Supplementary Materials

Computational Modeling of High-Entropy Alloys: Structures, Thermodynamics and Elasticity

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Empirical thermo-physical rules

The following equations are used to calculate those empirical thermos-physical parameters presented in the main text. These parameters are ideal configurational entropy (ΔS_{ideal}^{conf}), enthalpy of mixing of the liquid phase (ΔH_{mix}^{liq}),[1] atomic size difference (δ),[1] melting point of the alloy (T_m),[2] Ω-parameter,[2] valence electron concentration ($\overline{VEC}$),[3] the electronegativity difference ($\Delta\chi$),[4] the ϕ-parameter,[5] the η–parameter through the enthalpy of formation of the most stable binary compound ($|\Delta H_{ij}^{IM}|^{\max}$),[6] the average density ($\overline{\rho_m}$), the average bulk modulus ($\overline{B_m}$), and average shear modulus ($\overline{G_m}$):

$$\Delta S_{ideal}^{conf} = -R\sum_{i=1}^{N} c_i \ln c_i \tag{S1}$$

$$\Delta H_{mix}^{liq} = 4\sum_{i=1, i\neq j}^{N} \Delta H_{ij}^{liq} c_i c_j \tag{S2}$$

$$\delta = 100\,\% \sqrt{\sum_{i=1}^{N} c_i \left(1 - r_i / \sum_{j=1}^{N} c_j r_j\right)^2} \tag{S3}$$

$$\overline{T_m} = \sum_i c_i T_m^i \tag{S4}$$

$$\Omega = \frac{\overline{T_m}\Delta S_{ideal}^{conf}}{\left|\Delta H_{mix}^{liq}\right|} \tag{S5}$$

$$\overline{VEC} = \sum_i c_i VEC^i \tag{S6}$$

$$\Delta\chi = \sqrt{\sum_{i=1}^{N} c_i \left(\chi_i - \sum_{j=1}^{N} c_j \chi_j\right)^2} \tag{S7}$$

$$\phi = \frac{k_B \Delta S_{ideal}^{conf} - |\Delta H_{mix}^{liq}| / \overline{T_m}}{|S_E|} \tag{S8}$$

$$\eta = \frac{T_{ann}\Delta S_{ideal}^{conf}}{|\Delta H_{ij}^{IM}|^{\max}} \tag{S9}$$

$$\overline{\rho_m} = \frac{\sum_{i=1}^{N} c_i W_i}{\sum_{i=1}^{N} c_i W_i / \rho_i} \tag{S10}$$

$$\overline{B_m} = \sum_{i=1}^{N} c_i B_i \tag{S10}$$

$$\overline{G_m} = \sum_{i=1}^{N} c_i G_i \tag{S11}$$

where the individual items involved are defined as:

- c_i (and c_j) are the atomic percentage of the i^{th} (and j^{th}) element.
- r_i (and r_j) are the atomic radius of the i^{th} (and j^{th}) element.
- χ_i (and χ_j) are the Pauling electronegativity of the i^{th} (and j^{th}) element.
- T_m^i is the melting point of the i^{th} element.
- R is the gas constant (8.314 $J \cdot K^{-1} \cdot mol^{-1}$); k_B is the Boltzmann constant.
- S_E is the excessive entropy of mixing that is modeled as a function of atomic packing and atom size, and can be calculated following the procedure detailed in Ref.[5]

- ΔH_{ij}^{liq} is the enthalpy of mixing of equimolar *i-j* binary liquid alloy, which is taken from Ref.[7-9]
- H_{ij}^{IM} stands for the enthalpy of formation of the most stable compound of the *i-j* binary system, and can be found from Ref.[10]
- W_i, B_i, G_i, and ρ_i are the atomic weight, bulk modulus, shear modulus and density of the i^{th} element, respectively.

Table SI. Calculated empirical parameters for various equimolar single-phase alloys that were predicted using CALPHAD and phase diagram inspection with the FCC, BCC, and HCP structures.

