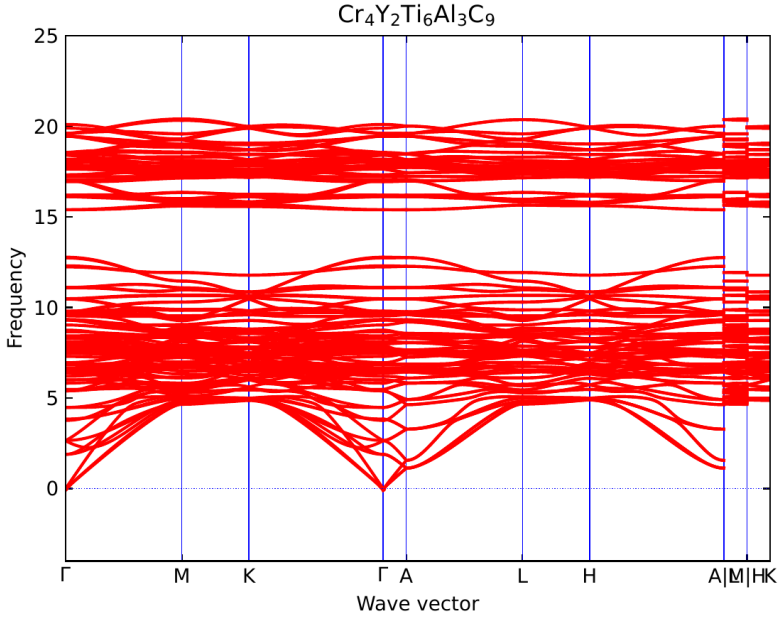

Figure S14. Phonon dispersion spectra for *s*-MAX phase $Cr_4Y_2Ti_6Al_3C_9$ with AFM3 spin configuration.

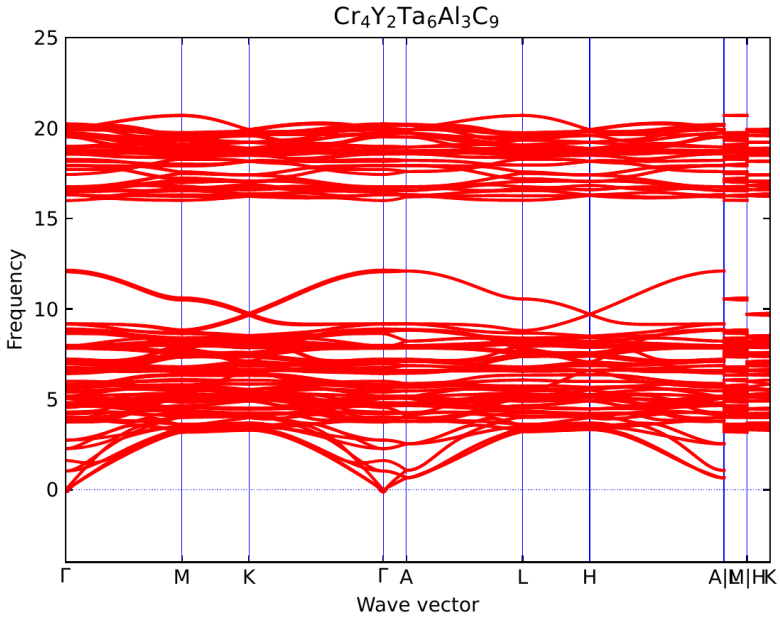

Figure S15. Phonon dispersion spectra for *s*-MAX phase $Cr_4Y_2Ta_6Al_3C_9$ with FM spin configuration.

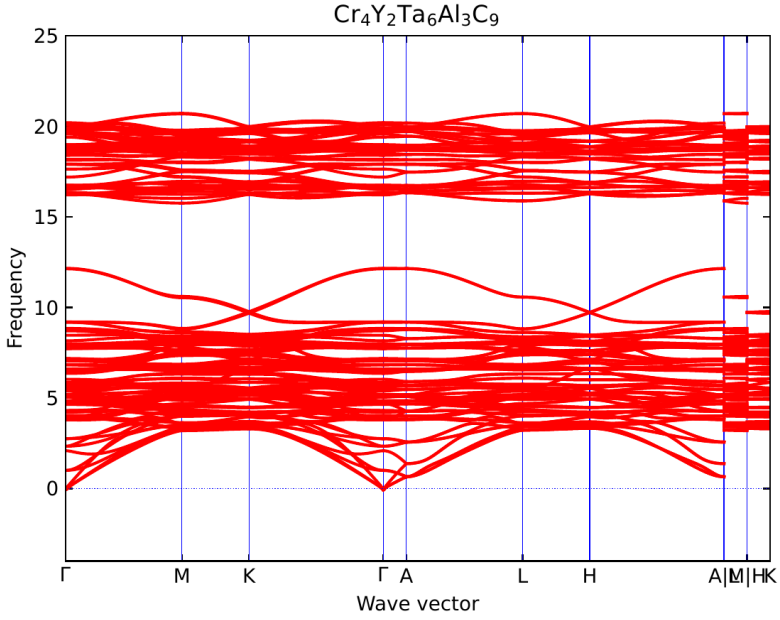

Figure S16. Phonon dispersion spectra for *s*-MAX phase $Cr_4Y_2Ta_6Al_3C_9$ with AFM1 spin configuration.

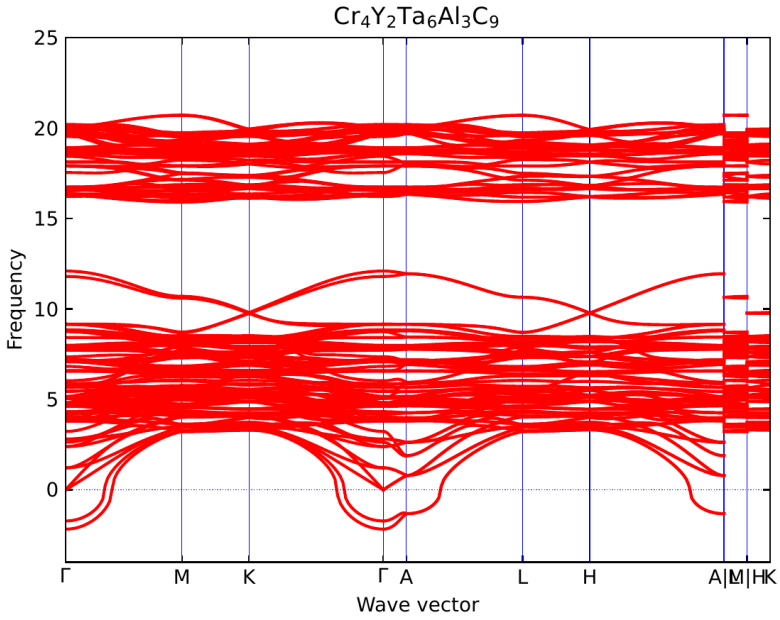

Figure S17. Phonon dispersion spectra for *s*-MAX phase $Cr_4Y_2Ta_6Al_3C_9$ with AFM2 spin configuration. Presence of imaginary frequencies indicate dynamical unstable structure.

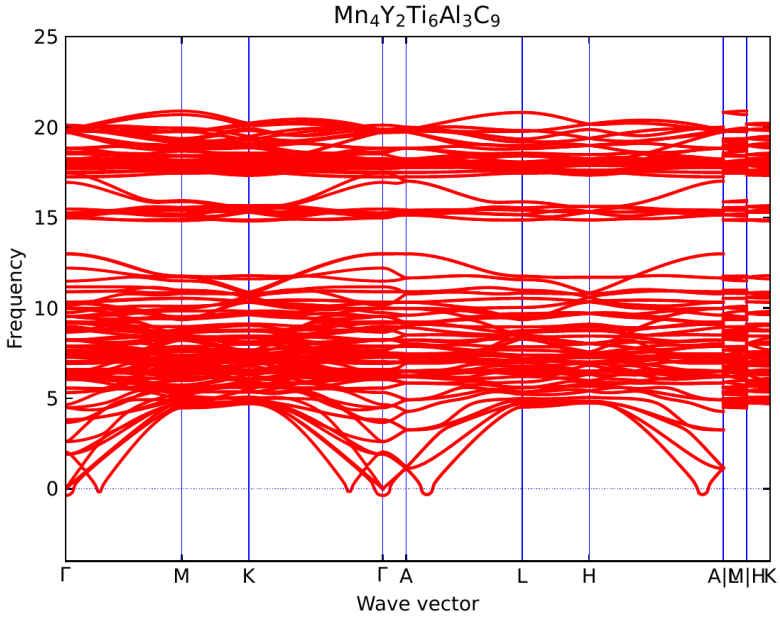

Figure S18. Phonon dispersion spectra for *s*-MAX phase $Mn_4Y_2Ti_6Al_3C_9$ with FM spin configuration. Presence of imaginary frequencies indicate dynamical unstable structure.

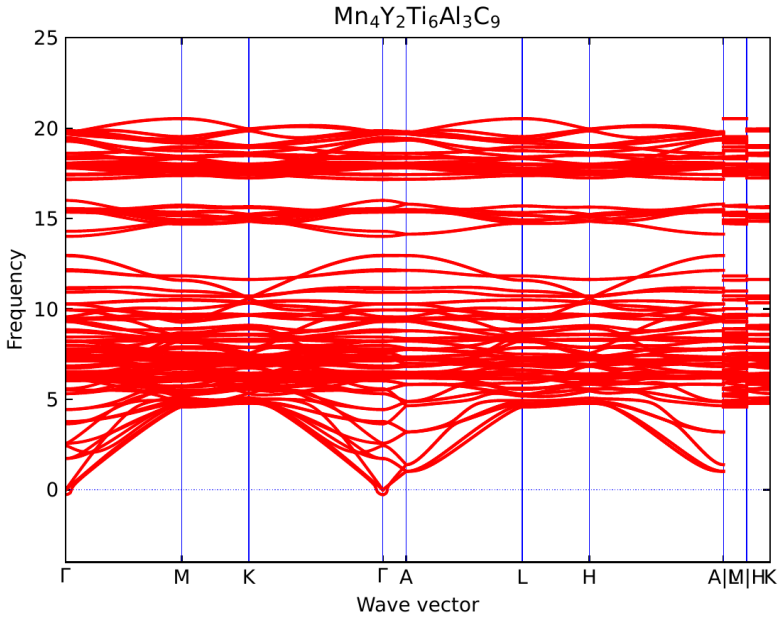

Figure S19. Phonon dispersion spectra for *s*-MAX phase $Mn_4Y_2Ti_6Al_3C_9$ with AFM5 spin configuration.

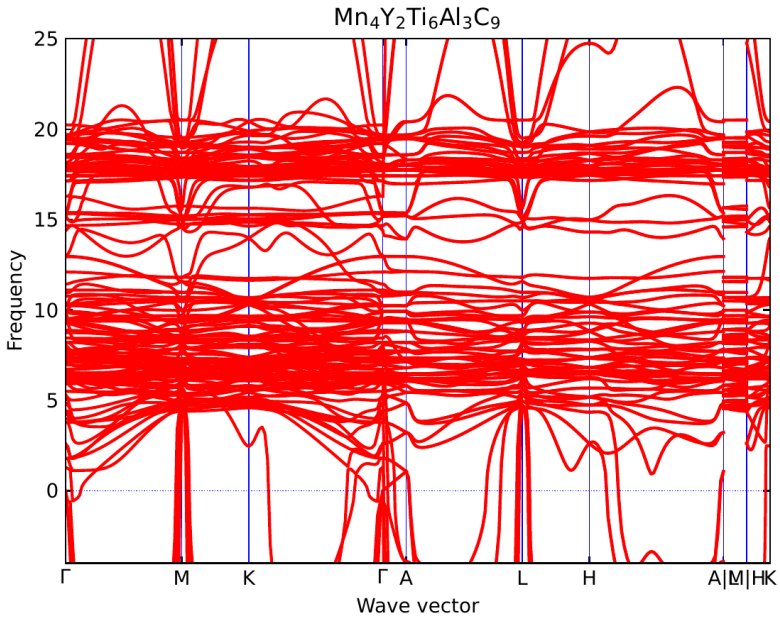

Figure S20. Phonon dispersion spectra for *s*-MAX phase $Mn_4Y_2Ti_6Al_3C_9$ with AFM6 spin configuration. Presence of imaginary frequencies indicate dynamical unstable structure.

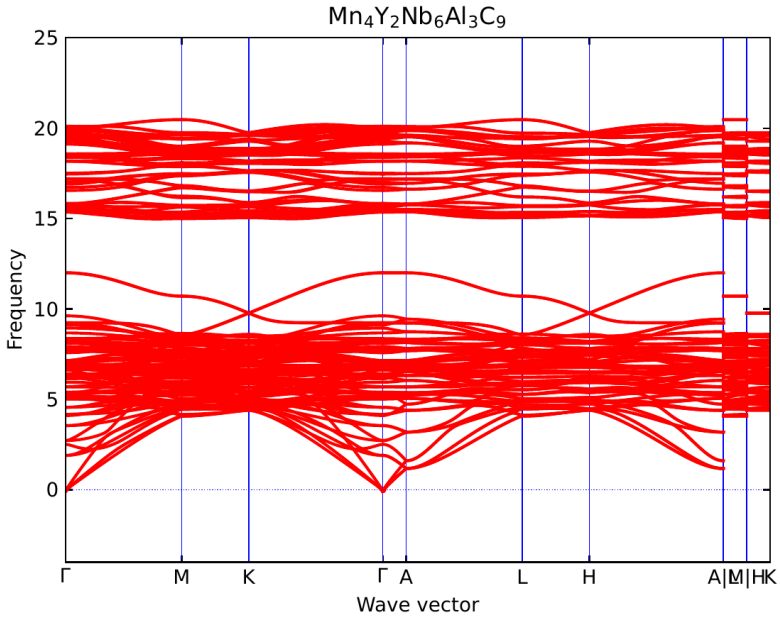

Figure S21. Phonon dispersion spectra for *s*-MAX phase $Mn_4Y_2Nb_6Al_3C_9$ with FM spin configuration.

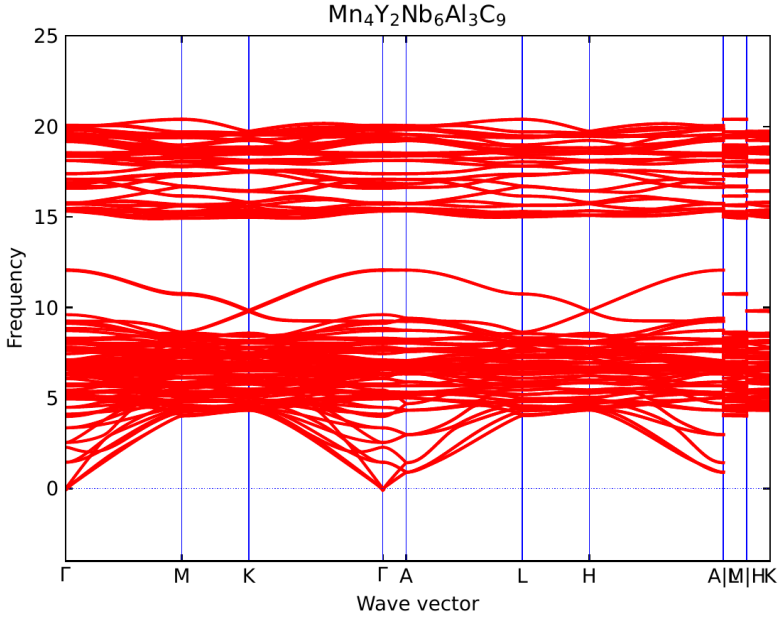

Figure S22. Phonon dispersion spectra for *s*-MAX phase $Mn_4Y_2Nb_6Al_3C_9$ with AFM4 spin configuration.

