Supplementary Information

Multi-objective optimization and system selection details

Pareto optimization technique is implemented and used in our calculation to simultaneously perform optimization of more than one property. This would help the calculation to focus on the optimal area of the search space. In general, from the total set of structures $\{S_n\}$ (n=1, .., N), and optimizing (let's say minimizing) multiple properties f_m (m=1, .., M), we say structure S_i dominates structure S_j ($i \neq j$) in terms of properties f_k, if $f_k(S_i) \leq f_k(S_j)$ for all properties, and $f_k(S_i) < f_k(S_j)$ in at least one of the properties. The set of structures not dominated by any other structures is, therefore, the set of Pareto optimal structures $\{S_t\}$ (t =1, .., T and $T \leq N$), and creates the first Pareto front. The set of these $\{S_t\}$ structures are then removed from the set of N individuals and the cycle is repeated to find successive Pareto fronts 2, 3,… until all N structures are classified. The set of structures belonging to the first Pareto front are assigned the highest rank, those in the second Pareto front the second highest rank, and so forth.

Selection of good parents is very important for the success of the algorithm. For selection of good parents, the roulette wheel selection method[1] is used and to each system the weight function $w_r > 0$ (r = 1, 2,.., N), derived from its fitness rank, is assigned. The probability of selection of each system with fitness rank *r* is defined as follow:

$$P_r = \frac{w_r}{n_r \times \sum w_r} \quad , \quad r = 1, 2, \dots, N \tag{1}$$

$$w_r = (N + 1 - r)^2 \tag{2}$$

where *N* is the last fitness ranking number, which is equal to the number of all systems in simple ranking and equal to the number of Pareto fronts in multi-objective Pareto ranking. n_r is equal to the number of systems having the same fitness ranking *r*.

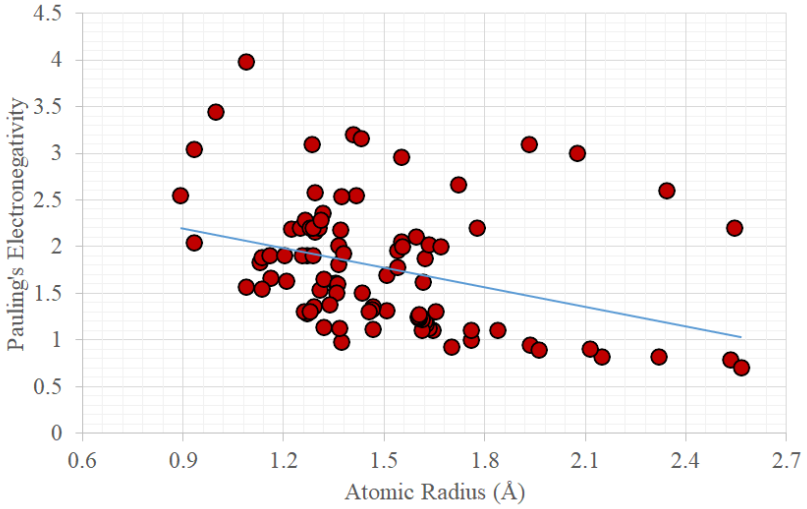

Fig 1. The electronegativities and atomic radii of the elements. The regression line is shown in blue.

Redefining the Mendeleev Number

Unlike Pettifor, who derived his MN empirically, we offer a nonempirical (and, therefore, more universal) definition. The most important chemical properties of an atom are (1) size R, (2) electronegativity χ, (3) polarizability α and (4) valence v. For simplicity, we excluded the valence, which is not constant for many elements. The polarizability was also disregarded in favor of the electronegativity because they are strongly correlated.[2] Thus, we only consider the electronegativity and atomic radius to define the MNs. In this work, the atomic radius R is defined as half the shortest interatomic distance in the relaxed (for most elements hypothetical) simple cubic structure of an element – see Table 1.

Table 1. Atomic radii of the elements that calculated and used in this work for redefining MN.

Element	Atomic radius R_a (Å)	Element	Atomic radius R_a (Å)	Element	Atomic radius R_a (Å)	Element	Atomic radius R_a (Å)
H	0.727	Mn	1.136	In	1.541	Ta	1.358
He	1.286	Fe	1.131	Sn	1.541	W	1.316
Li	1.374	Co	1.137	Sb	1.553	Re	1.287
Be	1.090	Ni	1.160	Te	1.596	Os	1.278
B	0.943	Cu	1.203	I	1.721	Ir	1.288
C	0.891	Zn	1.320	Xe	2.344	Pt	1.311
N	0.932	Ga	1.365	Cs	2.535	Au	1.374
O	0.997	Ge	1.365	Ba	1.962	Hg	1.556
F	1.089	As	1.369	La	1.647	Tl	1.617
Ne	1.409	Se	1.418	Ce	1.467	Pb	1.622
Na	1.701	Br	1.551	Pr	1.367	Bi	1.635
Mg	1.508	Kr	2.077	Nd	1.320	Po	1.670
Al	1.355	Rb	2.319	Pm	1.635	At	1.777
Si	1.269	Sr	1.935	Sm	1.626	Rn	2.544
P	1.223	Y	1.625	Eu	1.620	Fr	2.567
S	1.293	Zr	1.463	Gd	1.623	Ra	2.114
Cl	1.431	Nb	1.362	Tb	1.613	Ac	1.838
Ar	1.933	Mo	1.294	Dy	1.613	Th	1.655
K	2.151	Tc	1.257	Ho	1.604	Pa	1.436
Ca	1.761	Ru	1.249	Er	1.602	U	1.339
Sc	1.466	Rh	1.264	Tm	1.602	Np	1.291
Ti	1.308	Pd	1.306	Yb	1.759	Pu	1.271
V	1.209	Ag	1.379	Lu	1.605	Am	1.261
Cr	1.162	Cd	1.509	Hf	1.454	Cm	1.279

Looking at Fig. 1, one can see a clear correlation between these properties, which means that one of them, or better still, some combination of the two, can be approximately used as a single parameter approximately characterizing chemistry of the element. Therefore, we computed the regression line of the elements in the χ (Pauling electronegativity) and R (atomic radius) space (Fig. 1), and projected all the elements on it. The chemical scale equal to zero is assigned to the projection of the first element on the regression line, and the distance of the projections of other elements from this "zero" represents their chemical scale. The Mendeleev number - i.e. the integer version of the chemical scale, - is obtained as the sequence of the projected elements along the regression line. The redefined MN is shown in the Table 2.