Alloy	$\overline{\rho_m}$	$\overline{B_m}$	$\overline{G_m}$	ΔH_{mix}^{liq}	ΔS_{ideal}^{conf}	$\overline{T_m}$	Ω	δ [%]	ε [%]	Δχ	$\overline{VEC}$	ϕ	η
FCC structure													
CuMnNiZn	8.03	128	62	-3.5	11.53	1324	4.36	4.32	4.3	0.157	10	16.05	0.34
CuNiPdPt	13.32	183	57	-6.25	11.53	1739	3.21	4.61	4.62	0.17	10.2	12.96	0.684
CuNiPdPtRh	13.14	222	76	-4.48	13.38	1838	5.49	4.17	4.19	0.173	10	21.9	0.84
CoFeIrOsRh	15.44	291	148	-3.52	13.38	2372	9.02	3.52	3.53	0.185	8.6	33.46	2.87
CoIrNiOsRh	15.71	293	147	-0.8	13.38	2356	39.4	3.87	3.88	0.165	9	30.36	4.73
CoIrNiPdRh	13.38	248	111	0	13.38	2060	200	4.28	4.29	0.165	9.4	25.5	3.93
CoIrOsPtRh	18.02	303	144	-1.92	13.38	2418	16.85	3.53	3.56	0.148	9	35.64	1.72
Unknown[*a]													
IrNiOsPtRh	18.03	303	144	-1.12	13.38	2410	28.8	3.53	3.56	0.137	9.2	36.57	1.86
IrOsPtRhRu	18.35	311	163	-0.16	13.38	2586	216.29	1.27	1.26	0.0392	8.8	282.87	3.65
NiOsPtRhRu	15.93	283	136	-0.8	13.38	2384	39.88	3.47	3.49	0.137	9	38.2	1.84
CoCrFeMnNiOs	10.86	203	108	-5.44	14.9	2052	5.61	2.7	2.69	0.205	8	56.48	1.52
CoCrFeNiOsRh	11.72	246	120	-5.33	14.9	2172	6.07	3.3	3.29	0.214	8.33	39.04	1.43
CoCrFeNiOsRe	13.42	244	125	-3.33	14.9	2375	10.62	3.87	3.86	0.16	8	30.58	1.74
CoFeIrNiOsRh	14.49	273	136	-2.89	14.9	2265	11.68	3.75	3.75	0.18	8.83	33.5	1.98
CoFeIrNiPdRh	12.53	235	106	-2.33	14.9	2019	12.89	4.16	4.16	0.18	9.17	27.44	1.48
CoIrNiOsPtRh	16.76	283	132	-2.11	14.9	2303	16.25	4.13	4.15	0.166	9.17	28.7	1.83
CoIrNiPdPtRh	14.86	245	103	-1.33	14.9	2057	22.98	4.36	4.39	0.166	9.5	26.26	1.63
IrNiOsPtRhRu	17.09	289	149	-0.89	14.9	2443	40.95	3.22	3.25	0.125	9	49.34	2.1
CoCrFeMnNiOsRh	11.11	228	114	-6.86	16.18	2078	4.9	3.18	3.17	0.245	8.14	43.2	1.02