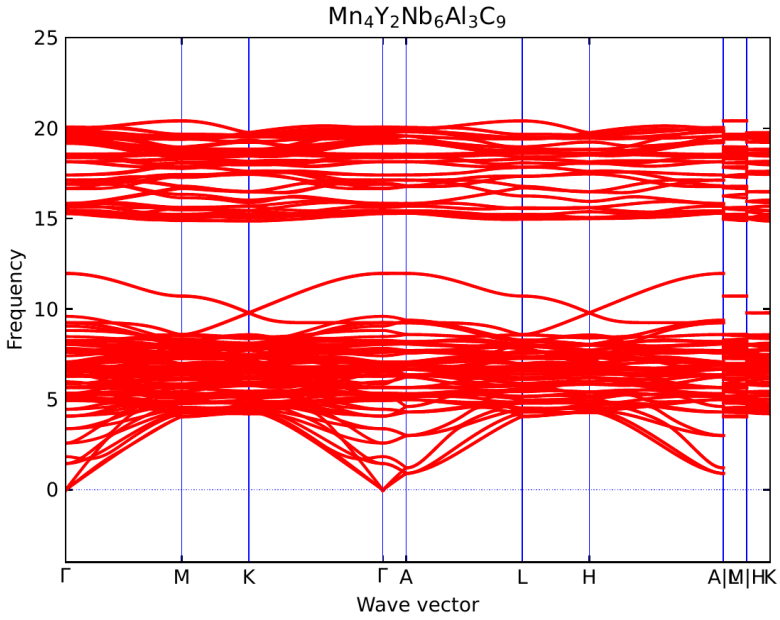

Figure S23. Phonon dispersion spectra for *s*-MAX phase $Mn_4Y_2Nb_6Al_3C_9$ with AFM6 spin configuration.

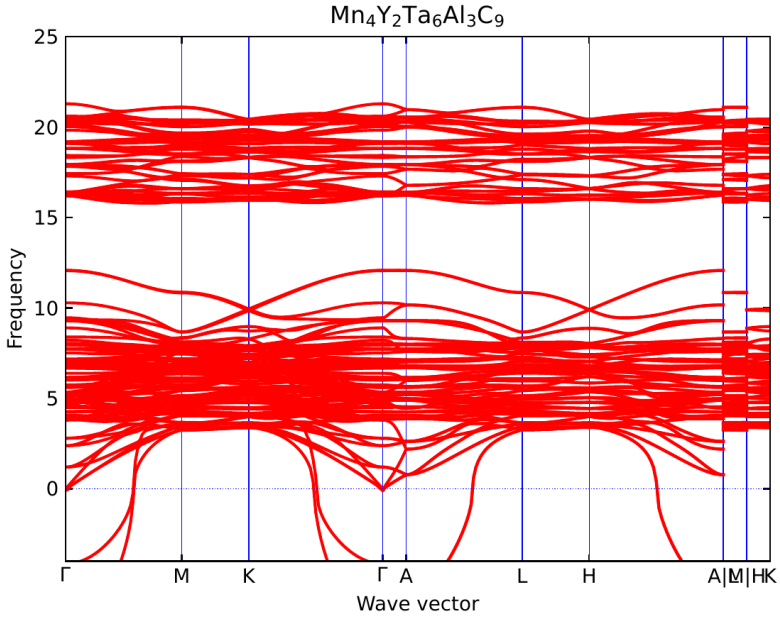

Figure S24. Phonon dispersion spectra for *s*-MAX phase $Mn_4Y_2Ta_6Al_3C_9$ with FM spin configuration. Presence of imaginary frequencies indicate dynamical unstable structure.

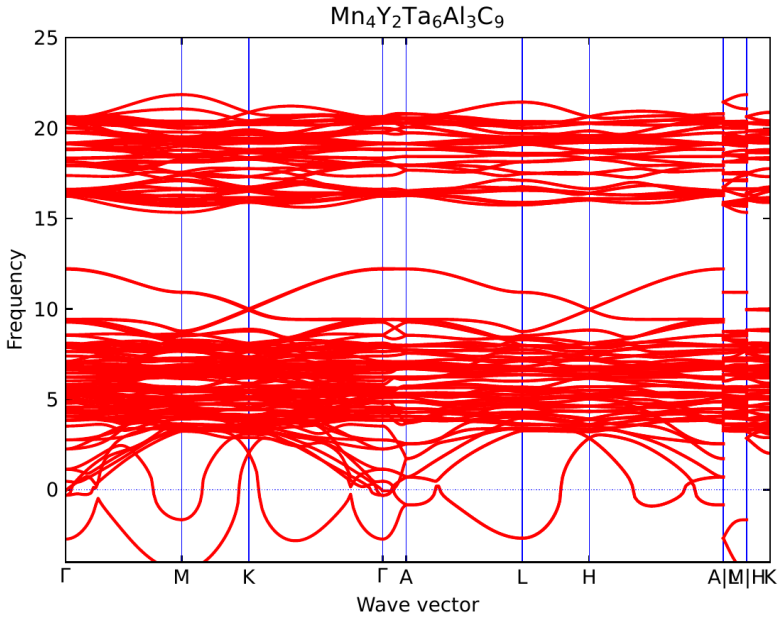

Figure S25. Phonon dispersion spectra for *s*-MAX phase $Mn_4Y_2Ta_6Al_3C_9$ with AFM1 spin configuration. Presence of imaginary frequencies indicate dynamical unstable structure.

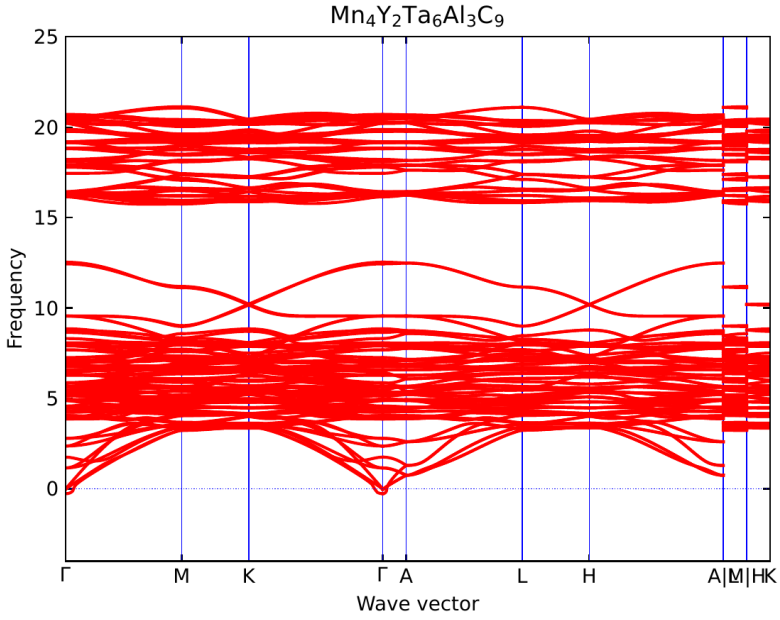

Figure S26. Phonon dispersion spectra for *s*-MAX phase $Mn_4Y_2Ta_6Al_3C_9$ with AFM2 spin configuration.

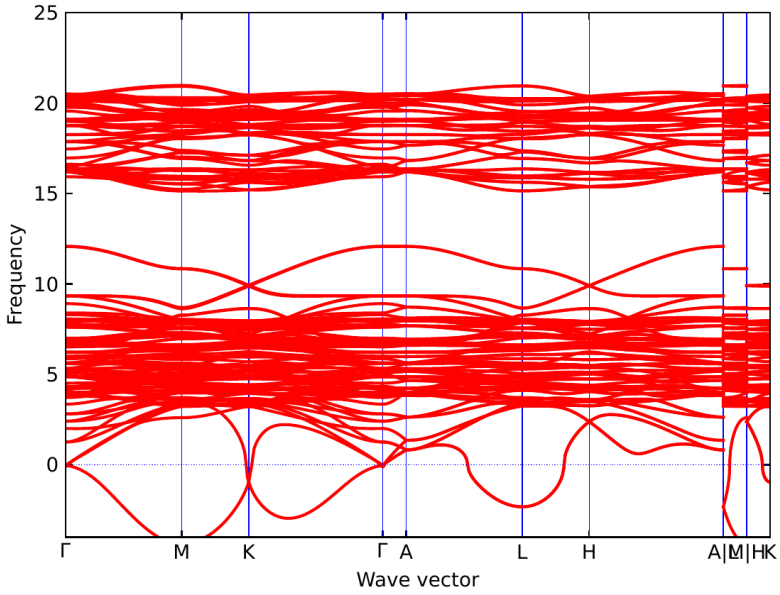

Figure S27. Phonon dispersion spectra for *s*-MAX phase $Mn_4Y_2Ta_6Al_3C_9$ with AFM6 spin configuration. Presence of imaginary frequencies indicate dynamical unstable structure.

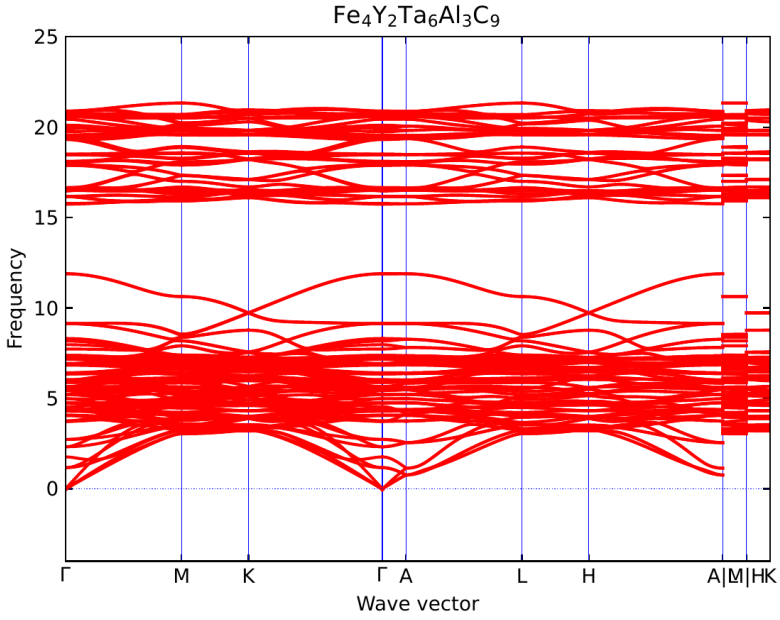

Figure S28. Phonon dispersion spectra for *s*-MAX phase $Fe_4Y_2Ta_6Al_3C_9$ with FM spin configuration.

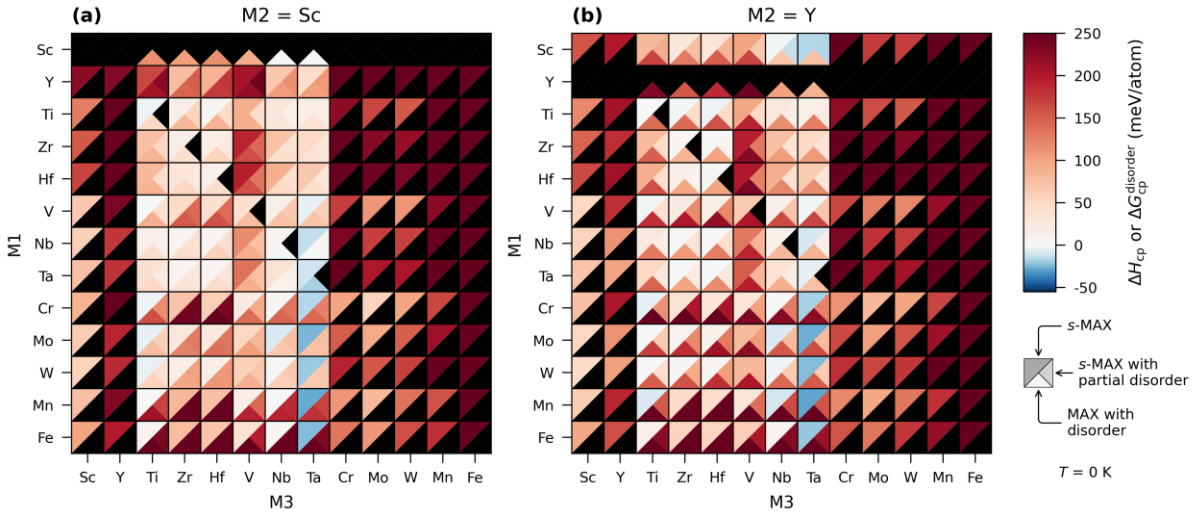

Figure S29. Stability heatmap evaluated at 0 K for 413 MAX phases upon mixing metals M1, M2, M3 in a 2:1:3 ratio with (a) M2 = Sc and (b) M2 = Y. For a given combination of M1 and M3, the right triangles indicate the stability for *s*-MAX with partial disorder, having in-plane order of M2 in the outer metal layer combined with disorder of M1 + M3, and the bottom triangles indicate the stability for MAX with disorder of M1, M2, and M3. Black triangles represent combinations of M1, M2 and M3 not considered.

Table S7. Calculated energy (E) and stability at 2000 K (ΔH_{cp}) for M2 = Y in *s*-MAX, *s*-MAX with disorder, and MAX with disorder for 312 MAX phases along with corresponding energy for their competing phases and identified set of most competing phases. Phases modelled with solid solution disorder have a contribution from configurational entropy evaluated at 2000 K. Competing phases in bold highlight when a MAX phase is part of the set of most competing phases.