Table 2. The redefined MN using our method for the first 96 elements of the Periodic Table.

1-20	Fr	Cs	Rb	K	Ra	Ba	Sr	Ac	Ca	Na	Rn	Yb	La	Pm	Tb	Sm	Gd	Eu	Y	Dy
21-40	Th	Ho	Er	Tm	Lu	Li	Ce	Mg	Pr	Hf	Xe	Zr	Nd	Sc	Tl	Pa	Pu	U	Cm	Am
41-60	Np	Cd	Pb	Ta	In	Po	At	Nb	Ti	Al	Bi	Sn	Zn	Hg	Te	Sb	Ga	V	Mn	Ag
61-80	Cr	Be	Kr	Ge	Re	Si	Tc	Cu	I	Fe	As	Ni	Co	Mo	Ar	Pd	Ir	Os	Pt	Ru
81-96	P	Rh	W	Se	Au	B	S	Br	Cl	H	Ne	He	C	N	O	F				

Input parameters

Pareto optimization of the hardness and stability was performed over all possible structures (with up to 12 atoms in the primitive cell) in the space of all possible binary compounds formed by 74 elements (i.e. excluding noble gases, rare earth elements and elements heavier than Pu). The input parameters of MendS were: Population size=30, percentage of chemical heredity=30%, percentage of reactive heredity=30%, percentage of mutation=20% and percentage of random systems=20%.

In each binary system, we ran evolutionary optimization with parameters: initial population size=100, subsequent population size=50, number of generations=6, percentage of heredity=40%, percentage of mutation=30%, percentage of random selection=30%.

The comprehensive multi-objective evolutionary algorithm runs as implemented in USPEX was performed on the selected promising binary systems with the following input parameters: initial population size=120, subsequent population size=60, number of generations=50, percentage of heredity=40%, percentage of transmutation=20%, percentage of softmutation=20%, percentage of random selection=20%.

The underlying ab initio structure relaxations and energy calculations were performed using density functional theory with projector augmented wave method (PAW) as implemented in the VASP code[3,4]. In spin-polarized calculations, the GGA-PE functional[5] was implemented. The cutoff energy of 600 eV, and k-mesh with the resolution of $0.06 \times \text{Å}^{-1}$ was used in all the VASP calculations. In 20 coevolutionary generations, 600 binary systems were studied. This calculation was done within 3 weeks using 280 cores, a surprisingly minor cost for a full exploration of the chemical space.

More details on the discussed systems

The crystal structure of several promising compounds presented in the Table. 1 of the paper, were shown in the Fig. 5a in the paper, and here, in Fig. 2, we show the crystal structure of the rest of the discussed compounds in this Table (Table. 1 in the paper).

We also show the convex hull diagram (Fig. 3) constructed during precise evolutionary search on some these binary systems – systems discussed in the Table. 1 of the paper.

In Table. 2, we show a full list of the studied systems during our MendS calculation. One can see that almost all the hard systems, or systems that reported to have a potential to be hard are found and studied in this single run.

Technicalities

(1) MendS works for all Unary, Binary, Ternary and Quaternary systems. (2) MendS can search for best systems at arbitrary pressures, because atomic radii and electronegativity can be computed for different pressures. (3) Calculations are highly parallelized and run efficiently on modern clusters and supercomputers.

