Coevolutionary search of materials with optimal properties in the space of all possible compounds

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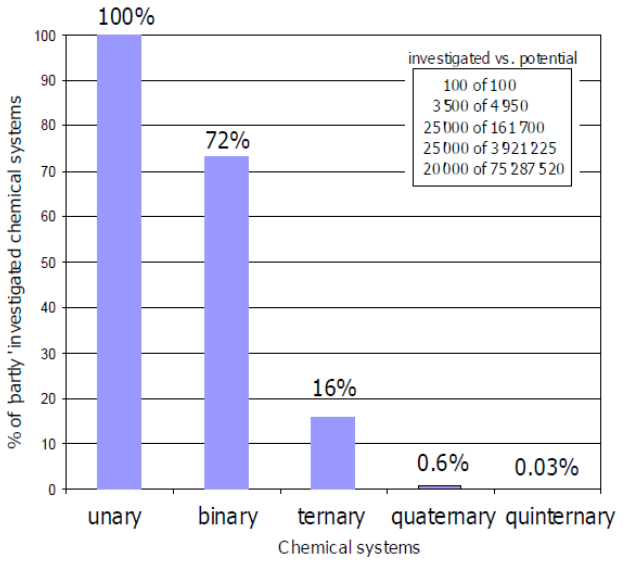
Outline

Search for materials with optimal target properties:

Mendelevian **S**erach-**MendS** (algorithm, method)[1][2].

- Defining a good chemical space.
- Multi-objective Pareto technique.

Results on searching (using MendS) for hard/superhard and low energy binary materials under zero pressure in the entire chemical space.



[1] Patent No: WO2018009090A1

[2] Paper in arxiv: 1807.00854 [cond-mat.mtrl-sci]

Villars, P. & IWATA, Sh. Chem. Met. Alloys, 6, 81-108, (2013).

Desired properties

Most optimal Materials

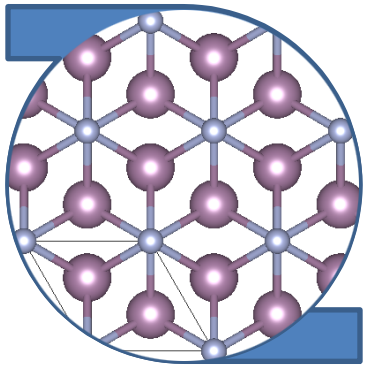
MendS

Which Materials? (i.e. X), & properties?

Most optimal phases and structures of X

USPEX

Structure search methods



Calculation of **Energy** and **Properties**. (i.e. magnetic, electronic, mechanical etc).

Search for the most optimal phases of a **specific** material.

Ab initio codes

Energy and Properties

What is coevolution and the difference of evolutionary algorithm and coevolutionary algorithm?