M1	M2	M3	Energy (eV/atom)				ΔH_{cp} (meV/atom)			Set of most competing phases
			s-MAX	*s*-MAX disorder	MAX disorder	Competing phases	*s*-MAX	*s*-MAX disorder	MAX disorder	
Sc	Y	Sc	-7.274441	N/A	-7.319607	-7.378699	104	N/A	59	AlY_3C_3 + Sc_3C_4 + Al_2Y + $AlSc_3C$
Sc	Y	Y	-7.222425	-7.248278	-7.289326	-7.370901	148	123	82	AlY_3C_3 + AlY_3C + $AlSc_3C$
Sc	Y	Ti	-7.664451	-7.715471	-7.682999	-7.756387	92	41	73	AlY_3C_3 + Sc_3C_4 + Al_2Y + $AlSc_3C$ + TiC
Sc	Y	Zr	-7.821275	-7.830334	-7.816137	-7.864289	43	34	48	ZrC + AlY_3C_3 + Sc_3C_4 + Al_2Y + $AlSc_3C$
Sc	Y	Hf	-8.097211	-8.100395	-8.077441	-8.144150	47	44	67	AlY_3C_3 + Sc_3C_4 + Al_2Y + $AlSc_3C$ + HfC
Sc	Y	V	-7.776448	-7.851325	-7.800757	-7.864765	88	13	64	**$Al_3Sc_3V_4Y_2C_6$** + AlY_3C_3 + Sc_3C_4 + Al_2Y + $AlSc_3C$
Sc	Y	Nb	-8.069941	-8.104246	-8.054367	-8.099963	30	-4	46	**$Al_3Nb_4Sc_3Y_2C_6$** + AlY_3C_3 + **$AlNbSc_2C_2$** + $AlSc_3C$
Sc	Y	Ta	-8.423133	-8.438820	-8.379775	-8.428856	6	-10	49	**$AlSc_2TaC_2$** + **$Al_3Sc_3Ta_4Y_2C_6$** + AlY_3C_3 + $AlSc_3C$
Sc	Y	Cr	-7.704789	N/A	N/A	-7.863484	159	N/A	N/A	**$Al_3Cr_4Sc_3Y_2C_6$** + $CrSc_2C_3$ + $Cr_2Y_2C_3$ + Al_2Y + $AlSc_3C$
Sc	Y	Mo	-8.049410	N/A	N/A	-8.108018	59	N/A	N/A	AlY_3C_3 + **$Al_3Mo_4Sc_3Y_2C_6$** + Sc_3C_4 + Al_2Y + $AlSc_3C$
Sc	Y	W	-8.421328	N/A	N/A	-8.448637	27	N/A	N/A	AlY_3C_3 + **$Al_3Sc_5W_4C_6$** + **$Al_3Sc_3W_4Y_2C_6$** + $AlSc_3C$
Sc	Y	Mn	-7.582825	N/A	N/A	-7.786626	204	N/A	N/A	$Mn_{13}Y_{10}C_{18}$ + AlY_3C_3 + Sc_3C_4 + $AlSc_3C$ + **$Al_3Mn_4Sc_2C_3$**
Sc	Y	Fe	-7.385990	N/A	N/A	-7.664674	279	N/A	N/A	Al_6Fe_6Sc + $FeSc_3C_4$ + AlY_3C_3 + AlY_3C + $AlSc_3C$
Y	Y	Ti	N/A	N/A	-7.605063	N/A	N/A	N/A	119	AlY_3C_3 + AlY_3C + Al_2Y + TiC
Y	Y	Zr	N/A	N/A	-7.773958	N/A	N/A	N/A	58	AlY_3C_3 + AlY_3C + Al_2Y + ZrC
Y	Y	Hf	N/A	N/A	-8.024707	N/A	N/A	N/A	87	AlY_3C_3 + AlY_3C + Al_2Y + HfC
Y	Y	V	N/A	N/A	-7.710820	N/A	N/A	N/A	118	V_6C_5 + AlY_3C + AlY_3C_3 + Al_2Y
Y	Y	Nb	N/A	N/A	-7.984852	N/A	N/A	N/A	21	**$Al_3Nb_7Y_2C_6$** + AlY_3C_3 + AlY_3C
Y	Y	Ta	N/A	N/A	-8.302899	N/A	N/A	N/A	17	AlY_3C + **$Al_3Ta_{10}Y_2C_9$** + AlY_3C_3 + Al_2Y
Ti	Y	Sc	-7.821739	-7.849020	-7.785277	-7.880073	58	31	95	AlY_3C_3 + AlY_3C + Al_2Y + $AlSc_3C$ + TiC
Ti	Y	Y	-7.719282	-7.716875	-7.722763	-7.853857	135	137	131	AlY_3C_3 + AlY_3C + Al_2Y + TiC
Ti	Y	Ti	-8.208747	N/A	-8.136670	-8.203091	-6	N/A	66	**$Al_3Ti_{10}Y_2C_9$** + **$AlTi_3C_2$** + AlY_2 + Al_2Y
Ti	Y	Zr	-8.317571	-8.320442	-8.238419	-8.317587	0	-3	79	**$Al_3Ti_7Y_2C_6$** + **$Al_3Ti_3Y_2Zr_4C_6$**
Ti	Y	Hf	-8.599722	-8.597916	-8.504123	-8.595740	-4	-2	92	$AlTi_3C_2$ + **$Al_3Hf_6Ti_4Y_2C_9$** + **$Al_3Hf_4Ti_6Y_2C_9$** + AlY_2 + Al_2Y
Ti	Y	V	-8.291892	-8.361959	-8.238690	-8.352156	60	-10	113	**$AlTi_2VC_2$** + **$Al_3Ti_3V_4Y_2C_6$** + AlY_3C + Al_2Y + TiC
Ti	Y	Nb	-8.535887	-8.566335	-8.462064	-8.549803	14	-17	88	**$Al_3Nb_4Ti_3Y_2C_6$** + **$AlNbTi_2C_2$** + **$Al_3Nb_4Ti_6Y_2C_9$** + AlY_3C + Al_2Y
Ti	Y	Ta	-8.875892	-8.894001	-8.783458	-8.878450	3	-16	95	AlY_2 + **$AlTaTi_2C_2$** + **$Al_3Ta_4Ti_3Y_2C_6$** + **$Al_3Ta_4Ti_6Y_2C_9$** + Al_2Y
Ti	Y	Cr	-8.195075	N/A	N/A	-8.345579	151	N/A	N/A	**$Al_3Cr_4Ti_6Y_2C_9$** + AlY_3C + Al_2Y + TiC + Cr
Ti	Y	Mo	-8.492983	N/A	N/A	-8.562756	70	N/A	N/A	$AlMo_3$ + **$Al_3Mo_4Y_2C_3$** + AlY_3C + Al_2Y + TiC
Ti	Y	W	-8.848920	N/A	N/A	-8.893417	44	N/A	N/A	**$Al_3Ti_3W_4Y_2C_6$** + AlY_3C + Al_2Y + TiC + W
Ti	Y	Mn	-8.089888	N/A	N/A	-8.264988	175	N/A	N/A	**$Al_3Mn_4Ti_6Y_2C_9$** + AlY_3C + Al_2Y + Mn + TiC
Ti	Y	Fe	-7.870992	N/A	N/A	-8.132706	262	N/A	N/A	Y_4C_7 + AlY_3C_3 + Al_8Fe_4Y + $AlFe_3$ + TiC
Zr	Y	Sc	-7.928272	-7.998159	-7.973262	-8.023942	96	26	51	ZrC + AlY_3C_3 + Al_2Y + AlY_3C + $AlSc_3C$
Zr	Y	Y	-7.876463	-7.920526	-7.935831	-7.997725	121	77	62	AlY_3C_3 + AlY_3C + Al_2Y + ZrC
Zr	Y	Ti	-8.278560	-8.353867	-8.298405	-8.352889	74	-1	54	**$AlTiZr_2C_2$** + AlY_2 + $Zr_{10}C_9$ + **$Al_3Ti_4Y_2Zr_3C_6$** + Al_2Y

Zr	Y	Zr	-8.443094	N/A	-8.442739	-8.447429	4	N/A	5	**$AlZr_3C_2$** + $Zr_{10}C_9$ + AlY_2 + Al_2Y
Zr	Y	Hf	-8.713805	-8.752510	-8.698820	-8.753961	40	1	55	**$AlHfZr_2C_2$** + **$Al_3Hf_6Y_2Zr_4C_9$** + **$Al_3Hf_4Y_2Zr_6C_9$** + AlY_2 + Al_2Y
Zr	Y	V	-8.341163	-8.423813	-8.373095	-8.470727	130	47	98	**$Al_3V_4Y_2C_3$** + AlY_3C + **$Al_3V_4Zr_2C_3$** + ZrC + Al_2Y
Zr	Y	Nb	-8.626146	-8.688952	-8.638967	-8.676640	50	-12	38	**$AlNbZr_2C_2$** + **$Al_3Nb_4Y_2Zr_3C_6$** + AlY_2 + Al_2Y + $Zr_{10}C_9$
Zr	Y	Ta	-8.960533	-9.009255	-8.953605	-8.994160	34	-15	41	**$Al_3Ta_4Y_2Zr_3C_6$** + AlY_2 + **$AlTaZr_2C_2$** + **$Al_3Ta_4Y_2Zr_6C_9$** + Al_2Y
Zr	Y	Cr	-8.240236	N/A	N/A	-8.478813	239	N/A	N/A	**$Al_3Cr_4Y_2C_3$** + Cr + $Cr_2Y_2C_3$ + Al_2Y + ZrC
Zr	Y	Mo	-8.556707	N/A	N/A	-8.706624	150	N/A	N/A	ZrC + $AlMo_3$ + **$Al_3Mo_4Y_2C_3$** + AlY_3C + Al_2Y
Zr	Y	W	-8.909381	N/A	N/A	-9.026369	117	N/A	N/A	ZrC + **$Al_3W_4Y_2Zr_3C_6$** + AlY_3C + Al_2Y + W
Zr	Y	Mn	-8.151572	N/A	N/A	-8.402190	251	N/A	N/A	**$Al_3Mn_4Y_2C_3$** + $Mn_{13}Y_{10}C_{18}$ + Al_2Y + Mn + ZrC
Zr	Y	Fe	-7.937978	N/A	N/A	-8.276574	339	N/A	N/A	Y_4C_7 + AlY_3C_3 + Al_8Fe_4Y + $AlFe_3$ + ZrC
Hf	Y	Sc	-8.280653	-8.357178	-8.318324	-8.397090	116	40	79	AlY_3C_3 + AlY_3C + Al_2Y + $AlSc_3C$ + HfC
Hf	Y	Y	-8.217765	-8.263960	-8.273587	-8.370874	153	107	97	AlY_3C_3 + AlY_3C + Al_2Y + HfC
Hf	Y	Ti	-8.633278	-8.719311	-8.645259	-8.722750	89	3	77	**$Al_3Hf_6Ti_4Y_2C_9$** + **$AlHf_2TiC_2$** + AlY_2 + **$AlHfTi_2C_2$** + Al_2Y
Hf	Y	Zr	-8.788269	-8.840760	-8.781228	-8.843531	55	3	62	**$AlHf_2Zr_2C_3$** + **$Al_3Hf_6Y_2Zr_4C_9$** + AlY_2 + Al_2Y
Hf	Y	Hf	-9.062544	N/A	-9.039222	-9.070646	8	N/A	31	**$AlHf_4C_3$** + AlY_2 + Al_2Y + HfC
Hf	Y	V	-8.694206	-8.789653	-8.717227	-8.843010	149	53	126	**$Al_3V_4Y_2C_3$** + AlY_3C + V_2C + Al_2Y + HfC
Hf	Y	Nb	-8.970490	-9.043670	-8.980020	-9.034369	64	-9	54	**$AlHf_2NbC_2$** + **$Al_3Hf_3Nb_4Y_2C_6$** + AlY_2 + Al_2Y + HfC
Hf	Y	Ta	-9.305135	-9.364382	-9.295271	-9.352621	47	-12	57	**$Al_3Hf_6Ta_4Y_2C_9$** + AlY_2 + **$AlHf_2TaC_2$** + Ta_2C + Al_2Y
Hf	Y	Cr	-8.592864	N/A	N/A	-8.851961	259	N/A	N/A	**$Al_3Cr_4Y_2C_3$** + Cr + $Cr_2Y_2C_3$ + Al_2Y + HfC
Hf	Y	Mo	-8.903652	N/A	N/A	-9.079773	176	N/A	N/A	AlY_3C + $AlMo_3$ + **$Al_3Mo_4Y_2C_3$** + Al_2Y + HfC
Hf	Y	W	-9.255557	N/A	N/A	-9.398340	143	N/A	N/A	**$Al_3W_4Y_2C_3$** + AlY_3C + Al_2Y + HfC + W
Hf	Y	Mn	-8.502784	N/A	N/A	-8.775338	273	N/A	N/A	**$Al_3Mn_4Y_2C_3$** + $Mn_{13}Y_{10}C_{18}$ + Al_2Y + Mn + HfC
Hf	Y	Fe	-8.287234	N/A	N/A	-8.649723	362	N/A	N/A	Y_4C_7 + AlY_3C_3 + Al_8Fe_4Y + $AlFe_3$ + HfC
V	Y	Sc	-8.026787	-8.018354	-7.930525	-8.020476	-6	2	90	**$Al_3Sc_2V_7C_6$** + AlY_3C_3 + AlY_3C + $AlSc_3C$
V	Y	Y	-7.911177	-7.857906	-7.863192	-7.992707	82	135	130	V_6C_5 + AlY_3C + AlY_3C_3 + Al_2Y
V	Y	Ti	-8.385343	-8.398680	-8.261496	-8.392566	7	-6	131	**$Al_3Ti_4V_3Y_2C_6$** + **$Al_3V_4Y_2C_3$** + AlY_3C + V_6C_5 + Al_2Y
V	Y	Zr	-8.462742	-8.425992	-8.339796	-8.474787	12	49	135	**$Al_3V_4Y_2C_3$** + ZrC
V	Y	Hf	-8.742074	-8.704252	-8.602544	-8.754648	13	50	152	**$Al_3V_4Y_2C_3$** + HfC
V	Y	V	-8.464609	N/A	-8.363728	-8.484387	20	N/A	121	**$Al_3V_4Y_2C_3$** + V_6C_5 + AlY_3C + Al_2Y
V	Y	Nb	-8.674798	-8.668776	-8.552142	-8.669206	-6	0	117	**$Al_3Nb_4V_3Y_2C_6$** + AlY_3C + **$Al_3V_4Y_2C_3$** + V_6C_5 + Al_2Y
V	Y	Ta	-9.005917	-8.991074	-8.866611	-8.989009	-17	-2	122	**$Al_3V_4Y_2C_3$** + **$Al_3Ta_4V_3Y_2C_6$** + AlY_3C + V_6C_5 + Al_2Y
V	Y	Cr	-8.365240	N/A	N/A	-8.471038	106	N/A	N/A	AlY_3C_3 + Al_3YC_3 + **$Al_3Cr_4Y_2C_3$** + V_6C_5 + Al_2Y
V	Y	Mo	-8.621877	N/A	N/A	-8.701224	79	N/A	N/A	V_6C_5 + AlY_3C_3 + Al_3YC_3 + **$Al_3Mo_4Y_2C_3$** + Al_2Y
V	Y	W	-8.966090	N/A	N/A	-9.017417	51	N/A	N/A	**$Al_3W_4Y_2C_3$** + Al_3YC_3 + WYC_2 + V_6C_5 + Al_2Y
V	Y	Mn	-8.265085	N/A	N/A	-8.396099	131	N/A	N/A	**$Al_3Mn_4Y_2C_3$** + V_6C_5 + Al_3YC_3 + $Mn_{13}Y_{10}C_{18}$ + Al_2Y
V	Y	Fe	-8.045873	N/A	N/A	-8.263867	218	N/A	N/A	Y_4C_7 + Al_8Fe_4Y + V_6C_5 + AlFe + $AlFe_2V$
Nb	Y	Sc	-8.286228	-8.338165	-8.268732	-8.321188	35	-17	52	AlY_3C + **$Al_3Nb_6Sc_4Y_2C_9$** + **$Al_3Nb_4Sc_5C_6$** + Al_2Y + **$Al_3Nb_7Sc_2C_6$**
Nb	Y	Y	-8.210631	-8.216222	-8.210575	-8.229252	19	13	19	**$Al_3Nb_7Y_2C_6$** + AlY_3C_3 + AlY_3C
Nb	Y	Ti	-8.606336	-8.663174	-8.572483	-8.649559	43	-14	77	**$Al_3Nb_7Y_2C_6$** + **$Al_3Nb_3Ti_4Y_2C_6$**
Nb	Y	Zr	-8.732031	-8.752074	-8.691864	-8.741522	9	-11	50	**$Al_3Nb_7Y_2C_6$** + **$Al_3Nb_3Y_2Zr_4C_6$**
Nb	Y	Hf	-9.002298	-9.018595	-8.947961	-9.007560	5	-11	60	**$Al_3Hf_4Nb_3Y_2C_6$** + **$Al_3Nb_7Y_2C_6$**
Nb	Y	V	-8.651488	-8.730813	-8.640201	-8.730907	79	0	91	**$Al_3Nb_7Y_2C_6$** + **$Al_3Nb_3V_4Y_2C_6$**
Nb	Y	Nb	-8.899231	N/A	-8.874150	-8.891288	-8	N/A	17	**$Al_3Nb_{10}Y_2C_9$** + **$Al_3Nb_4Y_2C_3$**
Nb	Y	Ta	-9.223859	-9.259037	-9.182860	-9.246962	23	-12	64	**$Al_3Nb_3Ta_4Y_2C_6$** + **$Al_3Nb_7Y_2C_6$**