CoCrFeMnOsReRh	13.01	255	129	-5.71	16.18	2326	6.58	3.73	3.73	0.245	7.71	33.86	1.14
CoCrFeMnNiOsRe	12.58	226	118	-4.16	16.18	2253	8.76	3.73	3.72	0.191	7.86	34.75	1.49
CoCrFeNiOsReRh	13.27	264	128	-3.92	16.18	2356	9.73	3.84	3.84	0.2	8.14	33.73	1.2
CoCrFeNiPdReRh	11.59	231	103	-3.84	16.18	2144	9.04	4.19	4.19	0.2	8.43	28.07	1.09
CoCrMnNiOsReRh	13.19	256	128	-5.88	16.18	2314	6.37	3.93	3.93	0.243	8	30.29	1.14
CoCrMnNiOsReW	14.36	246	130	-4.41	16.18	2522	9.26	4.74	4.74	0.261	7.57	21.94	1.67
CoFeMnNiOsReRh	13.3	258	123	-3.84	16.18	2261	9.54	3.99	3.99	0.225	8.29	31.14	1.11
CoFeIrMnNiOsRh	13.51	251	128	-6.69	16.18	2158	5.22	3.69	3.69	0.242	8.57	32.93	1
CrMnNiOsReRuW	14.71	252	144	-6.53	16.18	2642	6.55	4.33	4.33	0.277	7.43	25.29	1.75
CoFeMnOsReZn	12.88	219	113	-2.11	14.9	2093	14.77	4.42	4.43	0.206	8.5	24.51	1.28
BCC structure													
AlCrFeMn	5.98	132	76	-9.75	11.53	1611	1.9	5.32	5.28	0.104	6	6.49	0.287
AlCrFeMo	6.85	159	61	-7.25	11.53	1955	3.11	5.27	5.28	0.215	5.75	9.74	0.265
AlCrFeV	5.68	142	68	-11.75	11.53	1777	1.74	4.82	4.81	0.087	5.5	7.23	0.316
AlCrMnMo	6.77	147	60	-6.75	11.53	1882	3.21	5.48	5.5	0.243	5.5	9.16	0.445
AlCrMnTi	5.16	117	66	-18	11.53	1643	1.05	6.51	6.54	0.0485	5	0.47	0.252
AlCrMnV	5.61	129	67	-11.5	11.53	1704	1.71	5.02	5.01	0.0402	5.25	6.49	0.391
AlCrMoV	6.46	157	52	-8.25	11.53	2048	2.86	4.16	4.18	0.229	5	15.12	0.477
AlCrVW	8.92	177	87	-7.5	11.53	2248	3.45	4.28	4.3	0.315	5	15.66	0.524
AlFeMnV	5.76	132	59	-13.5	11.53	1612	1.38	5.17	5.17	0.105	5.75	4.02	0.287
AlFeMoV	6.61	159	44	-10.25	11.53	1956	2.2	4.45	4.47	0.221	5.5	11.14	0.266
AlFeTiV	5.04	129	50	-20.75	11.53	1717	0.954	5.37	5.4	0.108	5	-0.68	0.264
AlMnTiV	4.98	117	49	-19	11.53	1644	0.997	5.65	5.69	0.0383	4.75	-0.04	0.252
AlMoNbV	6.93	159	33	-11.5	11.53	2191	2.2	3.1	3.11	0.237	4.75	22.54	0.5
AlNbVW	9.16	179	68	-11.5	11.53	2390	2.4	3.06	3.07	0.323	4.75	24.85	0.545