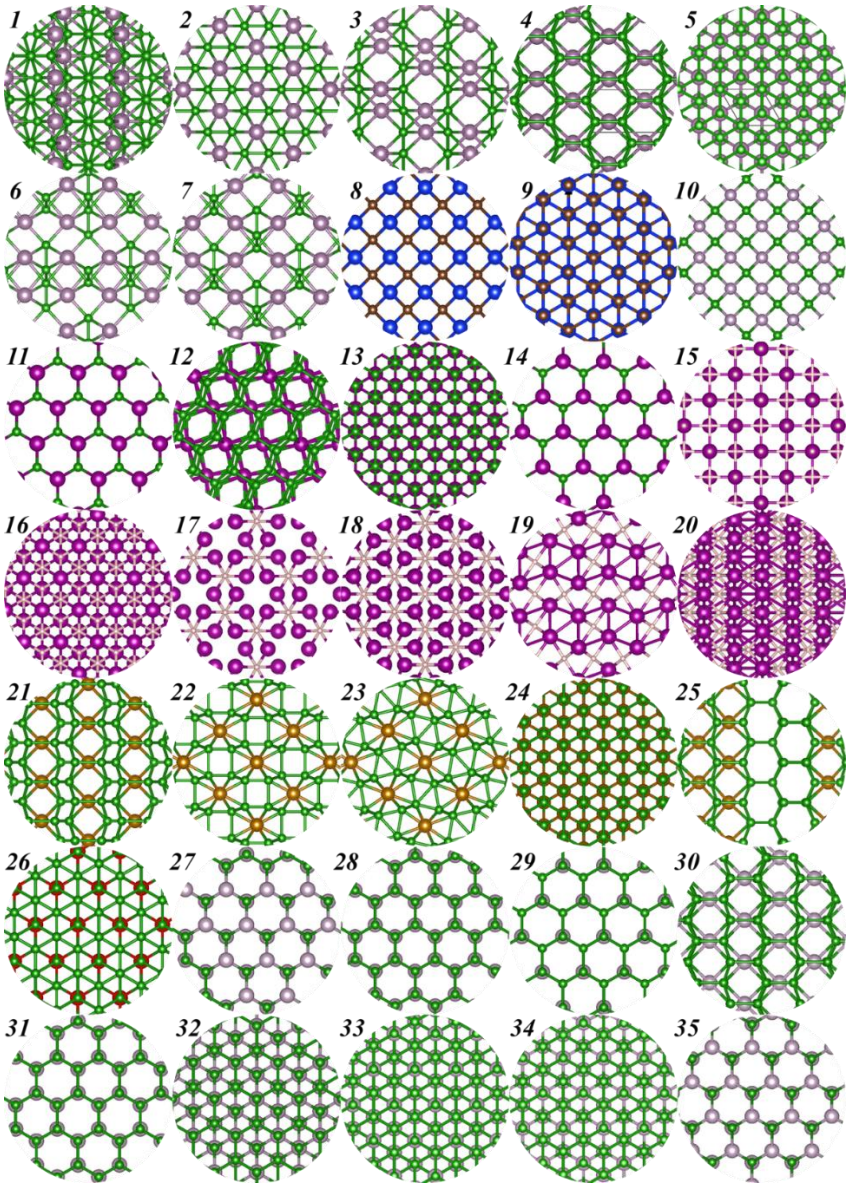

Fig 2. (1) A2/m-MoB_3, (2) $P6_3/mmc$-MoB_3, (3) $R\bar{3}m$-MoB_3, (4) Pmmn-MoB_4, (5) R3m-MoB_8, (6) Cmcm-Mo_2B_3, (7) Imm2-Mo_2B_3, (8) $F\bar{4}3m$-SiC, (9) R3m-SiC, (10) $F\bar{4}3m$-BP, (11) $P\bar{6}m2$-MnB_3, (12) $P2_1/c$-MnB_4, (13) $R\bar{3}m$-MnB_4, (14) $P\bar{6}m2$-MnB_5, (15) $Fm\bar{3}m$-MnH, (16) $R\bar{3}m$-MnH, (17) $P6_3/mcm$-Mn_3H_2, (18) R32-Mn_3H_2, (19) P2/m-Mn_4H_3, (20) A2/m-Mn_6H_5, (21) A2/m-FeB_4, (22) Immm-FeB_4, (23) Pnnm-FeB_4, (24) $R\bar{3}m$-FeB_4, (25) Pm-Fe_2B_{11}, (26) P3m1-VB_7, (27) $P\bar{3}m1$-TcB, (28) $P\bar{3}m1$-TcB_3, (29) $P\bar{6}m2$-TcB_3, (30) $P2_1/m$-TcB_4, (31) $P6_3mmc$-TcB_4, (32) $R\bar{3}m$-TcB_4, (33) R3m-TcB_7, (34) R3m-TcB_8, (35) $P\bar{6}m2$-Tc_3B_5.

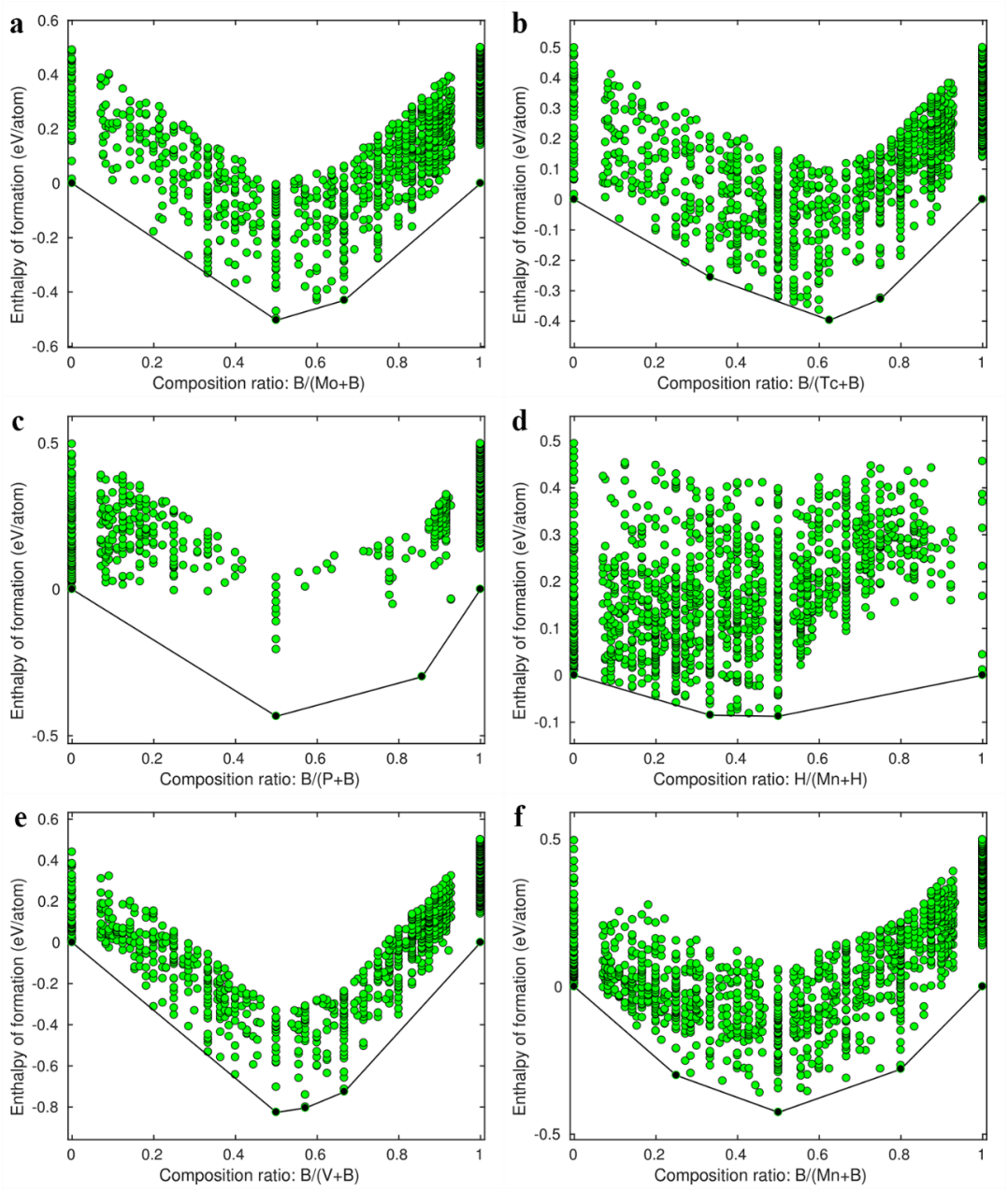

Fig 3. The convex hull plot of discussed systems in the Table. 1 of the paper. (a) Mo-B, (b) Tc-B, (c) B-P, (d) Mn-H, (e) V-B, and (f) Mn-B.