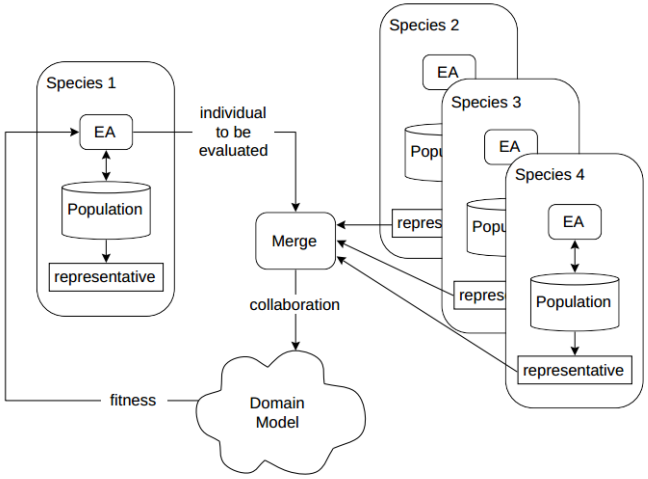
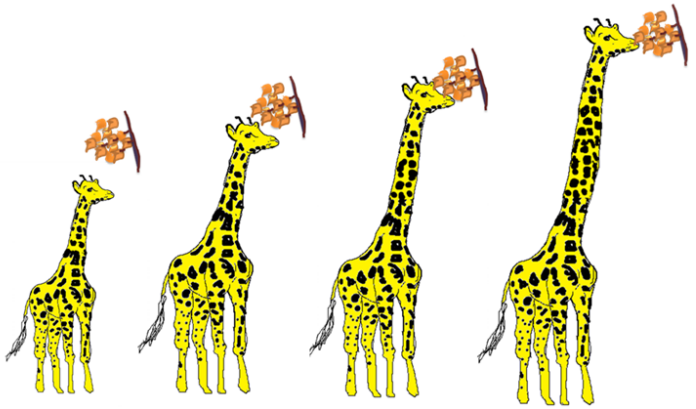
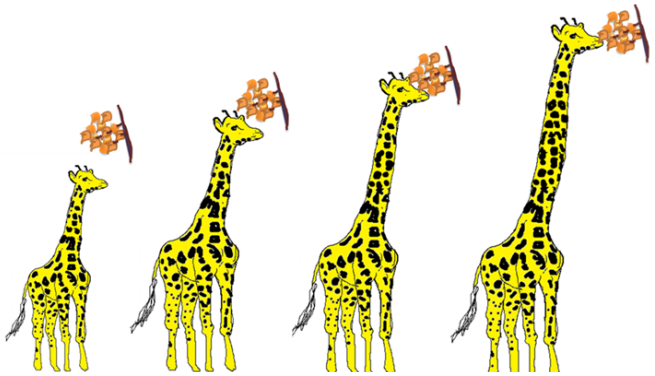


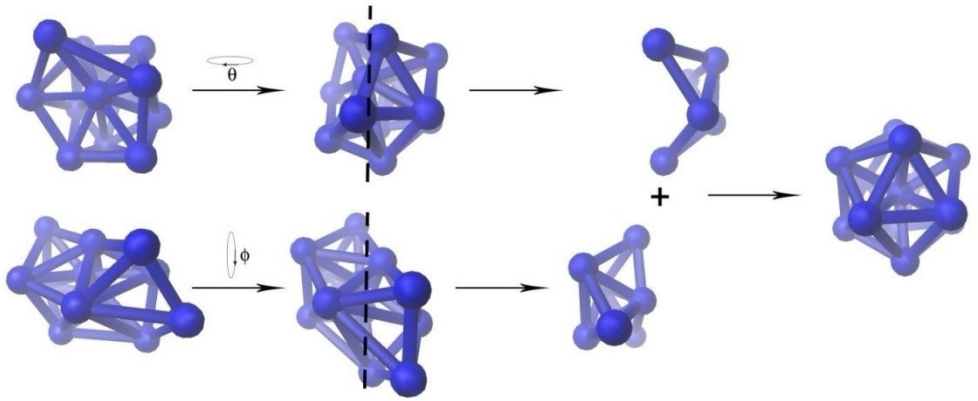
Figure 1: Cooperative coevolutionary architecture from the perspective of species number one

EA- Giraffe(one species only)



Child making in evolutionary algorithm is so obvious, but what about coevolutionary algorithm?





What is the child of

C-Fe & P-W

Chemical scale suggested by Pettifor (1984)

In 1984 Pettifor suggested two-dimensional map which every axis of this map are elements, he proposed to order these elements according to their Electronegativity and declared that in this way the excellent structural separation will be achieved and binary systems which have similar properties will be close together in the map!(*Solid. State. Commun.*, 51, 31-34 (1984)).