BaCaEuSr	3.28	12	7	0.5	11.53	1066	24.57	4.76	4.77	0.116	2.25	16.81	4.84
BaCaEuYb	4.22	16	8	0.5	11.53	1078	24.84	5.51	5.48	0.115	2.5	12.31	4.9
BaEuSrYb	4.35	15	7	0.5	11.53	1062	24.47	5.23	5.25	0.122	2.5	13.99	59.61
BaCaEuYb	4.22	16	8	0.5	11.53	1078	24.84	5.51	5.48	0.115	2.5	12.31	4.9
CaEuSrYb	4	17	8	0.5	11.53	1090	25.13	3.77	3.76	0.096	2.5	26.54	7.46
CrFeMnV	7.11	153	81	-2.25	11.53	1923	9.85	2.74	2.73	0.102	6.5	46.68	0.442
CrFeTiV	6.2	150	72	-9	11.53	2029	2.6	5.66	5.65	0.105	5.75	7.52	0.319
CrMnTiV	6.12	138	72	-4.5	11.53	1956	5.01	5.85	5.84	0.0512	5.5	9.18	0.345
CrMoNbV	8.15	180	55	-4	11.53	2502	7.21	5.05	5.07	0.23	5.5	13.48	1.24
CrMoTiV	6.94	165	57	-3.75	11.53	2300	7.07	4.82	4.83	0.242	5.25	14.81	0.406
FeMoTiV	7.08	168	48	-8	11.53	2208	3.18	5.08	5.11	0.238	5.75	10.66	0.3
MoNbReTa	13.93	243	76	-17	11.53	3099	2.1	2.84	2.84	0.259	5.75	25.81	0.901
MoNbReTi	10.67	220	70	-16.5	11.53	2762	1.93	2.68	2.69	0.249	5.5	26.54	0.898
MoNbReV	11.4	233	71	-13.25	11.53	2822	2.45	3.15	3.15	0.227	5.75	23.39	0.918
MoNbTaTi	10.03	178	43	-3	11.53	2719	10.45	2.01	2.02	0.268	5	89.82	0.926
MoNbTaV	10.68	190	44	-3.25	11.53	2780	9.86	3.56	3.58	0.257	5.25	28.35	0.946
MoNbTiV	7.35	168	37	-2.75	11.53	2443	10.24	3.41	3.43	0.249	5	30.99	0.961
MoNbTiW	10.42	205	66	-5.5	11.53	2821	5.91	2.12	2.12	0.353	5.25	73.3	1.11
MoNbVW	11.13	218	67	-4	11.53	2881	8.3	3.03	3.03	0.33	5.5	37.92	1.42
MoReTaTi	12.88	228	78	-16	11.53	2897	2.09	2.68	2.69	0.271	5.5	28.7	0.842
MoReTaV	13.75	240	79	-12.5	11.53	2957	2.73	3.15	3.15	0.254	5.75	24.99	0.86
MoReTaW	16.76	278	107	-11.75	11.53	3335	3.27	2.37	2.36	0.322	6	48.45	0.97
MoReTiV	10.25	218	72	-12.75	11.53	2620	2.37	2.88	2.88	0.243	5.5	27.42	0.911
MoReTiW	13.39	255	101	-11.5	11.53	2998	3	2.09	2.08	0.307	5.75	60.2	1.04
MoReVW	14.33	268	102	-6.25	11.53	3058	5.64	1.65	1.66	0.275	6	119.65	1.36

MoTiVW	10	203	68	-3.25	11.53	2679	9.5	2.78	2.78	0.346	5.25	45.96	1.05
NbReTaTi	12.33	213	82	-18	11.53	2860	1.83	2.61	2.63	0.157	5.25	26.85	0.831
NbReTaV	13.13	225	83	-16.25	11.53	2921	2.07	3.78	3.79	0.148	5.5	14.45	0.849
NbReTaW	16.05	263	112	-17.25	11.53	3299	2.2	2.72	2.73	0.334	5.75	29.38	0.959
NbReTiV	9.78	203	77	-16.25	11.53	2583	1.83	3.62	3.63	0.138	5.25	13.81	0.84
NbReTiW	12.81	240	105	-16.75	11.53	2961	2.04	2.57	2.57	0.324	5.5	30.69	0.963
NbReVW	13.67	253	106	-13.25	11.53	3022	2.63	3.16	3.16	0.305	5.75	24.38	0.983
NbTaTiW	12.07	198	78	-4.5	11.53	2919	7.48	1.71	1.72	0.354	5	118.29	1.68
NbTaVW	12.85	210	79	-4.5	11.53	2980	7.63	3.49	3.51	0.343	5.25	28.63	1.6
NbTiVW	9.54	188	73	-4	11.53	2642	7.61	3.35	3.36	0.335	5	31.1	1.79
ReTaTiV	12.05	210	85	-16	11.53	2718	1.96	3.62	3.63	0.156	5.25	14.87	0.79
ReTaTiW	15.01	248	113	-16.25	11.53	3096	2.2	2.57	2.57	0.346	5.5	32.83	0.9
ReTaVW	16	260	114	-12.5	11.53	3157	2.91	3.16	3.16	0.329	5.75	25.83	0.918
ReTiVW	12.55	238	108	-12.75	11.53	2820	2.55	2.9	2.9	0.319	5.5	28.49	0.98
TaTiVW	11.77	195	80	-4	11.53	2777	8	3.35	3.36	0.351	5	31.33	1.5
BaCaEuSrYb	3.87	15	7	0.64	13.38	1072	22.42	5.23	5.23	0.11	2.4	16.01	5.66
AlCrFeMnV	6.01	137	70	-10.4	13.38	1725	2.22	4.88	4.86	0.0941	5.8	10.45	0.357
AlCrFeMoV	6.7	159	58	-8.64	13.38	2001	3.1	4.71	4.72	0.206	5.6	14.11	0.315
AlCrMnTiV	5.34	125	63	-14.88	13.38	1751	1.57	5.84	5.85	0.0462	5	4.97	0.312
AlCrNbVW	8.84	175	77	-10.24	13.38	2348	3.07	4.79	4.82	0.295	5	13.81	0.622
HfMoNbTiZr	8.7	142	33	-1.6	13.38	2444	20.44	5.06	5.07	0.31	4.6	17.17	1.09
HfMoTaTiZr	10.21	148	39	-1.92	13.38	2552	17.79	5.06	5.07	0.311	4.6	17.04	1.01
MoNbTaTiW	11.75	204	66	-5.28	13.38	2914	7.39	2.12	2.13	0.357	5.2	88.83	1.15
MoNbReTiW	12.33	238	88	-13.44	13.38	2948	2.94	2.46	2.46	0.316	5.6	50.14	1.11
MoNbTiVW	9.69	196	62	-4.16	13.38	2693	8.66	3.07	3.08	0.336	5.2	43.45	1.23