Table 3. Binary systems that were calculated during the MendS run. “How created” specifies the variation operator that was used to create the compounds. In this column R=Randomly, CH=Chemical Heredity, RH=Reactive Heredity, M=Mutation.

Gen	Compound	How created	1th Parent	2nd Parent	Gen	Compound	How created	1th Parent	2nd Parent
1	Rh-B	R	-	-	2	Cr-Co	CH	B	Mo
1	Na-B	R	-	-	2	Rh-W	CH	C	Nb
1	Ca-Po	R	-	-	2	Rh-Rh	CH	Mo	C
1	Zr-Ge	R	-	-	2	Os-P	CH	Mo	Pt
1	H-N	R	-	-	2	Al-Si	CH	Mo	Np-Co
1	Y-N	R	-	-	2	V-Cr	CH	Os	Be
1	Ga-H	R	-	-	2	P-P	CH	Mo	Ru
1	La-Pt	R	-	-	2	Ga-S	CH	Nb-N	As
1	Sn-B	R	-	-	2	Re-C	CH	Nb-N	Rh
1	Ru-N	R	-	-	2	Mo-C	RH	C	Mo-Ir
1	Rb-Be	R	-	-	2	Fe-B	RH	Fe	B
1	W-C	R	-	-	2	As-Co	RH	As	Np-Co
1	Fe-Os	R	-	-	2	Al-Os	RH	Os-Ru	Bi-Al
1	Ti-Pd	R	-	-	2	As-Mo	RH	As	Mo
1	Th-Be	R	-	-	2	Co-Rh	RH	Co	Rh
1	Rb-Mo	R	-	-	2	Al-Be	RH	Be	Al-As
1	Ra-Zr	R	-	-	2	Ru-C	RH	Ru	W-C
1	Ca-Rh	R	-	-	2	W-H	RH	W-C	Ga-H
1	Np-Co	R	-	-	2	Pd-W	M	W	-
1	Rb-H	R	-	-	2	Sb-Rh	M	Rh	-
1	Bi-Al	R	-	-	2	Sn-N	M	Ru-N	-
1	Os-Ru	R	-	-	2	Ta-C	M	C	-
1	Li-Zn	R	-	-	2	In-Rh	M	Rh	-
1	Al-As	R	-	-	2	Mn-Be	M	Be	-
1	Mo-Ir	R	-	-	2	Pu-Ge	R	-	-
1	Zr-Fe	R	-	-	2	Li-Ir	R	-	-
1	Ac-Zn	R	-	-	2	Li-Fe	R	-	-
1	Nb-N	R	-	-	2	Ta-Po	R	-	-
1	Hf-Si	R	-	-	2	Sr-P	R	-	-
1	Pa-Ir	R	-	-	2	P-Cl	R	-	-
3	As-P	CH	C	F-B	4	Be-Fe	CH	C	Mn
3	Fe-Co	CH	C	C-Cr	4	Fe-Fe	CH	Cr	B-H
3	B-H	CH	Fe	C	4	Pd-Au	CH	As	Mo-H
3	Mo-H	CH	W-H	B	4	Cu-P	CH	V-Mo	Ru
3	Cu-Mo	CH	Ru	Co-Rh	4	Pb-Nb	CH	Cr	Fe
3	Ga-Os	CH	B	C	4	Ge-Ge	CH	B	Sn
3	Co-Ni	CH	V	B	4	Cr-Cr	CH	Fe	Mn
3	Cr-Cu	CH	Mn	Os	4	Ti-Ru	CH	Cr-Cu	Cr-Rh
3	Cu-Os	CH	Ir	Co-Rh	4	P-Pt	CH	As-P	Mo-H
3	Mn-B	RH	Mn	B	4	As-B	RH	B	As
3	V-P	RH	V	Os-P	4	B-C	RH	C	B-H
3	Pd-Os	RH	Pd	Al-Os	4	Fe-Cl	RH	Fe	Cl
3	V-Mo	RH	V	Mo-C	4	Np-Mn	RH	Mn	Np