Nb	Y	Cr	-8.553690	N/A	N/A	-8.715487	162	N/A	N/A	**$Al_3Nb_7Y_2C_6$** + **$Al_3Cr_4Nb_3Y_2C_6$**
Nb	Y	Mo	-8.805743	N/A	N/A	-8.936132	130	N/A	N/A	**$Al_3Nb_{10}Y_2C_9$** + **$Al_3Mo_4Nb_6Y_2C_9$** + **$Al_3Mo_4Y_2C_3$**
Nb	Y	W	-9.145150	N/A	N/A	-9.249982	105	N/A	N/A	**$Al_3W_4Y_2C_3$** + **$Al_3Nb_{10}Y_2C_9$** + WC
Nb	Y	Mn	-8.448077	N/A	N/A	-8.630719	183	N/A	N/A	**$Al_3Mn_4Nb_6Y_2C_9$** + **$Al_3Mn_4Y_2C_3$** + **$Al_3Nb_7Y_2C_6$**
Nb	Y	Fe	-8.239089	N/A	N/A	-8.488943	250	N/A	N/A	Al_8Fe_4Y + AlY_3C_3 + Y_4C_7 + $AlFe_3$ + Nb_6C_5
Ta	Y	Sc	-8.717271	-8.776071	-8.694703	-8.760948	44	-15	66	**$Al_3Sc_5Ta_4C_6$** + **$Al_3Sc_4Ta_6Y_2C_9$** + AlY_2 + Al_2Y
Ta	Y	Y	-8.639262	-8.644138	-8.631994	-8.647675	8	4	16	AlY_3C + **$Al_3Ta_{10}Y_2C_9$** + AlY_3C_3 + Al_2Y
Ta	Y	Ti	-9.026041	-9.094399	-8.996299	-9.078576	53	-16	82	**$Al_3Ta_6Ti_4Y_2C_9$** + **$Al_3Ta_3Ti_4Y_2C_6$** + Ta_2C + AlY_3C + Al_2Y
Ta	Y	Zr	-9.147861	-9.175583	-9.110968	-9.163774	16	-12	53	**$Al_3Ta_3Y_2Zr_4C_6$** + **$Al_3Ta_7Y_2C_6$**
Ta	Y	Hf	-9.417972	-9.442525	-9.367058	-9.431712	14	-11	65	**$Al_3Hf_4Ta_6Y_2C_9$** + **$Al_3Hf_4Ta_3Y_2C_6$** + AlY_3C + Ta_2C + Al_2Y
Ta	Y	V	-9.065401	-9.157216	-9.056690	-9.161270	96	4	105	**$Al_3Ta_7Y_2C_6$** + **$Al_3Ta_3V_4Y_2C_6$**
Ta	Y	Nb	-9.305707	-9.362872	-9.286582	-9.351110	45	-12	65	**$Al_3Nb_4Ta_3Y_2C_6$** + **$Al_3Ta_7Y_2C_6$**
Ta	Y	Ta	-9.627329	N/A	-9.592168	-9.622769	-5	N/A	31	AlY_3C + **$Al_3Ta_{10}Y_2C_9$** + Ta_2C + Al_2Y
Ta	Y	Cr	-8.967817	N/A	N/A	-9.147915	180	N/A	N/A	Cr + AlY_3C + **$Al_3Cr_4Ta_6Y_2C_9$** + **$Al_3Ta_7Y_2C_6$** + Al_2Y
Ta	Y	Mo	-9.204626	N/A	N/A	-9.369533	165	N/A	N/A	$AlMo_3$ + **$Al_3Ta_7Y_2C_6$** + AlY_3C + **$Al_3Mo_4Ta_6Y_2C_9$** + Al_2Y
Ta	Y	W	-9.538653	N/A	N/A	-9.680094	141	N/A	N/A	**$Al_3Ta_{10}Y_2C_9$** + **$Al_3Ta_6W_4Y_2C_9$** + AlY_3C + Al_2Y + W
Ta	Y	Mn	-8.857786	N/A	N/A	-9.069876	212	N/A	N/A	**$Al_3Mn_4Ta_6Y_2C_9$** + $AlMn_8Ta_3$ + AlY_3C + Mn + Al_2Y
Ta	Y	Fe	-8.651962	N/A	N/A	-8.925407	273	N/A	N/A	AlY_3C_3 + **$Al_3Ta_{10}Y_2C_9$** + Al_8Fe_4Y + **$Al_3Fe_4Ta_6Y_2C_9$** + $AlFe_2Ta$
Cr	Y	Sc	-8.019691	-7.949353	-7.885920	-8.019221	0	70	133	$CrSc_2C_3$ + $Cr_2Y_2C_3$ + **$Al_3Cr_4Sc_2C_3$** + Al_2Y + $AlSc_3C$
Cr	Y	Y	-7.896259	-7.792984	-7.828138	-7.989531	93	197	161	**$Al_3Cr_4Y_2C_3$** + $Cr_2Y_2C_3$ + AlY_3C_3 + Al_2Y
Cr	Y	Ti	-8.379553	-8.330735	-8.193583	-8.377073	-2	46	183	**$Al_3Cr_4Y_2C_3$** + **$Al_3Cr_4Ti_6Y_2C_9$**
Cr	Y	Zr	-8.441920	-8.343119	-8.270463	-8.476435	35	133	206	**$Al_3Cr_4Y_2C_3$** + ZrC
Cr	Y	Hf	-8.720713	-8.621560	-8.540643	-8.756296	36	135	216	**$Al_3Cr_4Y_2C_3$** + HfC
Cr	Y	V	-8.459449	-8.447778	-8.294266	-8.463626	4	16	169	**$Al_3Cr_4Y_2C_3$** + C + V_6C_5
Cr	Y	Nb	-8.654239	-8.586506	-8.480758	-8.643863	-10	57	163	**$Al_3Cr_4Y_2C_3$** + **$Al_3Cr_4Nb_6Y_2C_9$**
Cr	Y	Ta	-8.981642	-8.907985	-8.796082	-8.978851	-3	71	183	**$Al_3Cr_4Ta_6Y_2C_9$** + **$Al_3Cr_4Y_2C_3$**
Cr	Y	Cr	-8.368896	N/A	N/A	-8.420185	51	N/A	N/A	**$Al_3Cr_4Y_2C_3$** + C + Cr_3C_2
Cr	Y	Mo	-8.611605	N/A	N/A	-8.650371	39	N/A	N/A	C + Cr_3C_2 + **$Al_3Mo_4Y_2C_3$** + **$Al_3Cr_4Y_2C_3$**
Cr	Y	W	-8.947982	N/A	N/A	-8.984060	36	N/A	N/A	$Al_3Cr_4Y_2C_3$ + WC
Cr	Y	Mn	-8.267189	N/A	N/A	-8.352383	85	N/A	N/A	**$Al_3Cr_4Mn_2C_3$** + **$Al_3Cr_4Y_2C_3$** + $Mn_{13}Y_{10}C_{18}$ + C
Cr	Y	Fe	-8.051830	N/A	N/A	-8.220511	169	N/A	N/A	$Cr_2Y_2C_3$ + C + Cr_3C_2 + AlFe
Mo	Y	Sc	-8.351124	-8.341593	-8.262110	-8.320553	-31	-21	58	**$Al_3Mo_4Y_2C_3$** + Y_2C + **$Al_3Mo_4Sc_5C_6$** + Y_4C_5
Mo	Y	Y	-8.254839	-8.197846	-8.201411	-8.273322	18	75	72	**$Al_3Mo_4Y_2C_3$** + Y_2C + Y_4C_5
Mo	Y	Ti	-8.674347	-8.671951	-8.564583	-8.675449	1	3	111	**$Al_3Mo_4Y_2C_3$** + TiC
Mo	Y	Zr	-8.772904	-8.727339	-8.660732	-8.783350	10	56	123	ZrC + **$Al_3Mo_4Y_2C_3$**
Mo	Y	Hf	-9.042431	-8.996417	-8.916555	-9.063211	21	67	147	**$Al_3Mo_4Y_2C_3$** + HfC
Mo	Y	V	-8.719341	-8.742463	-8.636631	-8.770541	51	28	134	V_6C_5 + C + **$Al_3Mo_4Y_2C_3$**
Mo	Y	Nb	-8.944716	-8.918479	-8.836087	-8.948381	4	30	112	**$Al_3Mo_4Nb_6Y_2C_9$** + **$Al_3Mo_4Y_2C_3$**
Mo	Y	Ta	-9.266865	-9.231304	-9.143328	-9.280685	14	49	137	**$Al_3Mo_4Ta_6Y_2C_9$** + **$Al_3Mo_4Y_2C_3$**
Mo	Y	Cr	-8.626707	N/A	N/A	-8.727100	100	N/A	N/A	C + Cr_3C_2 + **$Al_3Mo_4Y_2C_3$**
Mo	Y	Mo	-8.861004	N/A	N/A	-8.926309	65	N/A	N/A	**$Al_3Mo_4Y_2C_3$** + C + Mo_2C
Mo	Y	W	-9.189738	N/A	N/A	-9.290975	101	N/A	N/A	**$Al_3Mo_4Y_2C_3$** + WC
Mo	Y	Mn	-8.516825	N/A	N/A	-8.636882	120	N/A	N/A	$AlMn_3C$ + **$Al_3Mo_4Y_2C_3$** + $Mn_{13}Y_{10}C_{18}$ + C + Mo_2C
Mo	Y	Fe	-8.308171	N/A	N/A	-8.502500	194	N/A	N/A	$Fe_{17}Y_2C_3$ + **$Al_3Mo_4Y_2C_3$** + C + Mo_2C + $AlFe_3C$

W	Y	Sc	-8.803201	-8.799689	-8.713789	-8.769490	-34	-30	56	**$Al_3Sc_5W_4C_6$** + **$Al_3W_4Y_5C_6$**
W	Y	Y	-8.707317	-8.648330	-8.646791	-8.706320	-1	58	60	WYC_2 + **$Al_3W_4Y_2C_3$** + AlY_3C_3 + AlY_3C
W	Y	Ti	-9.109045	-9.115395	-9.003292	-9.105382	-4	-10	102	**$Al_3W_4Y_2C_3$** + **$Al_3Ti_6W_4Y_2C_9$**
W	Y	Zr	-9.206314	-9.166012	-9.097638	-9.204483	-2	38	107	**$Al_3W_4Y_2C_3$** + ZrC
W	Y	Hf	-9.473588	-9.433683	-9.352350	-9.484345	11	51	132	**$Al_3W_4Y_2C_3$** + HfC
W	Y	V	-9.139393	-9.174451	-9.064743	-9.191674	52	17	127	**$Al_3W_4Y_2C_3$** + C + V_6C_5
W	Y	Nb	-9.358747	-9.342919	-9.264227	-9.365514	7	23	101	**$Al_3W_4Y_2C_3$** + **$Al_3Nb_{10}Y_2C_9$** + WC
W	Y	Ta	-9.677057	-9.650436	-9.567247	-9.695710	19	45	128	**$Al_3W_4Y_2C_3$** + **$Al_3Ta_6W_4Y_2C_9$**
W	Y	Cr	-9.048111	N/A	N/A	-9.166073	118	N/A	N/A	**$Al_3W_4Y_2C_3$** + **$Al_3Cr_4Y_2C_3$** + WC
W	Y	Mo	-9.260482	N/A	N/A	-9.396259	136	N/A	N/A	**$Al_3W_4Y_2C_3$** + **$Al_3Mo_4Y_2C_3$** + WC
W	Y	W	-9.581408	N/A	N/A	-9.712109	131	N/A	N/A	**$Al_3W_4Y_2C_3$** + WC
W	Y	Mn	-8.930785	N/A	N/A	-9.090642	160	N/A	N/A	**$Al_3Mn_4Y_2C_3$** + **$Al_3W_4Y_2C_3$** + WC
W	Y	Fe	-8.725375	N/A	N/A	-8.965760	240	N/A	N/A	WYC_2 + WC + AlFe
Mn	Y	Sc	-7.907964	-7.801639	-7.760049	-7.921180	13	120	161	$Mn_{13}Y_{10}C_{18}$ + AlY_3C_3 + Sc_3C_4 + $AlSc_3C$ + **$Al_3Mn_4Sc_2C_3$**
Mn	Y	Y	-7.787280	-7.679483	-7.725766	-7.897063	110	218	171	AlY_3C_3 + $Mn_{13}Y_{10}C_{18}$ + AlY_3C + Al_2Y
Mn	Y	Ti	-8.267289	-8.175421	-8.071949	-8.273203	6	98	201	**$Al_3Mn_4Ti_6Y_2C_9$** + **$Al_3Mn_4Y_2C_3$**
Mn	Y	Zr	-8.323268	-8.197330	-8.153501	-8.375861	53	179	222	**$Al_3Mn_4Y_2C_3$** + ZrC
Mn	Y	Hf	-8.601350	-8.469057	-8.412507	-8.655722	54	187	243	**$Al_3Mn_4Y_2C_3$** + HfC
Mn	Y	V	-8.348659	-8.302770	-8.178402	-8.363052	14	60	185	**$Al_3Mn_4Y_2C_3$** + V_6C_5 + C
Mn	Y	Nb	-8.536298	-8.437572	-8.363984	-8.541215	5	104	177	**$Al_3Mn_4Nb_6Y_2C_9$** + **$Al_3Mn_4Y_2C_3$**
Mn	Y	Ta	-8.863434	-8.759427	-8.673807	-8.876757	13	117	203	**$Al_3Mn_4Ta_6Y_2C_9$** + **$Al_3Mn_4Y_2C_3$**
Mn	Y	Cr	-8.250736	N/A	N/A	-8.327239	77	N/A	N/A	**$Al_3Cr_4Mn_2C_3$** + **$Al_3Cr_4Y_2C_3$** + **$Al_3Mn_4Y_2C_3$** + $Mn_{13}Y_{10}C_{18}$ + C
Mn	Y	Mo	-8.487644	N/A	N/A	-8.540406	53	N/A	N/A	$AlMn_3C$ + **$Al_3Mo_4Y_2C_3$** + $Mn_{13}Y_{10}C_{18}$ + C + MoO_2C
Mn	Y	W	-8.824769	N/A	N/A	-8.883486	59	N/A	N/A	**$Al_3Mn_4Y_2C_3$** + WC
Mn	Y	Mn	-8.137559	N/A	N/A	-8.237913	100	N/A	N/A	**$Al_3Mn_4Y_2C_3$** + $Mn_{13}Y_{10}C_{18}$ + C + $AlMn_3C$
Mn	Y	Fe	-7.922238	N/A	N/A	-8.124386	202	N/A	N/A	$AlFe_3C$ + $AlMn_3C$ + $Mn_{13}Y_{10}C_{18}$ + C + AlFe
Fe	Y	Sc	-7.707164	-7.562431	-7.545114	-7.743919	37	181	199	Y_3C_4 + $AlFe_3$ + Al_6Fe_6Sc + $FeSc_3C_4$ + Y_4C_5
Fe	Y	Y	-7.595915	-7.486691	-7.549905	-7.695219	99	209	145	$AlFe_3$ + Y_4C_7 + AlY_3C_3 + Al_8Fe_4Y
Fe	Y	Ti	-8.053777	-7.918880	-7.869561	-8.082774	29	164	213	Y_4C_7 + AlY_3C_3 + Al_8Fe_4Y + $AlFe_3$ + TiC
Fe	Y	Zr	-8.117974	-7.951633	-7.945807	-8.190675	73	239	245	Y_4C_7 + AlY_3C_3 + Al_8Fe_4Y + $AlFe_3$ + ZrC
Fe	Y	Hf	-8.395336	-8.220149	-8.208403	-8.470536	75	250	262	Y_4C_7 + AlY_3C_3 + Al_8Fe_4Y + $AlFe_3$ + HfC
Fe	Y	V	-8.130352	-8.054769	-7.965283	-8.179447	49	125	214	Y_4C_7 + $AlFe_3$ + V_6C_5 + AlFe
Fe	Y	Nb	-8.327642	-8.183748	-8.143122	-8.349531	22	166	206	AlFe + Y_4C_7 + $AlFe_3$ + Nb_6C_5
Fe	Y	Ta	-8.657302	-8.503718	-8.448340	-8.680220	23	177	232	AlY_3C_3 + Y_4C_7 + Al_8Fe_4Y + **$Al_3Fe_4Ta_6Y_2C_9$** + $AlFe_3$
Fe	Y	Cr	-8.032407	N/A	N/A	-8.149645	117	N/A	N/A	$AlFe_3C$ + $Cr_2Y_2C_3$ + C + Cr_3C_2 + AlFe
Fe	Y	Mo	-8.272897	N/A	N/A	-8.360375	87	N/A	N/A	$Fe_{17}Y_2C_3$ + **$Al_3Mo_4Y_2C_3$** + Y_4C_7 + C + $AlFe_3C$
Fe	Y	W	-8.608857	N/A	N/A	-8.706935	98	N/A	N/A	$AlFe_3C$ + WYC_2 + C + WC + AlFe
Fe	Y	Mn	-7.925943	N/A	N/A	-8.083038	157	N/A	N/A	$AlFe_3C$ + $AlMn_3C$ + $Mn_{13}Y_{10}C_{18}$ + C + AlFe
Fe	Y	Fe	-7.705634	N/A	N/A	-7.923610	218	N/A	N/A	Y_4C_7 + $AlFe_3C$ + AlFe + C

Table S8. Calculated energy (E) and stability at 2000 K (ΔH_{cp}) for M2 = Sc in *s*-MAX, *s*-MAX with disorder, and MAX with disorder for 312 MAX phases along with corresponding energy for their competing phases and identified set of most competing phases. Phases modelled with solid solution disorder have a contribution from configurational entropy evaluated at 2000 K. Competing phases in bold highlight when a MAX phase is part of the set of most competing phases.

