

Computationally discovered new materials

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Si No	Materials Formula	Total energy (eV)/for mula unit	Energy (eV/Atom)	Volume (Å ³ /atom)	Competing Phase 1	Space group	formation Energy 1 (eV/atom)	Competing phase 1 percentage	Competing Phase 2	Space group	formation Energy 2(eV/atom)	Competing phase 2 percentage	Competing Phase 3	Space group	formation Energy 3 (eV/atom)	Competing phase 3 percentage	Total formation energy of competing phases (eV)	Energy difference with competing phase (eV)	Formation energy difference (eV/atom)	New materials	Comments
1	Ag ₂ Al ₂ Ce	-19.5361	-3.90722	24.808	CeAl ₂	Fd3m	-4.563	1	Ag	P63/mmc	-2.764	2					-19.217	-0.31909	-0.06382	Yes	
2	Ag ₂ Al ₂ Th	-21.9739	-4.39477	20.798	ThAl ₂	P6/mmm	-5.418	1	Ag	P63/mmc	-2.764	2					-21.782	-0.19185	-0.03837	Yes	
3	Cd ₂ Al ₂ Ce	-16.0301	-3.20603	22.593	CeCd ₁₁	Pm-3m	-1.315	0.125	CeAl ₃	P63/mmc	-4.443	0.66	CeCd ₃	Fm-3m	-2.216	0.208	-15.6672	-0.36297	-0.07259	Yes	
4	Cd ₂ Ga ₂ Ce	-14.8794	-2.97589	22.123	CeCd ₁₁	Pm-3m	-1.315	0.18	CeGa ₃	P63/mmc	-4.044	0.36	CeGa ₂	P6/mmm	-4.303	0.45	-14.619	-0.26044	-0.05209	Yes	
5	Co ₂ Al ₂ Ce	-29.1445	-5.8289	16.74	AlCo	Pm-3m	-6.032	2	Ce	P63/mmc	-4.776	1					-28.904	-0.24051	-0.0481	Yes	
6	Co ₂ B ₂ Hf	-40.9287	-8.18573	10.12	HfCo ₃ B ₂	P6/mmm	-8.019	0.667	HfB ₂	P6/mmm	-8.794	0.333					-40.7942	-0.13445	-0.02689	Yes	
7	Co ₂ B ₂ Th	-37.6418	-7.52835	12.641	Th ₂ CoB ₁₀	Pbam	-7.445	0.0909	ThCo	Cmcm	-7.611	0.8181	CoB	Pnma	-7.295	1.09	-37.1687	-0.47302	-0.0946	Yes	
8	Co ₂ B ₂ Zr	-39.3587	-7.87173	10.342	ZrCo ₃ B ₂	R-3	-7.772	0.667	ZrB ₂	P6/mmm	-8.293	0.333					-39.3074	-0.05124	-0.01025	Yes	
9	Co ₂ Ga ₂ Ce	-27.7292	-5.54583	16.608	CeGa ₂	P6/mmm	-4.303	1	Co	Fm-3m	-7.09	2					-27.089	-0.64016	-0.12803	Yes	
10	Co ₂ Tl ₂ Ce	-40.028	-8.0056	55.204	CeTl ₃	Pm-3m	-3.238	0.5	CeTl	Pm-3m	-3.955	0.5	Co	Fm-3m	-7.09	2	-24.611	-15.417	-3.0834	Yes	
11	Cu ₂ Al ₂ Ce	-22.2397	-4.44795	17.289	AlCu	C2/m	-3.933	2	Ce ₃ Al ₂	C2/c	-4.305	0.5	CeAl ₂	Fd-3m	-4.563	-0.5	-19.65	-2.58973	-0.51795	Yes	
12	Cu ₂ Al ₂ Th	-24.2706	-4.85411	18.327	ThCu ₆	Pnma	-4.343	0.1666	AlCu ₃	Pmmn	-3.892	0.333	ThAl ₂	P6/mmm	-5.418	0.8333	-23.8012	-0.46939	-0.09388	Yes	
13	Cu ₂ Ga ₂ Ce	-21.128	-4.22559	17.839	CeGa ₂	P6/mmm	-4.303	1	Cu	Fm-3m	-3.716	2					-20.341	-0.78696	-0.15739	Yes	
14	Cu ₂ Ga ₂ Th	-22.907	-4.5814	18.16	ThGa ₂	I41/amd	-5.127	1	Cu	Fm-3m	-3.716	2					-22.813	-0.09399	-0.0188	Yes	
15	Fe ₂ Al ₂ Ce	-30.486	-6.09719	16.806	CeAl ₂	Fd-3m	-4.563	0.333	CeAl	Cmcm	-4.64	0.667	AlFe ₃	Fm-3m	-7.354	0.667	-30.3562	-0.1298	-0.02596	Yes	
16	Fe ₂ B ₂ Ce	-37.7133	-7.54266	12.532	CeFe ₄ B ₄	P42/n	-7.585	0.5	Ce	P4/mmm	-4.026	0.5					-36.1455	-1.56781	-0.31356	Yes	
17	Fe ₂ B ₂ Th	-39.484	-7.89679	13.079	Fe ₂ B	I4/mcm	-8.077	0.777	Th ₇ Fe ₃	P63mc	-7.81	0.1079	Th ₂ FeB ₁₀	Pbam	-7.527	0.1223	-39.2224	-0.26156	-0.05231	Yes	
18	Ir ₂ Al ₂ Ce	-34.524	-6.9048	17.289	CeAlIr	Pnma	-6.559	1	AlIr	Pm-3m	-7.247	1					-34.171	-0.35301	-0.0706	Yes	
19	Ir ₂ B ₂ Ce	-40.2509	-8.05019	14.639	CeB ₂ Ir ₂	Fddd	-7.873	1									-39.365	-0.88593	-0.17719	Yes	New Phase (I4/mmm)
20	Ir ₂ B ₂ Hf	-44.4562	-8.89124	12.42	HfB ₄ Ir ₃	P63/m	-8.431	0.3334	HfIr ₃	Pm-3m	-9.931	0.333	HfB ₂	P6/mmm	-8.794	0.333	-44.2119	-0.24435	-0.04887	Yes	
21	Ir ₂ Ga ₂ Ce	-32.8529	-6.57057	18.411	Ga ₂ Ir	Cmcm	-5.415	0.667	CeIr ₂	Fd-3m	-8.112	0.667	CeGa ₂	P6/mmm	-4.303	0.333	-31.2915	-1.56134	-0.31227	Yes	