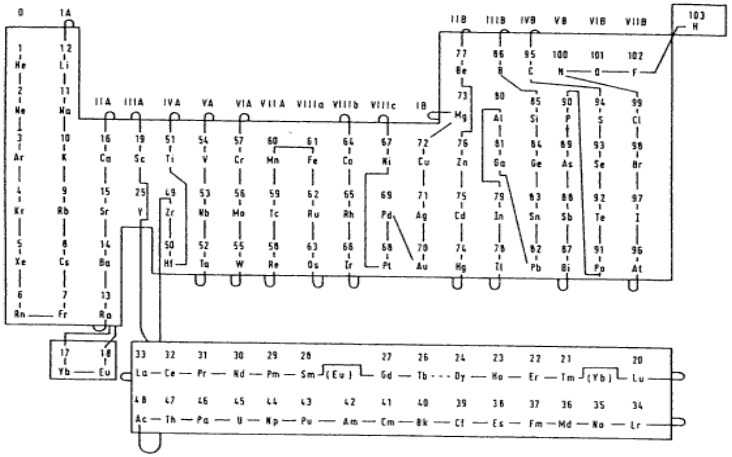
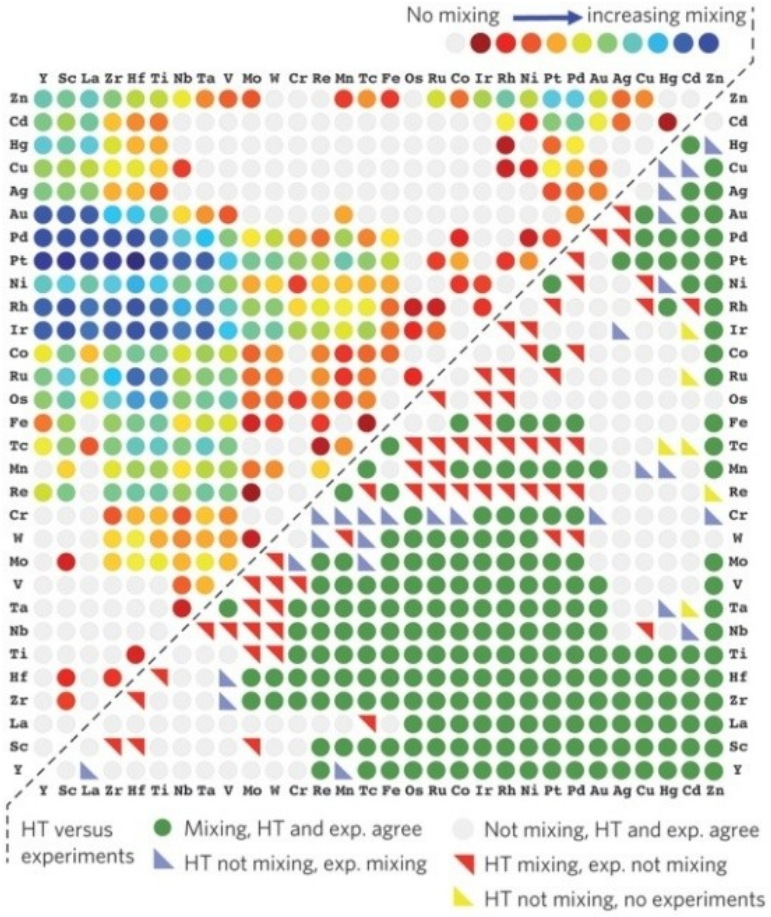


Fig. 1.8 The string running through this modified periodic table puts all the elements in sequential order, given by the ordering number $\mathcal{N}$. From Pettifor (1988).