M1	M2	M3	Energy (eV/atom)				ΔH_{cp} (meV/atom)			Set of most competing phases
			s-MAX	*s*-MAX disorder	MAX disorder	Competing phases	*s*-MAX	s-MAX disorder	MAX disorder	
Sc	Sc	Ti	N/A	N/A	-7.731297	N/A	N/A	N/A	24	Al_3ScC_3 + $AlSc_3C$ + TiC
Sc	Sc	Zr	N/A	N/A	-7.848280	N/A	N/A	N/A	15	Al_3ScC_3 + $AlSc_3C$ + ZrC
Sc	Sc	Hf	N/A	N/A	-8.115238	N/A	N/A	N/A	28	Al_3ScC_3 + $AlSc_3C$ + HfC
Sc	Sc	V	N/A	N/A	-7.865655	N/A	N/A	N/A	-2	**$Al_3Sc_5V_4C_6$** + Sc_3C_4 + Al_3ScC_3 + $AlSc_3C$
Sc	Sc	Nb	N/A	N/A	-8.108031	N/A	N/A	N/A	-7	Sc_3C_4 + **$Al_3Nb_4Sc_5C_6$** + Al_3ScC_3 + $AlSc_3C$
Sc	Sc	Ta	N/A	N/A	-8.438409	N/A	N/A	N/A	-8	Al_3ScC_3 + $AlSc_3C$ + **$AlSc_2Ta_2C_3$**
Y	Sc	Sc	-7.191372	-7.249638	-7.301166	-7.375956	185	126	75	AlY_3C_3 + Sc_3C_4 + Al_2Y + $AlSc_3C$
Y	Sc	Y	-7.165504	N/A	-7.273416	-7.353424	188	N/A	80	AlY_3C_3 + AlY_3C + $AlSc_3C$
Y	Sc	Ti	-7.552222	-7.585134	-7.635830	-7.741857	190	157	106	AlY_3C_3 + AlY_3C + Al_2Y + $AlSc_3C$ + TiC
Y	Sc	Zr	-7.742495	-7.747192	-7.797162	-7.849758	107	103	53	ZrC + AlY_3C_3 + Al_2Y + AlY_3C + $AlSc_3C$
Y	Sc	Hf	-8.014658	-8.009502	-8.051023	-8.129619	115	120	79	AlY_3C_3 + AlY_3C + Al_2Y + $AlSc_3C$ + HfC
Y	Sc	V	-7.643500	-7.679294	-7.748720	-7.851237	208	172	103	**$Al_3Sc_3V_4Y_2C_6$** + V_6C_5 + AlY_3C_3 + AlY_3C + Al_2Y
Y	Sc	Nb	-7.964906	-7.969913	-8.015558	-8.079724	115	110	64	**$Al_3Nb_4Sc_3Y_2C_6$** + AlY_3C + AlY_3C_3 + **$Al_3Nb_{10}Sc_2C_9$** + Al_2Y
Y	Sc	Ta	-8.313673	-8.297427	-8.336852	-8.408579	95	111	72	AlY_3C_3 + **$Al_3Sc_4Ta_6Y_2C_9$** + AlY_3C + Al_2Y
Y	Sc	Cr	-7.563387	N/A	N/A	-7.848776	285	N/A	N/A	AlY_3C_3 + $CrSc_2C_3$ + $Cr_2Y_2C_3$ + Al_2Y + $AlSc_3C$
Y	Sc	Mo	-7.928164	N/A	N/A	-8.091119	163	N/A	N/A	AlY_3C_3 + **$Al_3Mo_4Sc_3Y_2C_6$** + **$Al_3Mo_4Y_2C_3$** + AlY_3C + Y_4C_5
Y	Sc	W	-8.298330	N/A	N/A	-8.428397	130	N/A	N/A	AlY_3C_3 + **$Al_3Sc_3W_4Y_2C_6$** + **$Al_3W_4Y_5C_6$** + AlY_3C
Y	Sc	Mn	-7.464297	N/A	N/A	-7.776689	312	N/A	N/A	AlY_3C + $Mn_{13}Y_{10}C_{18}$ + AlY_3C_3 + $AlSc_3C$ + **$Al_3Mn_4Sc_2C_3$**
Y	Sc	Fe	-7.267754	N/A	N/A	-7.642149	374	N/A	N/A	$AlFe_3$ + Al_6Fe_6Sc + $FeSc_3C_4$ + AlY_3C_3 + Fe_2Sc
Ti	Sc	Sc	-7.806841	-7.838645	-7.859189	-7.880507	74	42	21	**$Al_3Sc_2Ti_{10}C_9$** + Al_3ScC_3 + $AlSc_3C$ + TiC
Ti	Sc	Y	-7.684379	-7.715216	-7.770348	-7.871335	187	156	101	AlY_3C_3 + AlY_3C + Al_2Y + $AlSc_3C$ + TiC
Ti	Sc	Ti	-8.210502	N/A	-8.237488	-8.227715	17	N/A	-10	Al_2Sc + **$Al_3Sc_2Ti_{10}C_9$** + $AlTi_2C$ + $AlSc_3C$
Ti	Sc	Zr	-8.295387	-8.304780	-8.314552	-8.341552	46	37	27	**$Al_3Sc_2Ti_7C_6$** + **$Al_3Sc_2Zr_7C_6$**
Ti	Sc	Hf	-8.581662	-8.586283	-8.589091	-8.607650	26	21	19	**$Al_3Sc_2Ti_7C_6$** + Al_2Sc + **$AlHfTi_2C_2$** + **$Al_3Hf_{10}Sc_2C_9$** + $AlSc_3C$
Ti	Sc	V	-8.307180	-8.376077	-8.356415	-8.371612	64	-4	15	**$Al_3Sc_2Ti_7C_6$** + **$Al_3Sc_2Ti_3V_4C_6$**
Ti	Sc	Nb	-8.530487	-8.565556	-8.567567	-8.563005	33	-3	-5	**$Al_3Sc_2Ti_7C_6$** + **$Al_3Nb_4Sc_2Ti_3C_6$**
Ti	Sc	Ta	-8.871746	-8.895544	-8.894482	-8.887682	16	-8	-7	**$Al_3Sc_2Ti_7C_6$** + **$Al_3Sc_2Ta_4Ti_3C_6$**
Ti	Sc	Cr	-8.210090	N/A	N/A	-8.365253	155	N/A	N/A	**$Al_3Cr_4Sc_2Ti_3C_6$** + **$Al_3Cr_4Sc_2C_3$** + **$Al_3Sc_2Ti_{10}C_9$**
Ti	Sc	Mo	-8.499002	N/A	N/A	-8.574495	75	N/A	N/A	**$Al_3Mo_4Sc_2Ti_3C_6$** + **$Al_3Sc_2Ti_{10}C_9$** + **$Al_3Mo_4Sc_2C_3$**
Ti	Sc	W	-8.853235	N/A	N/A	-8.916398	63	N/A	N/A	**$Al_3Sc_2Ti_6W_4C_9$** + **$Al_3Sc_2Ti_{10}C_9$** + $AlSc_3C$ + Al_2Sc + W
Ti	Sc	Mn	-8.099600	N/A	N/A	-8.294789	195	N/A	N/A	**$Al_3Sc_2Ti_{10}C_9$** + **$Al_3Mn_4Sc_2C_3$** + TiC
Ti	Sc	Fe	-7.877452	N/A	N/A	-8.161638	284	N/A	N/A	Al_8Fe_4Sc + **$Al_3Sc_2Ti_{10}C_9$** + Al_6Fe_6Sc + $FeSc_3C_4$ + TiC
Zr	Sc	Sc	-7.908491	-7.977311	-8.007301	-8.022612	114	45	15	**$Al_3Sc_2Zr_{10}C_9$** + Al_3ScC_3 + $AlSc_3C$ + ZrC
Zr	Sc	Y	-7.843529	-7.905914	-7.963705	-8.015203	172	109	51	ZrC + AlY_3C_3 + Al_2Y + AlY_3C + $AlSc_3C$
Zr	Sc	Ti	-8.268907	-8.334362	-8.356070	-8.376239	107	42	20	**$Al_3Sc_2Ti_7C_6$** + **$Al_3Sc_2Zr_7C_6$**

Zr	Sc	Zr	-8.415430	N/A	-8.480303	-8.475137	60	N/A	-5	Al_3Zr_2 + Al_3Zr_4 + **$Al_3Sc_2Zr_{10}C_9$** + $AlSc_3C$
Zr	Sc	Hf	-8.689273	-8.727105	-8.745783	-8.747823	59	21	2	**$AlHf_2Zr_2C_3$** + Al_2Sc + **$Al_3Hf_{10}Sc_2C_9$** + **$Al_3Sc_2Zr_7C_6$** + $AlSc_3C$
Zr	Sc	V	-8.340504	-8.411458	-8.441044	-8.498604	158	87	58	**$Al_3Sc_2V_7C_6$** + **$Al_3Sc_2V_4C_3$** + **$Al_3Sc_2Zr_{10}C_9$**
Zr	Sc	Nb	-8.612030	-8.670440	-8.699492	-8.695645	84	25	-4	**$Al_3Sc_2Zr_7C_6$** + **$Al_3Nb_4Sc_2Zr_3C_6$**
Zr	Sc	Ta	-8.947776	-8.992596	-9.019435	-9.015216	67	23	-4	**$Al_3Sc_2Zr_7C_6$** + **$Al_3Sc_2Ta_4Zr_3C_6$**
Zr	Sc	Cr	-8.234858	N/A	N/A	-8.504508	270	N/A	N/A	**$Al_3Cr_4Sc_2C_3$** + **$Al_3Sc_2Zr_{10}C_9$** + ZrC
Zr	Sc	Mo	-8.556387	N/A	N/A	-8.711679	155	N/A	N/A	ZrC + **$Al_3Mo_4Sc_2C_3$** + **$Al_3Sc_2Zr_{10}C_9$**
Zr	Sc	W	-8.910320	N/A	N/A	-9.029818	119	N/A	N/A	**$Al_3Sc_2Zr_{10}C_9$** + **$Al_3Sc_2W_4C_3$** + ZrC
Zr	Sc	Mn	-8.148246	N/A	N/A	-8.436894	289	N/A	N/A	**$Al_3Sc_2Zr_{10}C_9$** + **$Al_3Mn_4Sc_2C_3$** + ZrC
Zr	Sc	Fe	-7.933314	N/A	N/A	-8.305389	372	N/A	N/A	Al_8Fe_4Sc + Al_6Fe_6Sc + $FeSc_3C_4$ + $AlSc_3C$ + ZrC
Hf	Sc	Sc	-8.265045	-8.339947	-8.368200	-8.392580	128	53	24	Al_3Sc + Al_3ScC_3 + $AlSc_3C$ + HfC
Hf	Sc	Y	-8.187640	-8.256264	-8.305827	-8.388351	201	132	83	AlY_3C_3 + AlY_3C + Al_2Y + $AlSc_3C$ + HfC
Hf	Sc	Ti	-8.627431	-8.704611	-8.714699	-8.731038	104	26	16	**$Al_3Sc_2Ti_7C_6$** + Al_2Sc + **$AlHfTi_2C_2$** + **$Al_3Hf_{10}Sc_2C_9$** + $AlSc_3C$
Hf	Sc	Zr	-8.763410	-8.816218	-8.832168	-8.836996	74	21	5	**$AlHf_2Zr_2C_3$** + Al_2Sc + **$Al_3Hf_{10}Sc_2C_9$** + **$Al_3Sc_2Zr_7C_6$** + $AlSc_3C$
Hf	Sc	Hf	-9.040231	N/A	-9.098206	-9.093906	54	N/A	-4	Al_2Sc + Al_3Hf_4 + AlSc + $Al_3Hf_{10}Sc_2C_9$
Hf	Sc	V	-8.698834	-8.782960	-8.801334	-8.858649	160	76	57	**$Al_3Sc_2V_4C_3$** + **$Al_3Hf_{10}Sc_2C_9$** + HfC
Hf	Sc	Nb	-8.960254	-9.029720	-9.053261	-9.049036	89	19	-4	Al_2Sc + $AlSc_3C$ + **$Al_3Hf_{10}Sc_2C_9$** + $AlNb_2$ + **$Al_3Hf_3Nb_4Sc_2C_6$**
Hf	Sc	Ta	-9.296040	-9.352415	-9.373741	-9.368253	72	16	-5	**$Al_3Hf_7Sc_2C_6$** + **$Al_3Hf_3Sc_2Ta_4C_6$**
Hf	Sc	Cr	-8.595344	N/A	N/A	-8.868388	273	N/A	N/A	**$Al_3Cr_4Sc_2C_3$** + **$Al_3Hf_{10}Sc_2C_9$** + HfC
Hf	Sc	Mo	-8.906969	N/A	N/A	-9.076267	169	N/A	N/A	Al_8Mo_3 + **$Al_3Mo_4Sc_5C_6$** + **$Al_3Hf_{10}Sc_2C_9$** + $AlMo_3$ + HfC
Hf	Sc	W	-9.259050	N/A	N/A	-9.399538	140	N/A	N/A	**$Al_3Sc_2W_4C_3$** + **$Al_3Sc_5W_4C_6$** + Al_3Sc + HfC + W
Hf	Sc	Mn	-8.504099	N/A	N/A	-8.800774	297	N/A	N/A	**$Al_3Hf_{10}Sc_2C_9$** + **$Al_3Mn_4Sc_2C_3$** + HfC
Hf	Sc	Fe	-8.287260	N/A	N/A	-8.678537	391	N/A	N/A	Al_6Fe_6Sc + Al_8Fe_4Sc + $FeSc_3C_4$ + $AlSc_3C$ + HfC
V	Sc	Sc	-8.025090	-8.014456	-8.023980	-8.025609	1	11	2	**$AlSc_2VC_2$** + **$Al_3Sc_2V_7C_6$**
V	Sc	Y	-7.887632	-7.848328	-7.917268	-8.015427	128	167	98	**$Al_3Sc_3V_4Y_2C_6$** + V_6C_5 + AlY_3C_3 + AlY_3C + Al_2Y
V	Sc	Ti	-8.403675	-8.416321	-8.390493	-8.408426	5	-8	18	**$Al_3Sc_2V_7C_6$** + **$Al_3Sc_2Ti_4V_3C_6$**
V	Sc	Zr	-8.455114	-8.421007	-8.437901	-8.500321	45	79	62	**$Al_3Sc_2V_7C_6$** + **$Al_3Sc_2V_4C_3$** + **$Al_3Sc_2Zr_{10}C_9$**
V	Sc	Hf	-8.739477	-8.704130	-8.710366	-8.772513	33	68	62	**$Al_3Sc_2V_4C_3$** + HfC
V	Sc	V	-8.493888	N/A	-8.505473	-8.494815	1	N/A	-11	**$Al_3Sc_2V_4C_3$** + **$Al_3Sc_2V_{10}C_9$**
V	Sc	Nb	-8.682011	-8.678310	-8.679047	-8.705950	24	28	27	**$Al_3Sc_2V_7C_6$** + **$Al_3Nb_7Sc_2C_6$**
V	Sc	Ta	-9.014121	-9.003128	-8.999355	-9.022277	8	19	23	**$Al_3Sc_2V_7C_6$** + **$Al_3Sc_2V_4C_3$** + **$Al_3Sc_2Ta_{10}C_9$**
V	Sc	Cr	-8.389009	N/A	N/A	-8.498972	110	N/A	N/A	**$Al_3Cr_4Sc_2V_3C_6$** + **$Al_3Sc_2V_{10}C_9$** + **$Al_3Cr_4Sc_2C_3$**
V	Sc	Mo	-8.637956	N/A	N/A	-8.705803	68	N/A	N/A	Al_3ScC_3 + V_6C_5 + **$Al_3Mo_4Sc_2C_3$** + **$Al_3Mo_4Sc_5C_6$** + Al_8Mo_3
V	Sc	W	-8.981776	N/A	N/A	-9.033842	52	N/A	N/A	Al_3ScC_3 + **$Al_3V_4W_2C_3$** + **$Al_3Sc_5W_4C_6$** + WC + V_6C_5
V	Sc	Mn	-8.283358	N/A	N/A	-8.429583	146	N/A	N/A	V_6C_5 + **$Al_3Sc_2V_{10}C_9$** + Sc_3C_4 + Al_3ScC_3 + **$Al_3Mn_4Sc_2C_3$**
V	Sc	Fe	-8.057929	N/A	N/A	-8.289643	232	N/A	N/A	Al_6Fe_6Sc + Al_3ScC_3 + C + $FeSc_3C_4$ + V_6C_5
Nb	Sc	Sc	-8.271790	-8.320154	-8.341370	-8.327761	56	8	-14	**$Al_3Nb_7Sc_2C_6$** + **$AlNb_2Sc_2C_3$** + Al_2Sc + $AlSc_3C$
Nb	Sc	Y	-8.177514	-8.208223	-8.256752	-8.306620	129	98	50	**$Al_3Nb_4Sc_3Y_2C_6$** + AlY_3C + AlY_3C_3 + **$Al_3Nb_{10}Sc_2C_9$** + Al_2Y
Nb	Sc	Ti	-8.609904	-8.661122	-8.671511	-8.668988	59	8	-3	**$Al_3Nb_3Sc_2Ti_4C_6$** + **$Al_3Nb_7Sc_2C_6$**
Nb	Sc	Zr	-8.714923	-8.737101	-8.767426	-8.767932	53	31	1	**$Al_3Nb_3Sc_2Zr_4C_6$** + **$Al_3Nb_7Sc_2C_6$**
Nb	Sc	Hf	-8.990190	-9.007196	-9.031828	-9.033258	43	26	1	**$Al_3Hf_4Nb_3Sc_2C_6$** + **$Al_3Nb_7Sc_2C_6$**
Nb	Sc	V	-8.661688	-8.735783	-8.749951	-8.772775	111	37	23	**$Al_3Sc_2V_7C_6$** + **$Al_3Nb_7Sc_2C_6$**
Nb	Sc	Nb	-8.894075	N/A	-8.973252	-8.948237	54	N/A	-25	**$Al_3Nb_{10}Sc_2C_9$** + **$Al_3Nb_4Sc_2C_3$**
Nb	Sc	Ta	-9.221476	-9.256417	-9.287063	-9.288103	67	32	1	**$Al_3Nb_3Sc_2Ta_4C_6$** + **$Al_3Nb_7Sc_2C_6$**