MoNbReTaTi	11.95	216	70	-15.04	13.38	2867	2.55	2.66	2.67	0.253	5.4	39.73	0.968
MoNbReTaV	12.58	226	70	-13.28	13.38	2916	2.94	3.42	3.43	0.241	5.6	25.91	0.984
MoNbReTiV	9.87	208	65	-13.12	13.38	2646	2.7	3.27	3.28	0.233	5.4	27.06	0.999
MoNbReVW	13	248	89	-10.56	13.38	2997	3.8	2.83	2.83	0.296	5.8	41.96	1.13
MoReTaTiV	11.7	214	72	-12.8	13.38	2754	2.88	3.27	3.28	0.25	5.4	28.06	0.929
MoReTaTiW	14.11	244	94	-12.96	13.38	3056	3.16	2.46	2.46	0.337	5.6	51.95	1.03
MoReTaVW	14.87	254	95	-9.92	13.38	3105	4.19	2.83	2.83	0.32	5.8	43.36	1.05
MoReTiVW	12.09	236	90	-9.92	13.38	2835	3.82	2.6	2.59	0.31	5.6	50.22	1.14
MoTaTiVW	11.49	202	68	-4	13.38	2801	9.37	3.07	3.08	0.353	5.2	43.88	1.11
NbReTaTiW	13.63	232	98	-15.52	13.38	3027	2.61	2.54	2.55	0.322	5.4	44.35	1.02
NbReTaVW	14.34	242	99	-13.6	13.38	3075	3.03	3.39	3.4	0.311	5.6	26.9	1.04
NbReTaTiV	11.28	202	75	-14.24	13.38	2725	2.56	3.56	3.58	0.141	5.2	22.37	0.92
NbReTiVW	11.65	224	94	-13.44	13.38	2806	2.79	3.24	3.25	0.303	5.4	28.17	1.06
NbTaTiVW	11.08	190	72	-3.68	13.38	2772	10.08	3.26	3.28	0.32	5	39.81	1.73
NbTaTiVZr	8.48	146	46	0.32	13.38	2458	102.8	5.39	5.41	0.105	4.6	15.73	1.54
ReTaTiVW	13.47	230	100	-13.12	13.38	2914	2.97	3.24	3.25	0.319	5.4	29.11	0.983
AlCrMoNbVW	9.08	184	68	-8.33	14.9	2440	4.36	4.38	4.41	0.305	5.17	21.06	0.719
HfMoNbTaTiZr	9.95	152	39	-0.889	14.9	2585	43.33	4.7	4.7	0.284	4.67	22.56	1.14
HfMoTaTiVZr	9.69	150	41	-2.33	14.9	2491	15.9	6.07	6.09	0.285	4.67	13.15	1.1
MoNbReTaTiV	11.13	207	66	-12.33	14.9	2753	3.33	3.33	3.34	0.234	5.33	32.47	1.03
MoNbReTaTiW	13.11	232	85	-13.22	14.9	3005	3.39	2.53	2.54	0.326	5.5	56.48	1.13
MoNbReTaVW	13.68	240	86	-11.44	14.9	3046	3.96	3.13	3.13	0.314	5.67	39.1	1.14
MoNbReTiVW	11.43	225	81	-11.22	14.9	2821	3.74	2.99	2.99	0.307	5.5	42.02	1.19
MoNbTaTiVZr	8.75	160	42	-2.11	14.9	2531	17.86	5.27	5.27	0.257	4.83	17.27	1.11
MoReTaTiVW	12.95	230	87	-10.89	14.9	2911	3.98	2.99	2.99	0.323	5.5	42.93	1.09