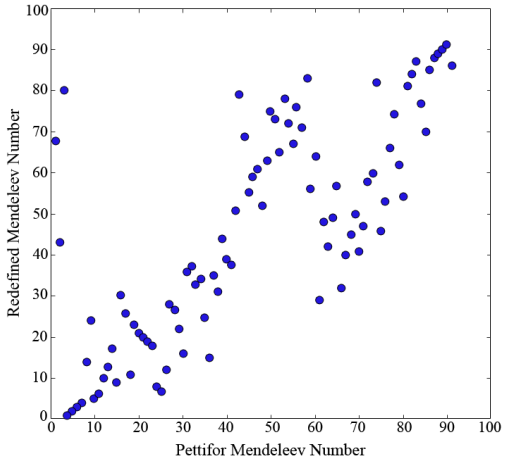
1	He	0.00	27	Gd	0.69	53	Nb	0.83	79	In	1.60
2	Ne	0.04	28	Sm	0.6925	54	V	0.84	80	Al	1.66
3	Ar	0.08	29	Pm	0.695	55	W	0.88	81	Ga	1.68
4	Kr	0.12	30	Nd	0.6975	56	Mo	0.885	82	Pb	1.80
5	Xe	0.16	31	Pr	0.70	57	Cr	0.89	83	Sn	1.84
6	Rn	0.20	32	Ce	0.7025	58	Re	0.935	84	Ge	1.90
7	Fr	0.23	33	La	0.705	59	Tc	0.94	85	Si	1.94
8	Cs	0.25	34	Lw	0.7075	60	Mn	0.945	86	B	2.00
9	Rb	0.30	35	No	0.71	61	Fe	0.99	87	Bi	2.04
10	K	0.35	36	Md	0.725	62	Ru	0.995	88	Sb	2.08
11	Na	0.40	37	Fm	0.715	63	Os	1.00	89	As	2.16
12	Li	0.45	38	Es	0.7175	64	Co	1.04	90	P	2.18
13	Ra	0.48	39	Cf	0.72	65	Rh	1.05	91	Po	2.28
14	Ba	0.50	40	Bk	0.7225	66	Ir	1.06	92	Te	2.32
15	Sr	0.55	41	Cm	0.725	67	Ni	1.09	93	Se	2.40
16	Ca	0.60	42	Am	0.7275	68	Pt	1.105	94	S	2.44
17	Yb	0.645	43	Pu	0.73	69	Pd	1.12	95	C	2.50
18	Eu	0.655	44	Np	0.7325	70	Au	1.16	96	At	2.52
19	Sc	0.66	45	U	0.735	71	Ag	1.18	97	I	2.56
20	Lu	0.67	46	Pa	0.7375	72	Cu	1.20	98	Br	2.64
21	Tm	0.675	47	Th	0.74	73	Mg	1.28	99	Cl	2.70
22	Er	0.6775	48	Ac	0.7425	74	Hg	1.32	100	N	3.00
23	Ho	0.68	49	Zr	0.76	75	Cd	1.36	101	O	3.50
24	Dy	0.6825	50	Hf	0.775	76	Zn	1.44	102	F	4.00
25	Y	0.685	51	Ti	0.79	77	Be	1.50	103	H	5.00
26	Tb	0.6875	52	Ta	0.82	78	Tl	1.56			