Gen	Compound	How created	1th Parent	2nd Parent	Gen	Compound	How created	1th Parent	2nd Parent
3	Cr-Ir	RH	Cr	Ir	4	Ca-C	RH	Ca	C
3	Sn-C	RH	Sn	C	4	Mn-P	RH	Mn	As-P
3	Cr-Rh	RH	Cr	Co-Rh	4	Pb-Mn	RH	Mn	Pb
3	Mn-Pd	RH	Mn	Pd-W	4	V-Ir	RH	V	Cr-Ir
3	As-C	RH	Mo-C	As-Mo	4	P-B	RH	B	P
3	Pt-Rh	M	Co-Rh	-	4	Cd-Mn	M	Mn	-
3	Se-C	M	Mo-C	-	4	Mn-C	M	C	-
3	Ge-W	M	Pd-W	-	4	Ge-Cr	M	Cr	-
3	Rh-C	M	Ru-C	-	4	Ge-C	M	C	-
3	Se-W	M	W-H	-	4	Fe-Rh	M	Fe	-
3	Mo-Ru	M	Mo	-	4	Ti-V	M	V	-
3	Li-Ta	R	-	-	4	V-V	R	-	-
3	Po-P	R	-	-	4	Ru-Rh	R	-	-
3	Sr-Cl	R	-	-	4	Bi-As	R	-	-
3	Zn-P	R	-	-	4	Mn-Rh	R	-	-
3	Al-Sb	R	-	-	4	Nb-C	R	-	-
3	Pb-V	R	-	-	4	Ge-Au	R	-	-
5	Al-Ru	CH	C	B	6	Fe-Se	CH	Cr-C	B-C
5	Be-Be	CH	Mn	B-C	6	Pd-Ir	CH	Fe	C
5	Fe-Ni	CH	Cr	B-C	6	Nb-Ga	CH	Cr-B	Cr-C
5	As-H	CH	Nb-C	B-H	6	Fe-Ru	CH	B	Mn-S
5	Zn-Cu	CH	V	Mn-Rh	6	Tc-Pt	CH	C	Co
5	Hg-Fe	CH	B	B-C	6	Al-P	CH	Mn-Pt	Be-B
5	Mo-P	CH	Cr	Mn-Rh	6	Cu-Cu	CH	P	Co
5	Si-Cu	CH	Be	Fe	6	Ru-H	CH	Mn-S	Cr
5	Co-Co	CH	Cr	B	6	Cu-Co	CH	Fe	Ni
5	Cr-C	RH	B-C	Ge-Cr	6	Mo-B	RH	B-H	Mo
5	P-H	RH	B-H	P-B	6	Cu-H	RH	P-H	Cu
5	Be-B	RH	B	Be	6	Fe-Mo	RH	Fe	Mo
5	Cr-B	RH	Ge-Cr	Mn-B	6	Ni-P	RH	Fe-Ni	Fe-P
5	Fe-Ir	RH	Fe	V-Ir	6	Si-B	RH	Si	B-H
5	Be-Rh	RH	Mn-Rh	Be	6	Cr-P	RH	P	Cr
5	Mn-Cu	RH	Mn	Cu-P	6	Fe-S	RH	Fe-Ni	Mn-S
5	Fe-P	RH	Fe	Cu-P	6	Mn-H	RH	P-H	Mn-Pt
5	Ir-H	RH	V-Ir	B-H	6	Mn-As	RH	Mn	As
5	Mo-Pd	M	Pd	-	6	Ge-Fe	M	Fe-Ir	-
5	Mn-S	M	Mn-C	-	6	Tc-Ni	M	Fe-Ni	-
5	Pd-Rh	M	Rh	-	6	Os-S	M	Mn-S	-
5	Sc-Nb	M	Nb	-	6	H-H	M	B-H	-
5	V-Ru	M	V-Ir	-	6	U-Mn	M	Mn	-
5	Mn-Pt	M	Mn-Rh	-	6	Be-Pt	M	Mn-Pt	-
5	K-Ti	R	-	-	6	Ca-Be	R	-	-
5	Hg-Ag	R	-	-	6	Mo-S	R	-	-
5	Po-Be	R	-	-	6	In-Br	R	-	-
5	Pu-Sn	R	-	-	6	Sc-Co	R	-	-
5	Cs-O	R	-	-	6	Cr-N	R	-	-
5	Ca-Th	R	-	-	6	Ga-V	R	-	-

Gen	Compound	How created	1th Parent	2nd Parent	Gen	Compound	How created	1th Parent	2nd Parent
7	Ni-B	CH	Cr-N	B-C	8	Ni-C	CH	Si-H	B-H
7	Co-Os	CH	Mo-S	B	8	Zn-Zn	CH	Ti	Tc
7	Os-Pt	CH	Mo-S	B	8	Ni-Ni	CH	Co	Fe-Ru
7	Zn-Fe	CH	Si-B	Cr	8	Al-H	CH	Mn-Fe	Cr-N
7	Ga-Ru	CH	Cr-P	Mn-H	8	Ge-Cu	CH	Te	Cr-B
7	Al-Cr	CH	Ru-H	Mn-H	8	Po-Fe	CH	Mn-Fe	C
7	Ni-Ru	CH	Tc-Pt	B	8	Tc-Br	CH	Cr-N	Te
7	Be-Co	CH	B-H	Mn	8	Ti-Ti	CH	Al-Cr	Ti-Cr
7	Co-Ru	CH	C	Cr-P	8	Tc-Ir	CH	Mn-C	Mo
7	Si-H	RH	Si	Mn-H	8	Mn-Tc	RH	Mn	Tc
7	Tc-P	RH	P	Tc	8	Cr-H	RH	Mn-H	Mn-Cr
7	Cr-Mo	RH	Mo-S	Cr	8	Tc-Fe	RH	Tc	Fe
7	S-B	RH	Mo-S	Si-B	8	Os-H	RH	Mn-H	Os-Pt
7	Tc-B	RH	B-C	Tc	8	Cr-Fe	RH	Cr-N	Mn-Fe
7	Co-B	RH	B-C	Co	8	Cr-Os	RH	Os	Mn-Cr
7	Mn-Cr	RH	Cr-N	Mn-H	8	Mn-N	RH	Ti-Mn	Cr-N
7	Mn-Co	RH	Co	Mn-As	8	Ti-Be	RH	Be	Ti-Cr
7	Mn-Fe	RH	Mn-As	Fe	8	Pd-B	RH	B-H	Pd
7	Fe-H	M	H	-	8	Zn-Mo	M	Cr-Mo	-
7	Tl-Ru	M	Ru-H	-	8	B-B	M	Tc-B	-
7	Ti-Cr	M	Cr	-	8	Sb-Ni	M	Ni	-
7	Te-Mn	M	Mn	-	8	V-Tc	M	Tc-B	-
7	Al-Pt	M	Al-P	-	8	Be-Ni	M	Be	-
7	Ti-Mn	M	Mn-As	-	8	Mn-Mo	M	Cr-Mo	-
7	Ca-Ni	R	-	-	8	Ac-Si	R	-	-
7	Zn-Be	R	-	-	8	Hf-Bi	R	-	-
7	Br-S	R	-	-	8	Pa-Si	R	-	-
7	In-Co	R	-	-	8	Pu-Tc	R	-	-
7	Rb-Sc	R	-	-	8	U-Se	R	-	-
7	Tc-Tc	R	-	-	8	Pd-O	R	-	-
9	P-C	CH	Os-H	B-H	10	Pa-P	CH	Rh	B-H
9	Co-Ir	CH	Mn-C	C	10	Si-Fe	CH	Mn	Cr-Ni
9	Ni-O	CH	Cr-Fe	Mn-N	10	Co-P	CH	V-B	B-H
9	Tc-Cu	CH	Mo	Cr	10	In-Ge	CH	Cr-B	Cr-H
9	Ga-Be	CH	Cr-B	Mn	10	V-Ni	CH	Tc-Ru	B
9	Cu-Ru	CH	Cr-H	Os	10	Ge-Ni	CH	Cr	Cr-N
9	Hg-Ni	CH	C	Cr-B	10	Hf-Be	CH	Mn	Cr-H
9	Cd-Be	CH	C	Mn-H	10	Nb-Co	CH	Cr	Si
9	Cu-Rh	CH	Cr-N	Os	10	Np-Cr	CH	Po	Fe
9	V-B	RH	V	B	10	C-O	RH	Ni-O	Tc-C
9	Ni-N	RH	Cr-N	Ni	10	Co-N	RH	Cr-N	Co
9	Mn-Ni	RH	Ni-C	Mn-H	10	Si-Tc	RH	Si	Tc-C
9	Cr-Ni	RH	Ni-C	Cr-Fe	10	Tc-H	RH	B-H	Tc
9	C-H	RH	B-H	C	10	Ga-C	RH	Ga	C
9	Tc-C	RH	C	Tc	10	Nb-V	RH	Nb-Ga	V-B
9	Ir-N	RH	Ir	Cr-N	10	Ga-Ni	RH	Ni	Ga-Be
9	Tc-Po	RH	Tc	Po	10	Be-N	RH	Be	Cr-N