Acknowledgment: This work has been performed under the course work of MSE 458 (Atomic scale computational materials science) in winter 2019 quarter.

22	Ir2Ga2Th	-34.7141	-6.94282	18.66 3	ThGaIr	P- 62m	-7.355	0.666 7	ThIr2	Fd-3m	-9.196	0.333	Ga2Ir	Cmc m	-5.415	0.6667	-34.5802	-0.13391	-0.02678	Yes	
23	Mn2B2Ce	-38.5945	-7.71891	12.63 4	MnB	Pnma	-8.352	2	Ce	P63/m mc	-4.776	1					-38.184	-0.41055	-0.08211	Yes	
24	Mo2Al2Ce	-35.6827	-7.13654	19.21	CeAl2	Fd- 3m	-4.563	0.333	CeAl	Cmcm	-4.64	0.6667	AlMo3	Pm- 3n	-9.308	0.6667	-35.4958	-0.18694	-0.03739	Yes	
25	Mo2B2Ce	-42.2349	-8.44698	14.20 9	BMo	I41/a md	-9.263	2	Ce	P63/m mc	-4.776	1					-41.828	-0.40688	-0.08138	Yes	
26	Mo2Ga2Ce	-34.6132	-6.92264	18.85 1	CeGa2	P6/m mm	-4.303	1	Mo	Im-3m	- 10.848	2					-34.605	-0.00818	-0.00164	Yes	
27	Nb2Al2Ce	-34.6042	-6.92084	20.97 9	CeAl	Cmc m	-4.64	1	Nb2Al	P42/m nm	-8.274	1					-34.102	-0.50218	-0.10044	Yes	
28	Nb2Ga2Ce	-33.7689	-6.75377	20.41 5	CeGa2	P6/m mm	-4.303	1	Nb	Im-3m	- 10.094	2					-33.097	-0.67185	-0.13437	Yes	
29	Ni2Al2Ce	-26.653	-5.33059	17.32 1	CeAlNi	P- 62m	-5.161	1	AlNi	Pm-3m	-5.326	1					-26.135	-0.51795	-0.10359	Yes	
30	Ni2B2Ce	-31.81	-6.362	13.06 8	CeB4	P4/m bm	-6.817	0.428 7	Ce3Ni 13B2	Cmm2	-5.89	0.1428	CeNi	Cmc m	-5.43	0.1428	-31.305	-0.50499	-0.101	Yes	
31	Ni2Ga2Ce	-25.2115	-5.0423	17.13 1	Ga3Ni5	Cmm m	-4.993	0.090 9	CeNi5	Cmm m	-5.655	0.1363	CeGa2 Ni	Cmm m	-4.712	0.8636	-24.5359	-0.67559	-0.13512	Yes	
32	Os2Al2Ce	-37.1683	-7.43366	18.56	Ce3Os	Pnma	-6.431	0.333	Os	P63/m mc	- 11.226	0.667	Al2Os	4/m mm	-6.801	1	-36.4472	-0.72106	-0.14421	Yes	
33	Os2B2Ce	-43.5821	-8.71641	15.05 1	CeB2Os2	F222	-8.52	1									-42.6	-0.98207	-0.19641	Yes	New phase(I 4/mm m)
34	Pd2Al2Ce	-27.4849	-5.49697	19.39 8	CeAl2Pd2	P4/n mm	-5.374	1									-26.87	-0.61487	-0.12297	Yes	New phase(I 4/mm m)
35	Pd2B2Ce	-31.6702	-6.33404	14.00 2	CeB6	Pm- 3m	-6.895	0.333	CePd3	Pm-3m	-5.768	0.6667					-31.2703	-0.39989	-0.07998	Yes	
36	Pd2Ga2Ce	-25.7766	-5.15531	19.27 9	CeGa3Pd 2	P6/m mm	-4.776	0.5	CeGaP d2	Pnma	-5.371	0.5					-25.07	-0.70656	-0.14131	Yes	
37	Pt2Al2Ce	-30.2447	-6.04893	18.96 9	CeAl2Pt3	P6/m mm	-6.155	0.166 6	CePt	Cmcm	-6.478	0.5	CeAl5 Pt3	Pnma	-5.661	0.333	-29.616	-0.62867	-0.12573	Yes	
38	Pt2B2Ce	-34.0578	-6.81155	13.84 3	CeB6	Pm- 3m	-6.895	0.2	CeBPt 2	P6222	-6.776	0.4	CeBPt 3	P4m m	-6.762	0.4	-34.0186	-0.03915	-0.00783	Yes	
39	Pt2Ga2Ce	-28.103	-5.6206	18.90 8	Ga3Pt2	P- 3m1	-4.842	0.222	CeGa3 Pt	Fmm2	-4.787	0.444	CePt2	Fd- 3m	-6.608	0.555	-27.0205	-1.08253	-0.21651	Yes	
40	Re2B2Ce	-44.9828	-8.99656	14.73 8	Ce2Re3B 6	C2/c	-8.278	0.266 6	Re3B	Cmcm	- 11.183	0.4	Ce	P63/ mmc	-4.776	0.4665	-44.4037	-0.57906	-0.11581	Yes	
41	Rh2Al2Ce	-31.8903	-6.37807	18.44 4	CeAlRh	Pnma	-6.021	1	AlRh	Pm-3m	-6.605	1					-31.273	-0.61734	-0.12347	Yes	
42	Rh2B2Ce	-36.8865	-7.37731	14.41 5	CeRh	Cmc m	-6.621	0.2	CeB4	P4/mb m	-6.817	0.2	CeB2R h3	P6/m mm	-7.281	0.6	-35.677	-1.20955	-0.24191	Yes	
43	Rh2Ga2Ce	-30.0984	-6.01968	18.38 8	CeGaRh	Pnma	-5.796	1	GaRh	Pm-3m	-5.84	1					-29.068	-1.03042	-0.20608	Yes	
44	Ru2Al2Ce	-34.0878	-6.81756	18.50 4	AlRu	Pm- 3m	-7.137	1.2	Al2Ru	Fddd	-6.277	0.2	Ce5Al 2Ru3	R3	-6.23	0.2	-33.355	-0.73278	-0.14656	Yes	
45	Ru2B2Ce	-39.8888	-7.97776	13.80 4	CeB2Ru2	Fddd	-7.776	1									-38.88	-1.0088	-0.20176	Yes	New phase(I 4/mm m)
46	Ta2Al2Ce	-37.679	-7.53581	20.78 4	Ta2Al	P42/ mm	-9.401	1	CeAl	Cmcm	-4.64	1					-37.483	-0.19603	-0.03921	Yes	
47	Ta2Ga2Ce	-36.7624	-7.35249	20.09 1	CeGa2	P6/m mm	-4.303	1	Ta	Im-3m	- 11.853	2					-36.615	-0.14744	-0.02949	Yes	