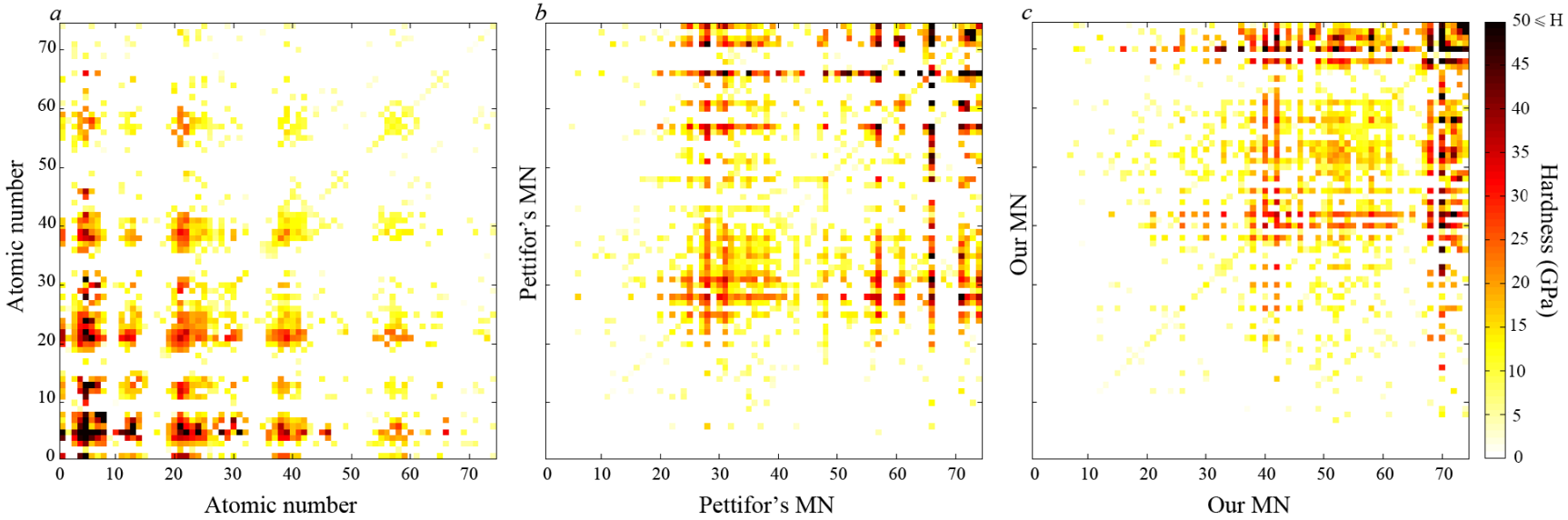
Well defined chemical space

- *New J. Phys.*, **18**, 093011 (2016).
- *J. Alloys. Compd.*, **317**, 26-38 (2001).
- *Solid. State. Commun.*, 51, 31-34 (1984).
- *Journal of Physics C*: Solid State Physics, 19, 3 (1986).