Gen	Compound	How created	1th Parent	2nd Parent	Gen	Compound	How created	1th Parent	2nd Parent
9	C-N	RH	Mn-N	C	10	Po-H	RH	B-H	Po
9	Zn-Mn	M	Mn	-	10	Re-Fe	M	Fe	-
9	Co-H	M	B-H	-	10	Zr-Be	M	Be	-
9	Cu-C	M	B-C	-	10	V-Re	M	V	-
9	V-Fe	M	Fe	-	10	Ga-Tc	M	Ga-Be	-
9	Tc-Ru	M	Tc-Ir	-	10	Cr-W	M	Cr-N	-
9	Si-C	M	Ni-C	-	10	Re-Cu	M	Cu	-
9	Y-Np	R	-	-	10	Sr-U	R	-	-
9	Li-Sn	R	-	-	10	Y-Zr	R	-	-
9	Sr-I	R	-	-	10	Al-Mn	R	-	-
9	Te-Co	R	-	-	10	Sb-Au	R	-	-
9	Rb-Ba	R	-	-	10	Ag-C	R	-	-
9	Hg-Be	R	-	-	10	Tl-Fe	R	-	-
11	V-Rh	CH	Mn	Al-Mn	12	P-N	CH	Br-O	B-H
11	Mo-Ni	CH	V-Re	Mn-H	12	Hg-Os	CH	B-H	B-C
11	Po-Cu	CH	V-Ni	C	12	Be-F	CH	Mn-O	O
11	Cd-Pt	CH	Ga-C	Np-Cr	12	Mo-Mo	CH	P	Si
11	Al-Co	CH	B	Ga-C	12	Mg-Fe	CH	Al-C	Zn-Cr
11	Mg-In	CH	B-C	Ni	12	Re-Ru	CH	Zn-Cr	Si
11	Zn-Cr	CH	V	Tc-H	12	Ta-Be	CH	Cr	Be
11	C-C	CH	B-H	O	12	Co-C	CH	B-H	Cr-O
11	Co-Mo	CH	Cr-W	Ni	12	Be-C	CH	B-H	Be-O
11	Al-C	RH	B-C	Al-Mn	12	Cr-Be	RH	Be	Cr-N
11	Cr-O	RH	O	Cr	12	Zn-V	RH	Zn-Cr	V
11	V-Si	RH	V	Si	12	B-O	RH	Mn-O	Cr-B
11	Mn-O	RH	Mn	O	12	Ga-Mo	RH	Mo	Ga
11	V-Mn	RH	Al-Mn	V	12	N-O	RH	O	Cr-N
11	V-Be	RH	Zr-Be	V	12	Be-Br	RH	Br	V-Be
11	Fe-N	RH	Fe	Cr-N	12	Nb-Cu	RH	Nb-Ga	Cu
11	Cr-Tc	RH	Tc	Cr-N	12	Ga-B	RH	Ga	B-C
11	Be-O	RH	Be	O	12	Zn-O	RH	O	Zn-Cr
11	Br-O	M	O	-	12	Pd-N	M	Fe-N	-
11	Tl-Mn	M	Mn	-	12	Ti-B	M	B-H	-
11	Pu-N	M	Cr-N	-	12	Si-O	M	Cr-O	-
11	Ge-B	M	B	-	12	Nb-Tc	M	Cr-Tc	-
11	Tc-Co	M	Tc-H	-	12	Pa-Be	M	Be	-
11	Tc-W	M	Tc	-	12	Si-S	M	Fe-S	-
11	Pu-Cu	R	-	-	12	Np-Os	R	-	-
11	Ba-Co	R	-	-	12	Te-Ru	R	-	-
11	Hf-Pa	R	-	-	12	Rb-Li	R	-	-
11	Cu-W	R	-	-	12	Y-Nb	R	-	-
11	Nb-P	R	-	-	12	Sc-I	R	-	-
11	Fr-Cu	R	-	-	12	Tl-Pd	R	-	-
13	N-N	CH	C	O	14	V-C	CH	Cr-B	Cr-N
13	P-Rh	CH	Ti	O	14	Ga-Rh	CH	Se	Mn-H
13	Pu-S	CH	Cr-N	Nb-Tc	14	Cu-Ni	CH	Ga	B
13	Sn-Ru	CH	Cr-B	Ga-Mo	14	Zr-Zn	CH	Nb-Mn	Cr