Nb	Sc	Cr	-8.553160	N/A	N/A	-8.760797	208	N/A	N/A	C + **$Al_3Cr_4Sc_2C_3$** + Cr_3C_2 + **$Al_3Nb_{10}Sc_2C_9$**
Nb	Sc	Mo	-8.803644	N/A	N/A	-8.966375	163	N/A	N/A	**$Al_3Mo_4Sc_2C_3$** + **$Al_3Nb_{10}Sc_2C_9$** + Mo_2C + C
Nb	Sc	W	-9.144434	N/A	N/A	-9.293819	149	N/A	N/A	**$Al_3Nb_{10}Sc_2C_9$** + **$Al_3Sc_2W_4C_3$** + WC
Nb	Sc	Mn	-8.444548	N/A	N/A	-8.688012	243	N/A	N/A	**$Al_3Nb_{10}Sc_2C_9$** + Mn_7C_3 + C + **$Al_3Mn_4Sc_2C_3$**
Nb	Sc	Fe	-8.232933	N/A	N/A	-8.547310	314	N/A	N/A	**$Al_3Nb_{10}Sc_2C_9$** + $AlFe_3C$ + $FeSc_3C_4$ + Al_6Fe_6Sc + C
Ta	Sc	Sc	-8.705748	-8.760745	-8.778140	-8.767514	62	7	-11	**$Al_3Sc_2Ta_7C_6$** + Al_2Sc + $AlSc_3C$ + **$AlSc_2Ta_2C_3$**
Ta	Sc	Y	-8.608807	-8.638403	-8.683974	-8.741255	132	103	57	AlY_3C_3 + **$Al_3Sc_4Ta_6Y_2C_9$** + AlY_3C + Al_2Y + **$Al_3Sc_2Ta_{10}C_9$**
Ta	Sc	Ti	-9.032971	-9.095544	-9.104414	-9.097713	65	2	-7	**$Al_3Sc_2Ta_7C_6$** + **$Al_3Sc_2Ta_3Ti_4C_6$**
Ta	Sc	Zr	-9.133845	-9.163557	-9.193520	-9.190632	57	27	-3	**$Al_3Sc_2Ta_7C_6$** + **$Al_3Sc_2Ta_3Zr_4C_6$**
Ta	Sc	Hf	-9.409018	-9.434168	-9.458268	-9.456361	47	22	-2	**$Al_3Hf_4Sc_2Ta_3C_6$** + **$Al_3Sc_2Ta_7C_6$**
Ta	Sc	V	-9.077398	-9.165361	-9.176446	-9.194545	117	29	18	**$Al_3Sc_2V_7C_6$** + **$Al_3Sc_2V_4C_3$** + **$Al_3Sc_2Ta_{10}C_9$**
Ta	Sc	Nb	-9.301096	-9.360967	-9.393054	-9.391353	90	30	-2	**$Al_3Nb_4Sc_2Ta_3C_6$** + **$Al_3Sc_2Ta_7C_6$**
Ta	Sc	Ta	-9.625490	N/A	-9.704221	-9.690498	65	N/A	-14	**$Al_3Sc_2Ta_{10}C_9$** + Ta_2C + Al_2Sc + $AlSc_3C$
Ta	Sc	Cr	-8.971178	N/A	N/A	-9.188522	217	N/A	N/A	Cr_3C_2 + **$Al_3Cr_4Sc_2C_3$** + C + **$Al_3Sc_2Ta_{10}C_9$**
Ta	Sc	Mo	-9.205414	N/A	N/A	-9.395478	190	N/A	N/A	**$Al_3Mo_4Sc_2C_3$** + **$Al_3Mo_4Sc_2Ta_6C_9$** + **$Al_3Sc_2Ta_{10}C_9$**
Ta	Sc	W	-9.541512	N/A	N/A	-9.721545	180	N/A	N/A	**$Al_3Sc_2W_4C_3$** + WC + **$Al_3Sc_2Ta_{10}C_9$**
Ta	Sc	Mn	-8.858517	N/A	N/A	-9.118708	260	N/A	N/A	**$Al_3Mn_4Sc_2Ta_6C_9$** + **$Al_3Sc_2Ta_{10}C_9$** + **$Al_3Mn_4Sc_2C_3$**
Ta	Sc	Fe	-8.649923	N/A	N/A	-8.979008	329	N/A	N/A	$AlFe_3C$ + **$Al_3Sc_2Ta_{10}C_9$** + Al_6Fe_6Sc + C + **$AlSc_2Ta_2C_3$**
Cr	Sc	Sc	-8.023653	-7.948063	-7.960345	-8.028884	5	81	69	$CrSc_2C_3$ + **$Al_3Cr_4Sc_2C_3$** + Al_3ScC_3 + $AlSc_3C$
Cr	Sc	Y	-7.878038	-7.774651	-7.869639	-8.012048	134	237	142	$CrSc_2C_3$ + $Cr_2Y_2C_3$ + **$Al_3Cr_4Sc_2C_3$** + Al_2Y
Cr	Sc	Ti	-8.403436	-8.351808	-8.315450	-8.402138	-1	50	87	**$Al_3Cr_4Sc_2Ti_6C_9$** + **$Al_3Cr_4Sc_2C_3$**
Cr	Sc	Zr	-8.439950	-8.337585	-8.366041	-8.505637	66	168	140	**$Al_3Cr_4Sc_2C_3$** + ZrC
Cr	Sc	Hf	-8.723509	-8.620989	-8.624656	-8.785499	62	165	161	**$Al_3Cr_4Sc_2C_3$** + HfC
Cr	Sc	V	-8.496635	-8.479714	-8.429839	-8.492828	-4	13	63	C + **$Al_3Cr_4Sc_2C_3$** + V_6C_5
Cr	Sc	Nb	-8.668520	-8.593597	-8.585343	-8.682945	14	89	98	C + **$Al_3Cr_4Sc_2C_3$** + Cr_3C_2 + **$Al_3Nb_{10}Sc_2C_9$**
Cr	Sc	Ta	-8.998904	-8.917803	-8.904670	-9.003739	5	86	99	Cr_3C_2 + **$Al_3Cr_4Sc_2C_3$** + C + **$Al_3Sc_2Ta_{10}C_9$**
Cr	Sc	Cr	-8.399410	N/A	N/A	-8.449388	50	N/A	N/A	**$Al_3Cr_4Sc_2C_3$** + Cr_3C_2 + C
Cr	Sc	Mo	-8.633177	N/A	N/A	-8.656558	23	N/A	N/A	**$Al_3Mo_4Sc_2C_3$** + C + **$Al_3Cr_4Sc_2C_3$** + Cr_3C_2
Cr	Sc	W	-8.969746	N/A	N/A	-9.013263	44	N/A	N/A	WC + **$Al_3Cr_4Sc_2C_3$**
Cr	Sc	Mn	-8.291818	N/A	N/A	-8.381773	90	N/A	N/A	**$Al_3Cr_4Sc_2C_3$** + C + Cr_3C_2 + **$Al_3Mn_4Sc_2C_3$**
Cr	Sc	Fe	-8.072188	N/A	N/A	-8.241861	170	N/A	N/A	Cr_3C_2 + Al_6Fe_6Sc + C + $CrScC_2$
Mo	Sc	Sc	-8.343723	-8.331111	-8.352041	-8.304827	-39	-26	-47	**$AlMoSc_2C_2$** + **$AlMo_2Sc_2C_3$** + **$Al_3Mo_4Sc_2C_3$**
Mo	Sc	Y	-8.226711	-8.190479	-8.253641	-8.325190	98	135	72	**$Al_3Mo_4Sc_3Y_2C_6$** + **$Al_3Mo_4Y_2C_3$** + Y_2C + Y_4C_5
Mo	Sc	Ti	-8.678754	-8.678001	-8.683806	-8.682463	4	4	-1	**$Al_3Mo_4Sc_2Ti_6C_9$** + **$Al_3Mo_4Sc_2C_3$**
Mo	Sc	Zr	-8.756376	-8.716577	-8.752085	-8.781864	25	65	30	ZrC + **$Al_3Mo_4Sc_2C_3$**
Mo	Sc	Hf	-9.030023	-8.989806	-9.016976	-9.061726	32	72	45	**$Al_3Mo_4Sc_2C_3$** + HfC
Mo	Sc	V	-8.736007	-8.755367	-8.758750	-8.769055	33	14	10	V_6C_5 + **$Al_3Mo_4Sc_2C_3$** + C
Mo	Sc	Nb	-8.942770	-8.916796	-8.950198	-8.955987	13	39	6	**$Al_3Mo_4Sc_2C_3$** + **$Al_3Nb_{10}Sc_2C_9$** + Mo_2C + C
Mo	Sc	Ta	-9.268140	-9.232236	-9.263010	-9.279536	11	47	17	**$Al_3Mo_4Sc_2C_3$** + **$Al_3Mo_4Sc_2Ta_6C_9$**
Mo	Sc	Cr	-8.628200	N/A	N/A	-8.725615	97	N/A	N/A	**$Al_3Mo_4Sc_2C_3$** + C + Cr_3C_2
Mo	Sc	Mo	-8.859495	N/A	N/A	-8.924824	65	N/A	N/A	**$Al_3Mo_4Sc_2C_3$** + C + Mo_2C
Mo	Sc	W	-9.190515	N/A	N/A	-9.289490	99	N/A	N/A	**$Al_3Mo_4Sc_2C_3$** + WC
Mo	Sc	Mn	-8.517067	N/A	N/A	-8.650039	133	N/A	N/A	Mo_2C + **$Al_3Mo_4Sc_2C_3$** + C + **$Al_3Mn_4Sc_2C_3$**
Mo	Sc	Fe	-8.303476	N/A	N/A	-8.514975	211	N/A	N/A	**$AlMo_2ScC_2$** + $AlFe_3C$ + C

W	Sc	Sc	-8.800000	-8.791314	-8.810939	-8.767261	-33	-24	-44	**$AlSc_2W_2C_3$** + **$Al_3Sc_2W_4C_3$** + **$AlSc_2WC_2$**
W	Sc	Y	-8.682403	-8.644018	-8.703367	-8.771240	89	127	68	**$Al_3Sc_3W_4Y_2C_6$** + **$Al_3W_4Y_5C_6$**
W	Sc	Ti	-9.118514	-9.123828	-9.133253	-9.128349	10	5	-5	**$Al_3Sc_2W_4C_3$** + **$Al_3Sc_2Ti_6W_4C_9$**
W	Sc	Zr	-9.194871	-9.157762	-9.196098	-9.206050	11	48	10	**$Al_3Sc_2W_4C_3$** + ZrC
W	Sc	Hf	-9.466969	-9.429595	-9.460184	-9.485911	19	56	26	**$Al_3Sc_2W_4C_3$** + HfC
W	Sc	V	-9.160042	-9.189986	-9.198394	-9.206453	46	16	8	Al_3ScC_3 + **$Al_3V_4W_2C_3$** + **$Al_3Sc_5W_4C_6$** + WC + V_6C_5
W	Sc	Nb	-9.361236	-9.344974	-9.386511	-9.398783	38	54	12	WC + **$Al_3Nb_{10}Sc_2C_9$** + **$Al_3Sc_2W_4C_3$**
W	Sc	Ta	-9.683703	-9.655452	-9.695510	-9.719577	36	64	24	**$Al_3Sc_2W_4C_3$** + WC + **$Al_3Sc_2Ta_{10}C_9$**
W	Sc	Cr	-9.052681	N/A	N/A	-9.188366	136	N/A	N/A	WC + **$Al_3Sc_2W_4C_3$** + **$Al_3Cr_4Sc_2C_3$**
W	Sc	Mo	-9.262135	N/A	N/A	-9.397769	136	N/A	N/A	**$Al_3Mo_4Sc_2C_3$** + WC + $AlMo_3$ + Al_8Mo_3 + **$Al_3Sc_5W_4C_6$**
W	Sc	W	-9.587919	N/A	N/A	-9.713675	126	N/A	N/A	**$Al_3Sc_2W_4C_3$** + WC
W	Sc	Mn	-8.934725	N/A	N/A	-9.120751	186	N/A	N/A	**$Al_3Sc_2W_4C_3$** + WC + **$Al_3Mn_4Sc_2C_3$**
W	Sc	Fe	-8.723120	N/A	N/A	-8.988298	265	N/A	N/A	Al_6Fe_6Sc + C + **$Al_3Sc_5W_4C_6$** + $FeSc_3C_4$ + WC
Mn	Sc	Sc	-7.920333	-7.789892	-7.815919	-7.927005	7	137	111	Sc_3C_4 + **$Al_3Mn_4Sc_2C_3$** + Sc_4C_3
Mn	Sc	Y	-7.776439	-7.656887	-7.761322	-7.917778	141	261	156	AlY_3C + $Mn_{13}Y_{10}C_{18}$ + AlY_3C_3 + $AlSc_3C$ + **$Al_3Mn_4Sc_2C_3$**
Mn	Sc	Ti	-8.298542	-8.194322	-8.160690	-8.307584	9	113	147	**$Al_3Mn_4Sc_2C_3$** + TiC
Mn	Sc	Zr	-8.331182	-8.185491	-8.220619	-8.415485	84	230	195	**$Al_3Mn_4Sc_2C_3$** + ZrC
Mn	Sc	Hf	-8.613649	-8.467820	-8.478981	-8.695346	82	228	216	**$Al_3Mn_4Sc_2C_3$** + HfC
Mn	Sc	V	-8.393828	-8.333913	-8.283715	-8.402676	9	69	119	V_6C_5 + C + **$Al_3Mn_4Sc_2C_3$**
Mn	Sc	Nb	-8.558886	-8.443110	-8.443956	-8.582452	24	139	138	**$Al_3Nb_{10}Sc_2C_9$** + Mn_7C_3 + C + **$Al_3Mn_4Sc_2C_3$**
Mn	Sc	Ta	-8.887062	-8.767920	-8.764243	-8.909187	22	141	145	**$Al_3Mn_4Sc_2Ta_6C_9$** + **$Al_3Mn_4Sc_2C_3$**
Mn	Sc	Cr	-8.290007	N/A	N/A	-8.359235	69	N/A	N/A	C + Cr_3C_2 + **$Al_3Mn_4Sc_2C_3$**
Mn	Sc	Mo	-8.517771	N/A	N/A	-8.558444	41	N/A	N/A	Mo_2C + C + **$Al_3Mn_4Sc_2C_3$**
Mn	Sc	W	-8.855421	N/A	N/A	-8.923110	68	N/A	N/A	WC + **$Al_3Mn_4Sc_2C_3$**
Mn	Sc	Mn	-8.172985	N/A	N/A	-8.265771	93	N/A	N/A	**$Al_3Mn_4Sc_2C_3$** + C + Mn_7C_3
Mn	Sc	Fe	-7.950557	N/A	N/A	-8.134614	184	N/A	N/A	$AlFe_3C$ + **$Al_3Mn_4Sc_2C_3$** + C + $FeSc_3C_4$ + Mn_7C_3
Fe	Sc	Sc	-7.727920	-7.547500	-7.588167	-7.767490	40	220	179	Al_6Fe_6Sc + Al_8Fe_4Sc + $FeSc_3C_4$ + $AlSc_3C$
Fe	Sc	Y	-7.598559	-7.462655	-7.541279	-7.728902	130	266	188	Y_3C_4 + $AlFe_3$ + Al_6Fe_6Sc + $FeSc_3C_4$ + Y_4C_5
Fe	Sc	Ti	-8.089752	-7.936357	-7.911909	-8.113389	24	177	201	$AlFe_3C$ + Al_6Fe_6Sc + C + $FeSc_3C_4$ + TiC
Fe	Sc	Zr	-8.134284	-7.936143	-7.989732	-8.221290	87	285	232	Al_6Fe_6Sc + $AlFe_3C$ + C + $FeSc_3C_4$ + ZrC
Fe	Sc	Hf	-8.415078	-8.211881	-8.242042	-8.501151	86	289	259	$AlFe_3C$ + Al_6Fe_6Sc + C + $FeSc_3C_4$ + HfC
Fe	Sc	V	-8.177902	-8.083160	-8.021952	-8.208481	31	125	187	$AlFe_3C$ + Al_6Fe_6Sc + C + $FeSc_3C_4$ + V_6C_5
Fe	Sc	Nb	-8.356386	-8.187438	-8.182604	-8.398144	42	211	216	**$Al_3Nb_{10}Sc_2C_9$** + $AlFe_3C$ + $FeSc_3C_4$ + Al_6Fe_6Sc + C
Fe	Sc	Ta	-8.687626	-8.511346	-8.499401	-8.723738	36	212	224	$AlFe_3C$ + **$Al_3Sc_2Ta_{10}C_9$** + Al_6Fe_6Sc + C + **$AlSc_2Ta_2C_3$**
Fe	Sc	Cr	-8.077054	N/A	N/A	-8.170694	94	N/A	N/A	Cr_3C_2 + Al_6Fe_6Sc + C + $AlFe_3C$ + $CrScC_2$
Fe	Sc	Mo	-8.308905	N/A	N/A	-8.376245	67	N/A	N/A	**$AlMo_2ScC_2$** + $AlFe_3C$ + **$Al_3Mo_4Sc_5C_6$** + C
Fe	Sc	W	-8.648207	N/A	N/A	-8.728915	81	N/A	N/A	Al_6Fe_6Sc + C + $AlFe_3C$ + $FeSc_3C_4$ + WC
Fe	Sc	Mn	-7.965249	N/A	N/A	-8.090895	126	N/A	N/A	$AlFe_3C$ + **$Al_3Mn_4Sc_2C_3$** + C + $FeSc_3C_4$ + Mn_7C_3
Fe	Sc	Fe	-7.740159	N/A	N/A	-7.950647	210	N/A	N/A	$AlFe_3C$ + Al_6Fe_6Sc + $FeSc_3C_4$ + C