NbReTaTiVW	12.57	220	90	-12.78	14.9	2886	3.37	3.29	3.3	0.299	5.33	33.64	1.08
CrMoNbTaTiVW	10.54	191	71	-4.9	16.18	2705	8.94	4.67	4.71	0.313	5.29	23.28	0.671
CrMoNbReTaVW	12.95	229	90	-9.96	16.18	2922	4.75	4.45	4.48	0.299	5.71	22.53	1.19
CrMoNbReTaTiVW	11.77	214	84	-10.19	17.29	2799	4.75	4.42	4.45	0.296	5.5	24.56	0.742
CrFeMoNbReRuTaVW	12.44	221	98	-15.31	18.27	2763	3.3	4.96	4.98	0.288	6.22	17.97	0.083
HCP structure													
CoCrReRu	12.87	233	135	-5	11.53	2504	5.77	3.86	3.87	0.192	7.5	22.01	1.89
CoOsReRu	16.73	294	162	-0.25	11.53	2785	128.4	3.64	3.67	0.155	8	30.24	2.06
CoPtReRu	16.45	250	122	-3	11.53	2469	9.49	4.12	4.15	0.177	8.5	21.39	0.699
CrIrMoRh	13.28	273	124	-16.5	11.53	2513	1.76	3.21	3.22	0.243	7.5	16.77	0.489
CrIrRhW	15.81	293	159	-13.5	11.53	2713	2.32	3.43	3.45	0.274	7.5	19.27	0.509
CrMoOsRu	13.23	254	133	-12.75	11.53	2747	2.48	3.18	3.18	0.229	7	23.59	3.17
CrOsRuW	15.77	274	168	-10.5	11.53	2947	3.24	3.43	3.43	0.265	7	23.37	2.93
CoPtReRu	16.45	250	122	-3	11.53	2469	9.49	4.12	4.15	0.177	8.5	21.39	0.699
IrMoPdRu	14.23	238	112	-9.75	11.53	2518	2.98	1.63	1.63	0.0173	8.25	98.72	0.489
IrMoRhW	16.13	310	135	-15	11.53	2892	2.22	1.85	1.85	0.0768	7.5	63.83	0.543
IrMoPtRu	16.58	250	116	-16.25	11.53	2571	1.82	1.74	1.74	0.0436	8.25	59.36	0.462
MoOsRuW	16.1	291	144	-12	11.53	3126	3	2.21	2.21	0.0768	7	54.03	3.11
MoPtRhRu	14.14	265	101	-14.75	11.53	2445	1.91	1.86	1.86	0.052	8.25	54.53	0.439
CoCrFeReRu	11.94	220	125	-4.32	13.38	2365	7.33	3.71	3.71	0.175	7.6	28.61	2.07
CoFeOsReRu	15.13	269	146	-1.76	13.38	2590	19.69	3.76	3.77	0.163	8	31.17	2.22
CoIrOsReRu	17.97	299	172	-1.44	13.38	2776	25.79	3.37	3.4	0.152	8.2	40.05	0.773
CoNiOsReRu	15.4	271	145	0.32	13.38	2574	107.62	4.1	4.12	0.149	8.4	27.37	1.69
CoOsPdReRu	15.71	271	138	2.88	13.38	2594	12.05	3.56	3.59	0.152	8.4	34.13	2.22
CoOsPtReRu	17.71	281	142	-2.08	13.38	2636	16.96	3.69	3.72	0.168	8.4	32.58	0.867