Gen	Compound	How created	1th Parent	2nd Parent	Gen	Compound	How created	1th Parent	2nd Parent
13	Re-Tc	CH	Ti	Mo	14	Pd-Ru	CH	P-Rh	C
13	Rh-O	CH	Zn-O	F	14	Ni-Ir	CH	B-N	P-Rh
13	Ru-Ru	CH	P	F	14	S-N	CH	O	Fe
13	In-Ru	CH	Si-S	C	14	Ti-Mo	CH	Cr	Fe
13	Au-C	CH	Fe	B-C	14	Zn-Tc	CH	Mo	V
13	P-O	RH	B-O	P	14	V-N	RH	Al-V	Cr-N
13	B-N	RH	P-N	Cr-B	14	Nb-Fe	RH	Nb-Mn	Fe-Se
13	Cr-Se	RH	Cr-Be	Fe-Se	14	As-O	RH	As	P-O
13	Cr-Ru	RH	Cr	Re-Ru	14	C-F	RH	C	F
13	Nb-Mo	RH	Nb-Ga	Ga-Mo	14	Nb-H	RH	Nb-Mn	Mn-H
13	Be-Mo	RH	Mo	Be-C	14	Nb-O	RH	Nb-Mn	O
13	Fe-Br	RH	Fe	Br	14	V-O	RH	Rh-O	V
13	Re-B	RH	Re	B	14	Ru-B	RH	Cr-B	Cr-Ru
13	Si-P	RH	Si	P	14	N-F	RH	B-N	F
13	Al-V	M	V	-	14	S-O	M	O	-
13	Pa-O	M	Si-O	-	14	Ta-Mn	M	Mn	-
13	Nb-Mn	M	Mn	-	14	Zn-N	M	B-N	-
13	Mn-I	M	Mn	-	14	Ir-O	M	P-O	-
13	Re-H	M	Mn-H	-	14	Si-N	M	Tc-N	-
13	Tc-N	M	P-N	-	14	Cu-B	M	Cr-B	-
13	Ac-C	R	-	-	14	Ac-Tl	R	-	-
13	Ga-As	R	-	-	14	Sb-I	R	-	-
13	Ge-As	R	-	-	14	Sb-Be	R	-	-
13	Ag-Ni	R	-	-	14	Pa-Tc	R	-	-
13	Hf-F	R	-	-	14	Ge-Si	R	-	-
13	Ca-Ac	R	-	-	14	U-Au	R	-	-
15	Ni-Br	CH	Si-N	N-F	16	Fe-C	CH	Mo-N	B
15	Ni-F	CH	Si-N	B-N	16	Y-Co	CH	Mn-H	Cr
15	Mo-N	CH	As-O	Ni-P	16	Ni-Os	CH	B-N	Si
15	I-Fe	CH	O	V-N	16	U-Co	CH	Cr-N	Cr
15	Cu-S	CH	Ta-Mn	F	16	Re-Au	CH	Mo	V-Ge
15	Si-Rh	CH	Pd	V-O	16	Tc-Mo	CH	B-C	Mo-N
15	Ag-W	CH	Nb-Fe	Cr-N	16	Mn-Au	CH	C	B-N
15	Pt-Au	CH	C	Ni	16	Ni-S	CH	B-N	Fe
15	Fe-O	CH	Cr-N	F	16	Zn-Si	CH	V	Ru
15	V-F	RH	N-F	V-C	16	Cr-Pt	RH	Pt	Cr-B
15	Ru-O	RH	V-O	Ru-B	16	As-Ir	RH	Ir	As
15	Zr-V	RH	Zr	V-N	16	Cr-Si	RH	Cr-N	Si
15	H-F	RH	Mn-H	N-F	16	Si-F	RH	Si	F
15	Tc-F	RH	F	Tc	16	B-F	RH	H-F	B-C
15	Cr-F	RH	N-F	Cr-N	16	Mo-O	RH	O	Mo-N
15	V-Ge	RH	V	Ge	16	Mn-Ru	RH	Mn-H	Ru
15	As-Ni	RH	As-O	Ni	16	As-F	RH	F	Cr-As
15	Cr-As	RH	As	Cr	16	Zr-O	RH	Zr-V	O
15	Bi-V	M	V-C	-	16	V-Ag	M	V	-
15	Si-Ir	M	Si-N	-	16	Nb-Si	M	Si	-
15	Cd-Ga	M	Nb-Ga	-	16	Pu-Ni	M	Ni	-