Table S9. Structural information for stable 312 *s*-MAX phases in Figure 4a. The space group symmetry is *Cmcm* (#63).

s-MAX phase	*a* (Å)	*b* (Å)	*c* (Å)	Wyckoff positions
$Cr_4Sc_2Nb_3Al_3C_6$	9.27402	5.35548	17.9620	Cr1 16h (0.16706, 0.16604, 0.62458) Sc1 8f (0.00000, 0.66819, 0.65152) Nb1 4a (0.00000, 0.00000, 0.00000) Nb2 8e (0.66197, 0.00000, 0.00000) Al1 4c (0.00000, 0.84446, 0.25000) Al2 8g (0.25559, 0.07733, 0.25000) C1 16h (0.17108, 0.16240, 0.07651) C2 8f (0.00000, 0.67524, 0.07759)
$Cr_4Sc_2Ti_3Al_3C_6$	9.15310	5.27548	17.7516	Cr1 16h (0.16666, 0.16642, 0.62188) Sc1 8f (0.00000, 0.66646, 0.65097) Ti1 4a (0.00000, 0.00000, 0.00000) Ti2 8e (0.66122, 0.00000, 0.00000) Al1 4c (0.00000, 0.84272, 0.25000) Al2 8g (0.25481, 0.07781, 0.25000) C1 16h (0.17196, 0.16093, 0.07364) C2 8f (0.00000, 0.67626, 0.07226)
$Cr_4Sc_2V_3Al_3C_6$	9.00360	5.19446	17.5198	Cr1 16h (0.16685, 0.16596, 0.61990) Sc1 8f (0.00000, 0.66820, 0.64977) V1 4a (0.00000, 0.00000, 0.00000) V2 8e (0.66056, 0.00000, 0.00000) Al1 4c (0.00000, 0.84072, 0.25000) Al2 8g (0.25458, 0.07730, 0.25000) C1 16h (0.17089, 0.16231, 0.06984) C2 8f (0.00000, 0.67398, 0.06923)
$Mo_4Sc_2Sc_3Al_3C_6$	9.54132	5.50662	18.9988	Mo1 16h (0.16649, 0.16653, 0.62739) Sc1 8f (0.00000, 0.66651, 0.64771) Sc2 4a (0.00000, 0.00000, 0.00000) Sc3 8e (0.66288, 0.00000, 0.00000) Al1 4c (0.00000, 0.85605, 0.25000) Al2 8g (0.26100, 0.07228, 0.25000) C1 16h (0.17109, 0.16217, 0.07666) C2 8f (0.00000, 0.67531, 0.07512)
$Ti_4Sc_2Ti_3Al_3C_6$	9.38236	5.41252	18.8164	Ti1 16h (0.16723, 0.16615, 0.62275) Sc1 8f (0.00000, 0.66648, 0.64159) Ti2 4a (0.00000, 0.00000, 0.00000) Ti3 8e (0.66337, 0.00000, 0.00000) Al1 4c (0.00000, 0.85722, 0.25000) Al2 8g (0.26267, 0.07027, 0.25000) C1 16h (0.16887, 0.16484, 0.06816) C2 8f (0.00000, 0.67106, 0.06735)
$V_4Sc_2Nb_3Al_3C_6$	9.35320	5.39208	18.3494	V1 16h (0.16642, 0.16613, 0.62428) Sc1 8f (0.00000, 0.66726, 0.64852) Nb1 4a (0.00000, 0.00000, 0.00000) Nb2 8e (0.66137, 0.00000, 0.00000) Al1 4c (0.00000, 0.84994, 0.25000) Al2 8g (0.25713, 0.07687, 0.25000) C1 16h (0.16977, 0.16366, 0.07455) C2 8f (0.00000, 0.67192, 0.07505)
$V_4Sc_2Sc_3Al_3C_6$	9.40532	5.43478	18.7800	V1 16h (0.16697, 0.16630, 0.62575) Sc1 8f (0.00000, 0.66612, 0.64892) Sc2 4a (0.00000, 0.00000, 0.00000) Sc3 8e (0.66315, 0.00000, 0.00000) Al1 4c (0.00000, 0.85037, 0.25000) Al2 8g (0.25904, 0.07432, 0.25000) C1 16h (0.17394, 0.15953, 0.07912) C2 8f (0.00000, 0.68110, 0.07848)

$V_4Sc_2Ta_3Al_3C_6$	9.33932	5.38508	18.2909	V1 16h (0.16637, 0.16589, 0.62410) Sc1 8f (0.00000, 0.66705, 0.64853) Ta1 4a (0.00000, 0.00000, 0.00000) Ta2 8e (0.66139, 0.00000, 0.00000) Al1 4c (0.00000, 0.85067, 0.25000) Al2 8g (0.25733, 0.07685, 0.25000) C1 16h (0.16921, 0.16438, 0.07318) C2 8f (0.00000, 0.67077, 0.07378)
$V_4Sc_2Ti_3Al_3C_6$	9.22464	5.32256	18.1818	V1 16h (0.16679, 0.16646, 0.12240) Sc1 8f (0.00000, 0.66613, 0.14691) Ti1 4a (0.00000, 0.00000, 0.00000) Ti2 8e (0.33805, 0.00000, 0.00000) Al1 4c (0.00000, 0.14988, 0.25000) Al2 8g (0.75771, 0.42423, 0.25000) C1 16h (0.17083, 0.16232, 0.57141) C2 8f (0.00000, 0.67465, 0.57036)
$V_4Sc_2V_3Al_3C_6$	9.10130	5.24054	17.9093	V1 16h (0.16669, 0.16599, 0.61989) Sc1 8f (0.00000, 0.66692, 0.64637) V2 4a (0.00000, 0.00000, 0.00000) V3 8e (0.65961, 0.00000, 0.00000) Al1 4c (0.00000, 0.84842, 0.25000) Al2 8g (0.25691, 0.07660, 0.25000) C1 16h (0.16905, 0.16435, 0.06758) C2 8f (0.00000, 0.67061, 0.06723)
$W_4Sc_2Sc_3Al_3C_6$	9.53154	5.50152	19.0189	W1 16h (0.16661, 0.16682, 0.12777) Sc1 8f (0.00000, 0.66684, 0.14784) Sc2 4a (0.00000, 0.00000, 0.00000) Sc3 8e (0.33762, 0.00000, 0.00000) Al1 4c (0.00000, 0.13881, 0.25000) Al2 8g (0.76360, 0.43053, 0.25000) C1 16h (0.17090, 0.16219, 0.57659) C2 8f (0.00000, 0.67529, 0.57520)

Table S10. Structural information for stable 312 *s*-MAX phases in Figure 4b. The space group symmetry is *Cmcm* (#63).

s-MAX phase	*a* (Å)	*b* (Å)	*c* (Å)	Wyckoff positions
$Cr_4Y_2Nb_3Al_3C_6$	9.39748	5.42488	18.3574	Cr1 16h (0.16704, 0.16587, 0.62145) Y1 8f (0.00000, 0.66801, 0.65506) Nb1 4a (0.00000, 0.00000, 0.00000) Nb2 8e (0.66089, 0.00000, 0.00000) Al1 4c (0.00000, 0.83666, 0.25000) Al2 8g (0.25230, 0.07971, 0.25000) C1 16h (0.17461, 0.15861, 0.07401) C2 8f (0.00000, 0.68183, 0.07495)
$Cr_4Y_2Sc_3Al_3C_6$	9.46970	5.46798	18.6993	Cr1 16h (0.16716, 0.16698, 0.62305) Y1 8f (0.00000, 0.66722, 0.65669) Sc1 4a (0.00000, 0.00000, 0.00000) Sc2 8e (0.66088, 0.00000, 0.00000) Al1 4c (0.00000, 0.83769, 0.25000) Al2 8g (0.25247, 0.08060, 0.25000) C1 16h (0.17940, 0.15342, 0.07929) C2 8f (0.00000, 0.69127, 0.07840)
$Cr_4Y_2Ta_3Al_3C_6$	9.41122	5.42106	18.1970	Cr1 16h (0.16711, 0.16580, 0.62024) Y1 8f (0.00000, 0.66819, 0.65560) Ta1 4a (0.00000, 0.00000, 0.00000) Ta2 8e (0.66055, 0.00000, 0.00000) Al1 4c (0.00000, 0.83565, 0.25000) Al2 8g (0.25233, 0.07958, 0.25000) C1 16h (0.17358, 0.15944, 0.07313) C2 8f (0.00000, 0.67945, 0.07370)
$Cr_4Y_2Ti_3Al_3C_6$	9.28584	5.35764	18.1522	Cr1 16h (0.16686, 0.16646, 0.61858) Y1 8f (0.00000, 0.66644, 0.65429) Ti1 4a (0.00000, 0.00000, 0.00000) Ti2 8e (0.66006, 0.00000, 0.00000) Al1 4c (0.00000, 0.83656, 0.25000) Al2 8g (0.25181, 0.08053, 0.25000) C1 16h (0.17575, 0.15679, 0.07152) C2 8f (0.00000, 0.68284, 0.06983)
$Mo_4Y_2Sc_3Al_3C_6$	9.68950	5.59260	19.2008	Mo1 16h (0.16644, 0.16657, 0.62478) Y1 8f (0.00000, 0.66618, 0.65412) Sc1 4a (0.00000, 0.00000, 0.00000) Sc2 8e (0.66144, 0.00000, 0.00000) Al1 4c (0.00000, 0.84281, 0.25000) Al2 8g (0.25398, 0.07918, 0.25000) C1 16h (0.17485, 0.15833, 0.07562) C2 8f (0.00000, 0.68215, 0.07369)
$Nb_4Y_2Hf_3Al_3C_6$	9.85988	5.68852	19.4546	Nb1 16h (0.16695, 0.16636, 0.62545) Y1 8f (0.00000, 0.66647, 0.64998) Hf1 4a (0.00000, 0.00000, 0.00000) Hf2 8e (0.66235, 0.00000, 0.00000) Al1 4c (0.00000, 0.84532, 0.25000) Al2 8g (0.25475, 0.07853, 0.25000) C1 16h (0.17079, 0.16235, 0.07063) C2 8f (0.00000, 0.67466, 0.06990)
$Nb_4Y_2Nb_3Al_3C_6$	9.75650	5.62162	19.2582	Nb1 16h (0.16641, 0.16601, 0.62334) Y1 8f (0.00000, 0.66672, 0.64968) Nb1 4a (0.00000, 0.00000, 0.00000) Nb2 8e (0.65961, 0.00000, 0.00000) Al1 4c (0.00000, 0.84353, 0.25000) Al2 8g (0.25381, 0.08019, 0.25000) C1 16h (0.16878, 0.16463, 0.06825) C2 8f (0.00000, 0.66978, 0.06843)

$Nb_4Y_2Sc_3Al_3C_6$	9.84884	5.69082	19.6321	Nb1 16h (0.16708, 0.16631, 0.62504) Y1 8f (0.00000, 0.66597, 0.65104) Sc1 4a (0.00000, 0.00000, 0.00000) Sc2 8e (0.66215, 0.00000, 0.00000) Al1 4c (0.00000, 0.84355, 0.25000) Al2 8g (0.25562, 0.07747, 0.25000) C1 16h (0.17339, 0.16028, 0.07329) C2 8f (0.00000, 0.68041, 0.07235)
$Nb_4Y_2Ta_3Al_3C_6$	9.71956	5.60716	19.2309	Nb1 16h (0.16629, 0.16578, 0.62345) Y1 8f (0.00000, 0.66651, 0.64976) Ta1 4a (0.00000, 0.00000, 0.00000) Ta2 8e (0.65962, 0.00000, 0.00000) Al1 4c (0.00000, 0.84346, 0.25000) Al2 8g (0.25392, 0.08040, 0.25000) C1 16h (0.16831, 0.16530, 0.06683) C2 8f (0.00000, 0.66870, 0.06716)
$Nb_4Y_2Zr_3Al_3C_6$	9.91838	5.72190	19.5571	Nb1 16h (0.16689, 0.16653, 0.62614) Y1 8f (0.00000, 0.66665, 0.65049) Zr1 4a (0.00000, 0.00000, 0.00000) Zr2 8e (0.66252, 0.00000, 0.00000) Al1 4c (0.00000, 0.84575, 0.25000) Al2 8g (0.25509, 0.07799, 0.25000) C1 16h (0.17144, 0.16163, 0.07276) C2 8f (0.00000, 0.67588, 0.07211)
$Sc_4Y_2Ta_3Al_3C_6$	9.77462	5.63968	20.0516	Sc1 16h (0.16710, 0.16625, 0.62312) Y1 8f (0.00000, 0.66682, 0.64359) Ta1 4a (0.00000, 0.00000, 0.00000) Ta2 8e (0.66396, 0.00000, 0.00000) Al1 4c (0.00000, 0.84297, 0.25000) Al2 8g (0.25551, 0.07790, 0.25000) C1 16h (0.16674, 0.16686, 0.06313) C2 8f (0.00000, 0.66705, 0.06238)
$Sc_4Y_2W_3Al_3C_6$	9.69730	5.57644	19.7180	Sc1 16h (0.16755, 0.16484, 0.62105) Y1 8f (0.00000, 0.66685, 0.64446) W1 4a (0.00000, 0.00000, 0.00000) W2 8e (0.65723, 0.00000, 0.00000) Al1 4c (0.00000, 0.84339, 0.25000) Al2 8g (0.25455, 0.07973, 0.25000) C1 16h (0.16479, 0.16941, 0.06133) C2 8f (0.00000, 0.66402, 0.06232)
$Ta_4Y_2Hf_3Al_3C_6$	9.83164	5.67348	19.4042	Ta1 16h (0.16704, 0.16641, 0.62546) Y1 8f (0.00000, 0.66661, 0.65084) Hf1 4a (0.00000, 0.00000, 0.00000) Hf2 8e (0.66176, 0.00000, 0.00000) Al1 4c (0.00000, 0.84729, 0.25000) Al2 8g (0.25578, 0.07752, 0.25000) C1 16h (0.17129, 0.16187, 0.07129) C2 8f (0.00000, 0.67572, 0.07075)
$Ta_4Y_2Ta_3Al_3C_6$	9.69738	5.59332	19.1877	Ta1 16h (0.16644, 0.16541, 0.62334) Y1 8f (0.00000, 0.66598, 0.65061) Ta2 4a (0.00000, 0.00000, 0.00000) Ta3 8e (0.65837, 0.00000, 0.00000) Al1 4c (0.00000, 0.84567, 0.25000) Al2 8g (0.25480, 0.07938, 0.25000) C1 16h (0.16897, 0.16493, 0.06754) C2 8f (0.00000, 0.66978, 0.06817)