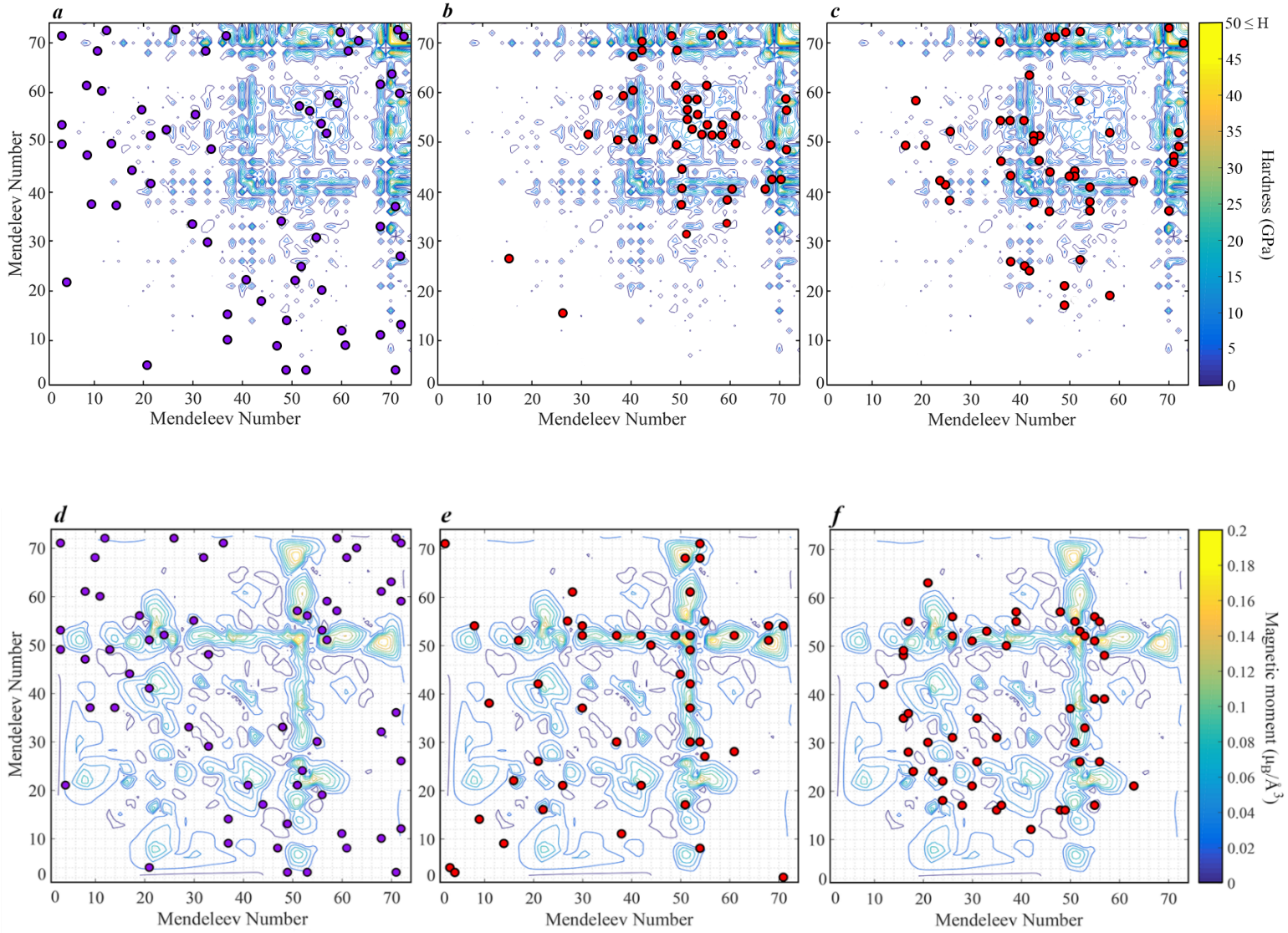


Our redefined MN, and it's comparison with the Pettifor's MN.