CoOsReRhRu	15.85	311	160	0.16	13.38	2675	223.76	3.31	3.33	0.168	8.2	43	1.13
CoOsReRuTc	15.63	291	156	-0.16	13.38	2714	226.99	3.37	3.4	0.15	7.8	41.48	2.33
CrIrMoRhW	14.61	280	131	-14.4	13.38	2749	2.55	3.39	3.4	0.246	7.2	24.83	0.599
CrMoOsRuW	14.58	265	138	-11.2	13.38	2937	3.51	3.45	3.46	0.238	6.8	28	3.39
MoPdRhRuTc	11.69	258	104	-6.72	13.38	2400	4.78	1.58	1.58	0.13	8	145.65	0.738
210 quaternary RE HEAs[*b]													
378 quinary RE HEAs[*b]													
210 senary RE HEAs[*b]													
120 septenary RE HEAs[*b]													
45 octonary RE HEAs[*b]													
10 Ennead RE HEAs[*b]													
1 decadal RE HEA[*b]													
DHCP structure													
CeNdPmPr	6.93	29	16	0	11.53	1237	200**	0.455	0.455	0.0071	3	1914.43	inf
CeLaPmPr	6.7	28	15	0	11.53	1211	200**	1.41	1.41	0.0122	3	198.59	inf
CeLaNdPr	6.64	28	15	0	11.53	1192	200**	1.27	1.27	0.015	3	241.79	inf
CeLaNdPm	6.76	29	16	0	11.53	1233	200**	1.47	1.46	0.015	3	182.45	inf
LaNdPmPr	6.78	30	16	0	11.53	1268	200**	1.47	1.46	0.015	3	182.45	inf
CeLaNdPmPr	6.76	29	15	0	13.38	1228	200**	1.32	1.31	0.014	3	262.39	inf

[*a] The crystal structures of these compositions were not suggested in Ref.[10] although the majority of them likely prefer an FCC structure.

*[b] These numbers represent the total number of equimolar compositions for quaternary, quinary, senary, septenary, octonary, ennead and decadal systems respectively, which comprises arbitrary selection of RE elements from the Dy-Er-Gd-Ho-Lu-Sc-Sm-Tb-Tm-Y system.[11]

**Since the enthalpy of mixing is zero for these alloys, the Ω–parameter will be infinity. In order to show these compositions in Figure 1(b), the Ω-parameter is set as 200 arbitrarily to demonstrate that they have an extremely large Ω-parameter.

Table SII. DFT-calculated lattice parameter [a, Å], single-crystal elastic constants, polycrystalline bulk modulus, polycrystalline shear modulus, and polycrystalline Poisson's ratio for those pure elements that constitute the BCC HEAs in the present work as presented in Figure 6, based on the study by Feng and Widom.[12]

BCC	*Cr.cI2*	*Hf.cI2*	*Mo.cI2*	*Nb.cI2*	*Ta.cI2*	*Ti.cI2*	*V.cI2*	*Zr.cI2*	*W.cI2*
a	2.857	3.541	3.159	3.322	3.319	3.254	2.99	3.571	3.184
C_{11}	444	73	469	247	268	95	278	87	519
C_{12}	62	116	159	137	161	115	143	93	199
C_{44}	99	53	101	17	79	41	24	34	141
B	188	102	263	173	197	108	188	91	306
G	129	-54	120	28	67	-10	37	5	149
ν	0.22	0.83	0.3	0.42	0.35	0.55	0.41	0.47	0.29

Table SIII. DFT-calculated lattice parameter [a, Å], single-crystal elastic constants [GPa], polycrystalline bulk modulus [GPa], polycrystalline shear modulus [GPa], and polycrystalline Poisson's ratio for those pure elements that constitute FCC HEAs in the present work as presented in Figure 6, based on the work by Gao et al.[13] and the present work. "FM" stands for ferromagnetism, and "AFM" stands for antiferromagnetism.