$Ta_4Y_2Zr_3Al_3C_6$	9.88990	5.70658	19.5130	Ta1 16h (0.16699, 0.16656, 0.62616) Y1 8f (0.00000, 0.66678, 0.65124) Zr1 4a (0.00000, 0.00000, 0.00000) Zr2 8e (0.66197, 0.00000, 0.00000) Al1 4c (0.00000, 0.84788, 0.25000) Al2 8g (0.25619, 0.07694, 0.25000) C1 16h (0.17194, 0.16118, 0.07348) C2 8f (0.00000, 0.67695, 0.07302)
$Ti_4Y_2Hf_3Al_3C_6$	9.73618	5.62158	19.3803	Ti1 16h (0.16727, 0.16585, 0.62424) Y1 8f (0.00000, 0.66690, 0.65178) Hf1 4a (0.00000, 0.00000, 0.00000) Hf2 8e (0.66358, 0.00000, 0.00000) Al1 4c (0.00000, 0.84188, 0.25000) Al2 8g (0.25503, 0.07825, 0.25000) C1 16h (0.17243, 0.16104, 0.07173) C2 8f (0.00000, 0.67796, 0.07104)
$Ti_4Y_2Nb_3Al_3C_6$	9.61848	5.55534	19.0851	Ti1 16h (0.16702, 0.16617, 0.62231) Y1 8f (0.00000, 0.66634, 0.65019) Nb1 4a (0.00000, 0.00000, 0.00000) Nb2 8e (0.66125, 0.00000, 0.00000) Al1 4c (0.00000, 0.84189, 0.25000) Al2 8g (0.25387, 0.07971, 0.25000) C1 16h (0.17021, 0.16315, 0.06919) C2 8f (0.00000, 0.67380, 0.06924)
$Ti_4Y_2Ta_3Al_3C_6$	9.59750	5.54100	19.0527	Ti1 16h (0.16708, 0.16608, 0.62220) Y1 8f (0.00000, 0.66653, 0.65016) Ta1 4a (0.00000, 0.00000, 0.00000) Ta2 8e (0.66137, 0.00000, 0.00000) Al1 4c (0.00000, 0.84158, 0.25000) Al2 8g (0.25365, 0.07996, 0.25000) C1 16h (0.16986, 0.16349, 0.06803) C2 8f (0.00000, 0.67305, 0.06811)
$Ti_4Y_2Ti_3Al_3C_6$	9.50266	5.48562	19.0256	Ti1 16h (0.16730, 0.16586, 0.62070) Y1 8f (0.00000, 0.66664, 0.65000) Ti2 4a (0.00000, 0.00000, 0.00000) Ti3 8e (0.66244, 0.00000, 0.00000) Al1 4c (0.00000, 0.83981, 0.25000) Al2 8g (0.25372, 0.07971, 0.25000) C1 16h (0.17171, 0.16201, 0.06691) C2 8f (0.00000, 0.67665, 0.06572)
$Ti_4Y_2Zr_3Al_3C_6$	9.79690	5.65686	19.4776	Ti1 16h (0.16723, 0.16587, 0.62511) Y1 8f (0.00000, 0.66686, 0.65212) Zr1 4a (0.00000, 0.00000, 0.00000) Zr2 8e (0.66379, 0.00000, 0.00000) Al1 4c (0.00000, 0.84272, 0.25000) Al2 8g (0.25539, 0.07796, 0.25000) C1 16h (0.17306, 0.16041, 0.07364) C2 8f (0.00000, 0.67927, 0.07309)
$V_4Y_2Nb_3Al_3C_6$	9.48500	5.45944	18.6786	V1 16h (0.16654, 0.16610, 0.62112) Y1 8f (0.00000, 0.66700, 0.65355) Nb1 4a (0.00000, 0.00000, 0.00000) Nb2 8e (0.66011, 0.00000, 0.00000) Al1 4c (0.00000, 0.83824, 0.25000) Al2 8g (0.25255, 0.08002, 0.25000) C1 16h (0.17277, 0.16022, 0.07234) C2 8f (0.00000, 0.67769, 0.07280)

$V_4Y_2Sc_3Al_3C_6$	9.54492	5.51588	19.0893	V1 16h (0.16719, 0.16661, 0.62321) Y1 8f (0.00000, 0.66675, 0.65452) Sc1 4a (0.00000, 0.00000, 0.00000) Sc2 8e (0.66186, 0.00000, 0.00000) Al1 4c (0.00000, 0.83992, 0.25000) Al2 8g (0.25364, 0.07951, 0.25000) C1 16h (0.17820, 0.15524, 0.07744) C2 8f (0.00000, 0.68919, 0.07673)
$V_4Y_2Ta_3Al_3C_6$	9.47180	5.45090	18.6219	V1 16h (0.16656, 0.16597, 0.62075) Y1 8f (0.00000, 0.66689, 0.65366) Ta1 4a (0.00000, 0.00000, 0.00000) Ta2 8e (0.66011, 0.00000, 0.00000) Al1 4c (0.00000, 0.83826, 0.25000) Al2 8g (0.25264, 0.07991, 0.25000) C1 16h (0.17194, 0.16125, 0.07097) C2 8f (0.00000, 0.67606, 0.07147)
$V_4Y_2Ti_3Al_3C_6$	9.35580	5.39918	18.5316	V1 16h (0.16702, 0.16656, 0.61940) Y1 8f (0.00000, 0.66617, 0.65226) Ti1 4a (0.00000, 0.00000, 0.00000) Ti2 8e (0.66074, 0.00000, 0.00000) Al1 4c (0.00000, 0.83954, 0.25000) Al2 8g (0.25244, 0.08097, 0.25000) C1 16h (0.17411, 0.15891, 0.06964) C2 8f (0.00000, 0.68084, 0.06841)
$W_4Y_2Sc_3Al_3C_6$	9.68142	5.58758	19.1954	W1 16h (0.16666, 0.16666, 0.62534) Y1 8f (0.00000, 0.66657, 0.65436) Sc1 4a (0.00000, 0.00000, 0.00000) Sc2 8e (0.66097, 0.00000, 0.00000) Al1 4c (0.00000, 0.84405, 0.25000) Al2 8g (0.25490, 0.07795, 0.25000) C1 16h (0.17462, 0.15845, 0.07550) C2 8f (0.00000, 0.68217, 0.07403)
$W_4Y_2Ti_3Al_3C_6$	9.51082	5.48124	18.7262	W1 16h (0.16608, 0.16601, 0.62099) Y1 8f (0.00000, 0.66555, 0.65317) Ti1 4a (0.00000, 0.00000, 0.00000) Ti2 8e (0.65836, 0.00000, 0.00000) Al1 4c (0.00000, 0.84069, 0.25000) Al2 8g (0.25335, 0.07901, 0.25000) C1 16h (0.17126, 0.16229, 0.06816) C2 8f (0.00000, 0.67354, 0.06649)
$W_4Y_2Y_3Al_3C_6$	9.91592	5.72488	19.7763	W1 16h (0.16665, 0.16667, 0.62970) Y1 8f (0.00000, 0.66699, 0.65730) Y2 4a (0.00000, 0.00000, 0.00000) Y3 8e (0.66225, 0.00000, 0.00000) Al1 4c (0.00000, 0.84647, 0.25000) Al2 8g (0.25639, 0.07673, 0.25000) C1 16h (0.17642, 0.15667, 0.08387) C2 8f (0.00000, 0.68575, 0.08305)
$W_4Y_2Zr_3Al_3C_6$	9.76122	5.62278	19.1930	W1 16h (0.16620, 0.16686, 0.62589) Y1 8f (0.00000, 0.66712, 0.65553) Zr1 4a (0.00000, 0.00000, 0.00000) Zr2 8e (0.66078, 0.00000, 0.00000) Al1 4c (0.00000, 0.84315, 0.25000) Al2 8g (0.25439, 0.07777, 0.25000) C1 16h (0.17247, 0.16056, 0.07588) C2 8f (0.00000, 0.67614, 0.07545)

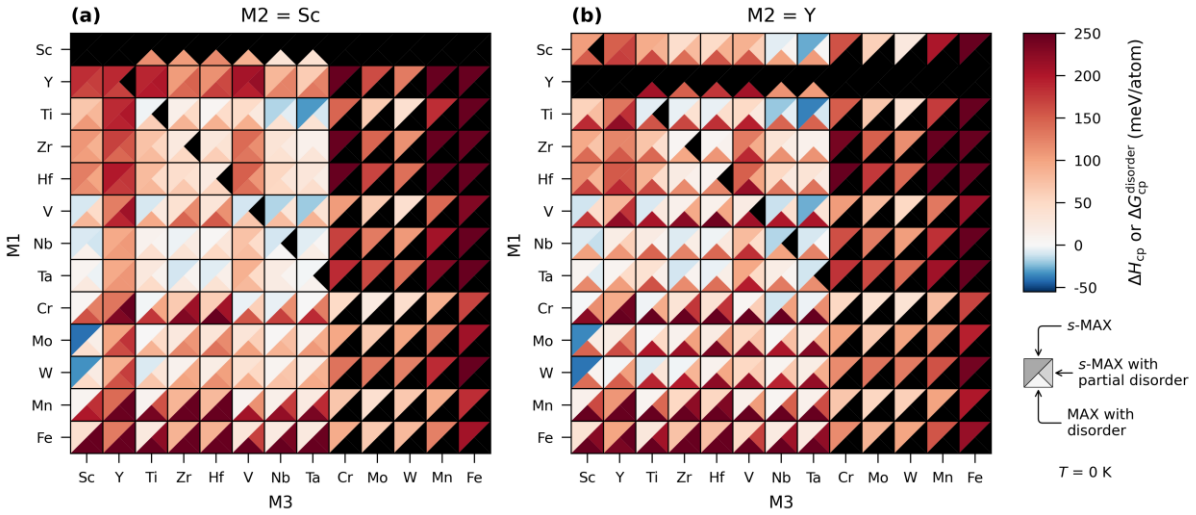

Figure S30. Stability heatmap evaluated at 0 K for 312 MAX phases upon mixing metals M1, M2, M3 in a 4:2:3 ratio with (a) M2 = Sc and (b) M2 = Y. For a given combination of M1 and M3, the right triangles indicate the stability for *s*-MAX with partial disorder, having in-plane order of M2 in the outer metal layer combined with disorder of M1 + M3, and the bottom triangles indicate the stability for MAX with disorder of M1, M2, and M3. Black triangles represent combinations of M1, M2 and M3 not considered.

Table S11. Atomic radius and electronegativity (Pauling scale) considered for M and A. [1, 2]

M	Atomic radius r_M (Å)	Electronegativity (Pauling scale)
Sc	1.62	1.36
Y	1.80	1.22
Ti	1.47	1.54
Zr	1.60	1.33
Hf	1.59	1.30
V	1.35	1.63
Nb	1.46	1.60
Ta	1.46	1.50
Cr	1.29	1.66
Mo	1.39	2.16
W	1.39	2.36
Mn	1.27	1.55
Fe	1.26	1.83
Al	1.43	1.61

Table S12. Calculated stability for synthesized 211 *i*-MAX phases being part of compositions in Figure S2. Data evaluated at 2000 K. Deviations from 2:1 metal ratio in reported composition is noted.

i-MAX phase	ΔH_{cp} (meV/atom)	Set of most competing phase	Notes	Exp. ref.
$Mo_4Sc_2Al_3C_3$	-40	$(Sc_{0.67}Mo_{0.33})_3AlC_2$ (312 MAX with disorder) + $AlMo_3$ + Mo_2ScAlC_2 (312 *o*-MAX) + Al_8Mo_3	Deviation from ideal 2:1 ratio of Mo:Sc have been reported[3]	4
$Mo_4Y_2Al_3C_3$	-99	Al_3YC_3 + $AlMo_3$ + AlY_3C_3 + C		5
$W_4Sc_2Al_3C_3$	-25	Al_3Sc + W_2ScAlC_2 (312 *o*-MAX) + W		6
$W_4Y_2Al_3C_3$	-35	WYC_2 + WC + Al_2Y + W		6
$Cr_4Sc_2Al_3C_3$	-98	Al_3Sc + $CrSc_2C_3$ + Cr_2AlC (211 MAX) + Sc_3AlC		7
$Cr_4Y_2Al_3C_3$	-39	Cr_7C_3 + $Cr_2Y_2C_3$ + Cr_2AlC (211 MAX) + Al_2Y		7
$Cr_4Zr_2Al_3C_3$	-65	Al_3Zr + Cr_2AlC (211 MAX) + $AlCr_2$ + ZrC		8
$V_4Sc_2Al_3C_3$	-29	V_2AlC (211 MAX) + Al_2Sc + $V_{12}Al_3C_8$ (413 MAX with ordered C-vacancies) + Sc_3AlC		9
$V_4Zr_2Al_3C_3$	-48	Zr_3AlC_2 (312 MAX) + Al_3Zr_2 + V_2AlC (211 MAX) + V_2C		5

Table S13. Calculated stability for synthesized 312 *o*-MAX phase being part of compositions in Figure S3. Data evaluated at 2000 K. Deviations from 2:1 metal ratio in reported composition is noted.

o-MAX phase	ΔH_{cp} (meV/atom)	Set of most competing phase	Notes	Exp. ref.
Cr_2TiAlC_2	-3	$Cr_2Ti_2AlC_3$ (413 *o*-MAX) + Cr_2AlC (211 MAX)	Intermixing shown to stabilize *o*-MAX phase	10 11
Cr_2VAlC_2	24	$(Cr_{0.67}V_{0.33})_2AlC$ (211 MAX with disorder) + C + Cr_3C_2 + V_6C_5	Reported composition $(Cr_{0.75}V_{0.25})_2VAlC_2$ Intermixing shown to stabilize *o*-MAX phase	12 11
Mo_2TiAlC_2	-16	$AlMo_3$ + C + $Mo_2Ti_2AlC_3$ (413 *o*-MAX) + Al_8Mo_3	Reported composition $Mo_2TiAlC_{1.7}$ Intermixing shown to stabilize *o*-MAX phase	13 11
Mo_2ScAlC_2	-13	$(Mo_{0.67}Sc_{0.33})_4AlC_3$ (413 MAX with disorder) + $Mo_4Sc_2Al_3C_3$ (211 *i*-MAX) + C + Mo_2C		14

Table S14. Calculated stability for synthesized 413 *o*-MAX phase being part of compositions in Figure S4. Data evaluated at 2000 K. Deviations from 2:2 metal ratio in reported composition is noted.

o-MAX phase	ΔH_{cp} (meV/atom)	Set of most competing phase	Notes	Exp. ref.
$Cr_2Ti_2AlC_3$	2	Cr_2TiC_2 (312 *o*-MAX) + TiC	Reported composition $Cr_{2.5}Ti_{1.5}AlC_3$ or $Cr_2(Ti_{0.75}Cr_{0.25})_2AlC_3$	15, 16
$Cr_2V_2AlC_3$	23	Cr_3C_2 + $(Cr_{0.67}V_{0.33})_2AlC$ (211 MAX with disorder) + C + V_6C_5	Reported composition $(Cr_{0.7}V_{0.3})_2(V_{0.8}Cr_{0.2})_4AlC_3$, i.e., intermixing of metal sites	12
$Mo_2Ti_2AlC_3$	-18	Mo_2TiAlC_2 (312 *o*-MAX) + TiC	Reported composition $Mo_2Ti_{1.9}Al_{0.9}C_{2.5}$	17
$Mo_2Nb_2AlC_3$	22	$AlMo_3$ + C + Al_8Mo_3 + Nb_6C_5	Some intermixing of metal sites and reported compostion deviates from ideal 2:2 ratio of Mo:Nb ($Mo_{2+\alpha}Nb_{2-\alpha}AlC_3$)	18

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