Gen	Compound	How created	1th Parent	2nd Parent	Gen	Compound	How created	1th Parent	2nd Parent
15	Mg-C	M	V-C	-	16	O-F	M	F	-
15	Hg-F	M	N-F	-	16	Tc-As	M	Cr-As	-
15	Pu-H	M	Mn-H	-	16	Ir-B	M	B-N	-
15	Sr-Co	R	-	-	16	K-Sb	R	-	-
15	Ag-Mn	R	-	-	16	Li-Cu	R	-	-
15	Ga-At	R	-	-	16	In-S	R	-	-
15	Ti-Cu	R	-	-	16	Ac-F	R	-	-
15	Ag-Pd	R	-	-	16	Pu-F	R	-	-
15	U-Si	R	-	-	16	Hg-Te	R	-	-
17	Ga-O	CH	Fe-C	Cr-N	18	Ta-Ru	CH	Si-Mo	Cr-N
17	Zn-Co	CH	B-H	Cr-B	18	Bi-Fe	CH	Cr-N	B-C
17	Ni-Rh	CH	Si	B-C	18	Ag-Fe	CH	C	B-C
17	Cd-Tc	CH	Cr-Si	Mo	18	Re-P	CH	Cr-Pd	Mo
17	Fe-Pt	CH	O	Cr-N	18	Mg-As	CH	B-C	Nb-B
17	Rh-N	CH	C	Mo-O	18	Al-Fe	CH	Mn	Cr
17	Al-Mo	CH	Tc	Tc-As	18	Co-S	CH	B-C	Cr-Au
17	I-S	CH	Mo-O	B-N	18	Zn-Ge	CH	B-N	C
17	Co-O	CH	Fe-C	F	18	Zn-B	CH	Mn-H	Cr
17	Mn-Si	RH	Mn	Cr-Si	18	Tc-Au	RH	Tc	Au
17	V-H	RH	V	Mn-H	18	Al-Rh	RH	Rh	Al-Mo
17	Mn-F	RH	Mn	O-F	18	H-O	RH	O-F	B-H
17	Ir-C	RH	Fe-C	Ir-B	18	Si-Pt	RH	Mn-Si	Pt
17	Tc-O	RH	O-F	Tc-As	18	Nb-Cr	RH	Cr	Nb
17	Si-Mo	RH	Tc-Mo	Si	18	Mo-F	RH	Mo	O-F
17	As-N	RH	Cr-N	As	18	Pd-C	RH	Cr-Pd	B-C
17	Pt-F	RH	Cr-Pt	F	18	Mo-Rh	RH	Mo	Rh
17	Nb-B	RH	Nb-Si	B-N	18	Ga-F	RH	F	Ga-O
17	Pa-Mn	M	Mn	-	18	Hg-Cr	M	Cr	-
17	Hg-H	M	B-H	-	18	Pu-Pt	M	Pt	-
17	Ag-Tc	M	Tc	-	18	Cd-Pd	M	Pd	-
17	In-C	M	C	-	18	Ti-N	M	Cr-N	-
17	Cr-Au	M	Cr-N	-	18	Ag-N	M	B-N	-
17	Cr-Pd	M	Cr-B	-	18	Zr-Mn	M	Mn-H	-
17	Mg-Be	R	-	-	18	Ta-Mo	R	-	-
17	Ba-Hg	R	-	-	18	Hf-Ni	R	-	-
17	Hg-Ir	R	-	-	18	U-Cu	R	-	-
17	Bi-At	R	-	-	18	Ga-Po	R	-	-
17	Pa-Sb	R	-	-	18	Li-Tl	R	-	-
17	Ru-Br	R	-	-	18	Os-Se	R	-	-
19	Tc-Rh	CH	Pd	Cr-N	20	Re-I	CH	Br	Cr-N
19	S-Cl	CH	Ni	O	20	Be-Cu	CH	Mn	Os-B
19	Th-Rh	CH	C-C	Mo-Rh	20	I-Os	CH	Re	Tc-Rh
19	Ir-Rh	CH	Se	P	20	Bi-Ni	CH	Tc-Rh	Os-B
19	Au-S	CH	Se	C	20	Be-S	CH	Mn-H	B-H
19	Br-C	CH	O-F	B-N	20	Ta-Co	CH	Zr-Cr	Zr-Ni
19	Ti-C	CH	B-H	B-N	20	Sn-Al	CH	Zr-Cr	Re-Re
19	Zr-Nb	CH	Cr	Mn	20	Ag-Mo	CH	As	Mn-Re

Gen	Compound	How created	1th Parent	2nd Parent	Gen	Compound	How created	1th Parent	2nd Parent
19	Rh-H	CH	B-N	Mo	20	Cl-H	CH	B	C-C
19	Mn-Re	RH	Zr-Mn	Re-P	20	Zr-C	RH	C	Zr-Ni
19	Zr-B	RH	Zr-Mn	B	20	Os-Rh	RH	Rh	Os-B
19	Ta-O	RH	O	Ta-Mo	20	Rh-Cl	RH	S-Cl	Rh-H
19	Zr-Ni	RH	Ni	Zr-Mn	20	Mn-Os	RH	Os-B	Mn
19	Zr-Cr	RH	Zr-Mn	Cr-N	20	S-F	RH	S	F
19	As-Rh	RH	As	Rh	20	Re-Os	RH	Re	Os-B
19	Pt-N	RH	Cr-N	Pt	20	Si-Os	RH	Os-B	Si
19	Re-F	RH	Re-P	O-F	20	Zr-Rh	RH	Rh	Zr-B
19	Mn-Se	RH	Se	Mn	20	Re-Ir	RH	Re	Ir-Rh
19	Os-B	M	B	-	20	Re-Rh	M	Rh-H	-
19	Re-Si	M	Re	-	20	Pt-B	M	B-N	-
19	Se-F	M	F	-	20	Ti-As	M	Ti-C	-
19	Bi-Cr	M	Cr-N	-	20	Ta-Cr	M	Cr	-
19	Co-F	M	F	-	20	Ti-Si	M	Si	-
19	Cd-Au	M	Tc-Au	-	20	W-B	M	B-C	-
19	Pu-Ru	R	-	-	20	K-Pd	R	-	-
19	I-N	R	-	-	20	At-C	R	-	-
19	Ac-Be	R	-	-	20	At-O	R	-	-
19	Li-C	R	-	-	20	Li-Ti	R	-	-
19	U-Pt	R	-	-	20	Rb-Na	R	-	-
19	Zn-Os	R	-	-	20	Pb-C	R	-	-

References

1. Lipowski, A. & Lipowska, D. Roulette-wheel selection via stochastic acceptance. *Phys. A Stat. Mech. its Appl.* **391**, 2193–2196 (2012).

2. Nagle, J. K. Atomic polarizability and electronegativity. *J. Am. Chem. Soc.* **112**, 4741–4747 (1990).

3. Kresse, G. & Furthmüller, J. Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set. *Phys. Rev. B* **54**, 11169–11186 (1996).

4. Kresse, G. & Joubert, D. From ultrasoft pseudopotentials to the projector augmented-wave method. *Phys. Rev. B* **59**, 1758–1775 (1999).

5. Perdew, J. P., Burke, K. & Ernzerhof, M. Generalized Gradient Approximation Made Simple. *Phys. Rev. Lett.* **77**, 3865–3868 (1996).