FCC	*Co.hP2_FM*	*Co.cF4*	*Cr.cF4*	*Cr.cI2_AFM*	*Fe.cF4_FM*	*Fe.cF4_AFM*	*Mn.cF4*	*Ni.cF4*
a	3.523	3.523	3.625	2.870	3.482	*a*=3.680 *b*=*c*=3.429	3.508	3.508
C_{11}	361	288	26	434	311	263	400	278
C_{12}	169	168	348	59	107	101	225	159
C_{44}	97	142	-87	96	192	267	178	133
C_{13}	114					101		
C_{33}	406					334		
C_{66}	96					177		
B	208	208	240	184	175	196	283	199
G	101	101	-112	126	149	132	134	96
v	0.292	0.292	0.775	0.22	0.168	0.225	0.296	0.291

Table SIV. DFT-calculated lattice parameter [a, Å], single-crystal elastic constants [GPa], polycrystalline bulk modulus [GPa], polycrystalline shear modulus [GPa], polycrystalline Poisson's ratio, and in comparison with their average values estimated using the ROM for single-phase HEAs studied by Gao et al.,[13] Feng and Widom,[12] Tian et al., [14] and Ge et al.[15]

No.	Alloys	$\overline{a}$	a	$\overline{C_{11}}$	C_{11}	$\overline{C_{12}}$	C_{12}	$\overline{C_{44}}$	C_{44}	$\overline{B}$	B	$\overline{G}$	G	$\overline{\nu}$	ν
1	NbTiVZr[12]	3.284	3.300	177	161	122	103	29	29	134	122	19	29	0.43	0.39
2	NbTiVZr[14]	3.285	3.303	173	160	121	114	29	19	139	130	16	20	0.41	0.43
3	CrMoNbV[12]	3.082	3.089	360	354	125	143	60	51	201	213	65	69	0.35	0.35
4	HfNbTaZr[12]	3.438	3.441	169	159	127	108	45	41	133	125	14	34	0.45	0.38
5	MoNbTaW[12]	3.246	3.246	376	371	164	160	84	69	229	230	76	82	0.35	0.34
6	MoNbTiZr[14]	3.327	3.322	220	203	128	122	47	30	159	148	36	34	0.39	0.39
7	MoNbTaTiV[16]	3.212	3.213	278	262	147	141	54	43	185	181	65	51	0.34	0.37
8	MoNbTiVZr[14]	3.261	3.266	230	209	131	123	42	27	164	152	36	33	0.39	0.40
9	CoCrFeNi[13]	3.346	3.551	328	224	123	132	141	131	192	209	118	86	0.24	0.28
10	CoCrFeMnNi[13]	3.378	3.545	342	243	144	134	148	141	210	168	121	96	0.26	0.26
11	CrMoTi[15]			322	332	102.8	125	85	78.2	175.9	194		88		0.3
12	MoNbTi[15]			290.9	279	128.1	126	61.5	69.7	182.4	178		73		0.32
13	MoNbV[15]			313	340	137.1	139	60.4	65.6	195.7	206		78		0.33
14	MoTiV[15]			284.9	280	122.9	124	66.4	68.6	176.9	176		72		0.32
15	AlMoNbV[15]			261.4	262	117.9	138	52.4	97.5	165.8	180		81		0.3
16	CrMoTiV[15]			298.7	324	106.9	131	74.5	70.1	170.8	196		80		0.32
17	MoNbTiV[15]			275.3	278	125.8	128	57	67	175.7	178		70		0.33

For average property calculations, the properties of BCC Ti, BCC Cr, and ferromagnetic FCC Fe were used for the alloys cited in Ref. 12-14, 16

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