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48	Tc2B2Ce	-41.1764	-8.23528	14.336	CeB4	P4/m bm	-6.817	0.2857	Ce	P63/m mc	-4.776	0.714	Tc7B3	P63 mc	-9.573	0.2857	-40.5014	-0.67496	-0.13499	Yes	
49	V2B2Hf	-44.5157	-8.90314	11.412	HfB2	P6/m mm	-8.794	0.333	V3B2	P4/mb m	-8.75	0.667	Hf	P63/ mmc	-9.955	0.667	-44.5122	-0.00345	-0.00069	Yes	
50	V2B2Zr	-42.9658	-8.59316	11.619	ZrB2	P6/m mm	-8.293	0.333	V3B2	P4/mb m	-8.75	0.667	Zr	P63/ mmc	-8.547	0.667	-43.0747	0.108844	0.021769	No	Metast able
51	Rh2B2Th	-38.6315	-7.7263	14.639	ThB4	P4/m bm	-7.446	0.25	ThRh2	P63/m mc	-8.146	0.5	ThB4Rh4	P42/ nmc	-7.618	0.25	-38.667	0.035507	0.007101	No	Metast able
52	Nb2Ga2Th	-35.5811	-7.11621	20.716	Nb3Ga2	P4/m bm	-7.633	0.5	Nb	Im-3m	-10.094	0.5	ThGa	Pnma	-5.747	1	-35.6235	0.042448	0.00849	No	Metast able
53	Ni2B2Hf	-37.5917	-7.51833	10.265	HfB2	P6/m mm	-8.794	0.777	Ni3B	Pnma	-6.111	0.444	HfNi3	R-3m	-7.093	0.222	-37.6774	0.085695	0.017139	No	Metast able

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