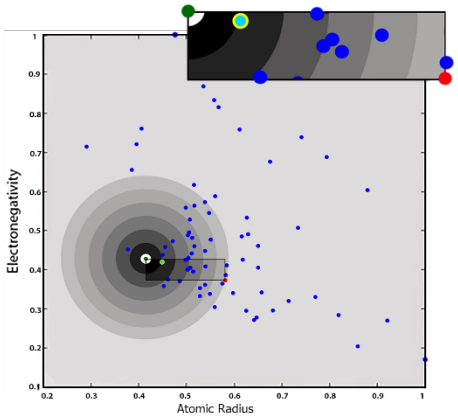


Efficiency of the algorithm in system selection and improving the Pareto front

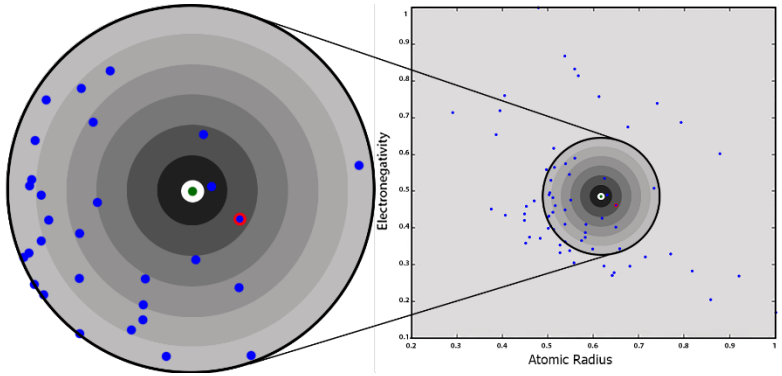


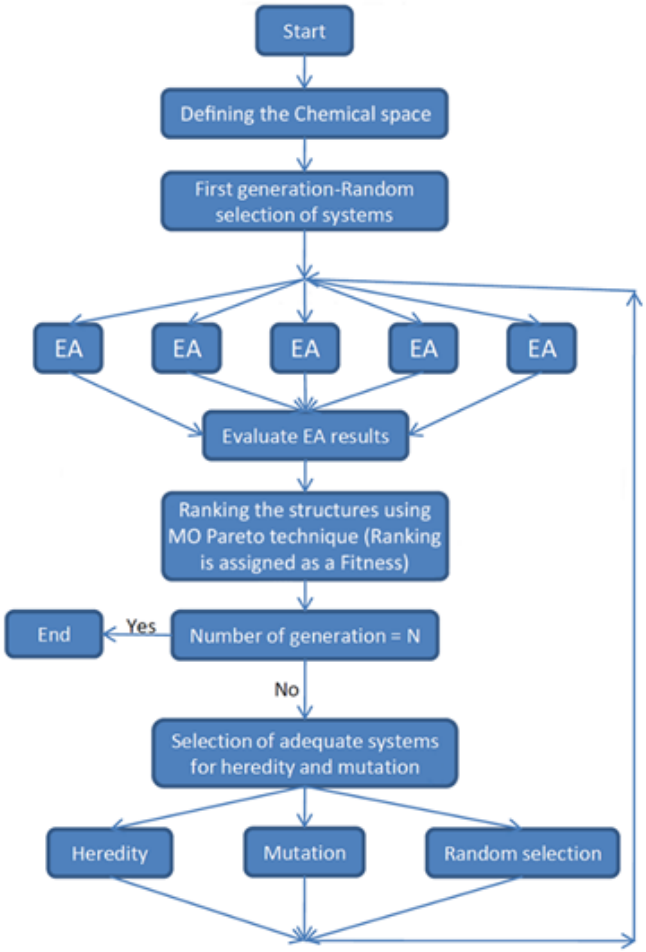
MendS algorithm and its important Variation operators

Finding the child of two parent red and green using **chemical heredity operator.**

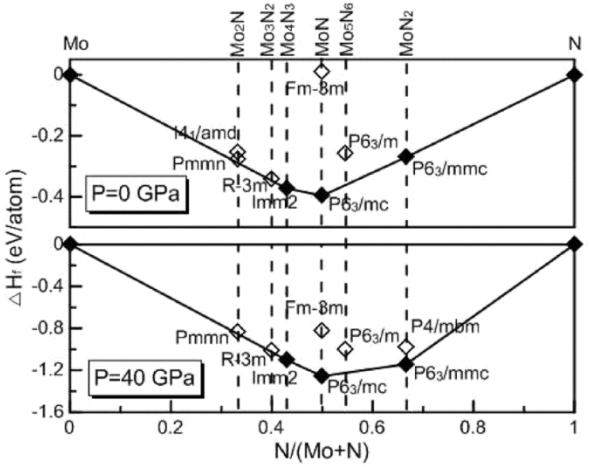


Using **chemical mutation operator** we mutate an atom to find

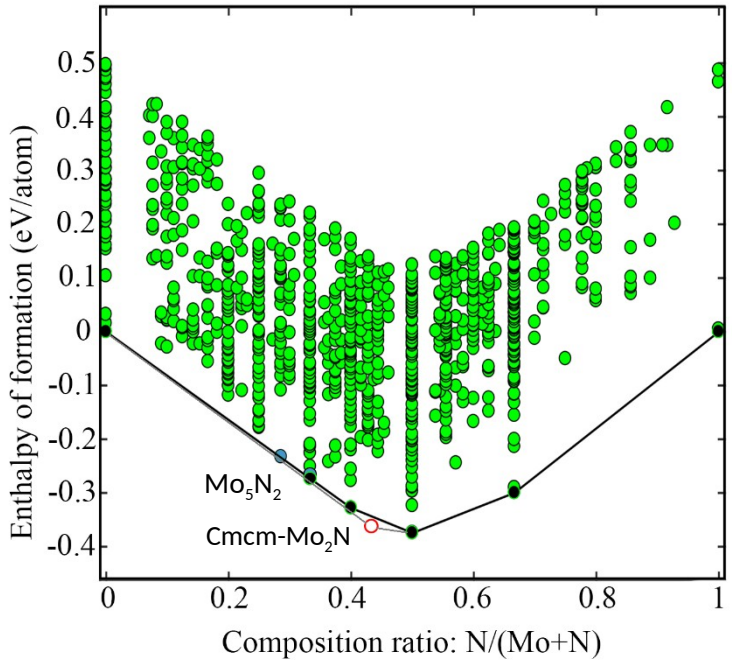


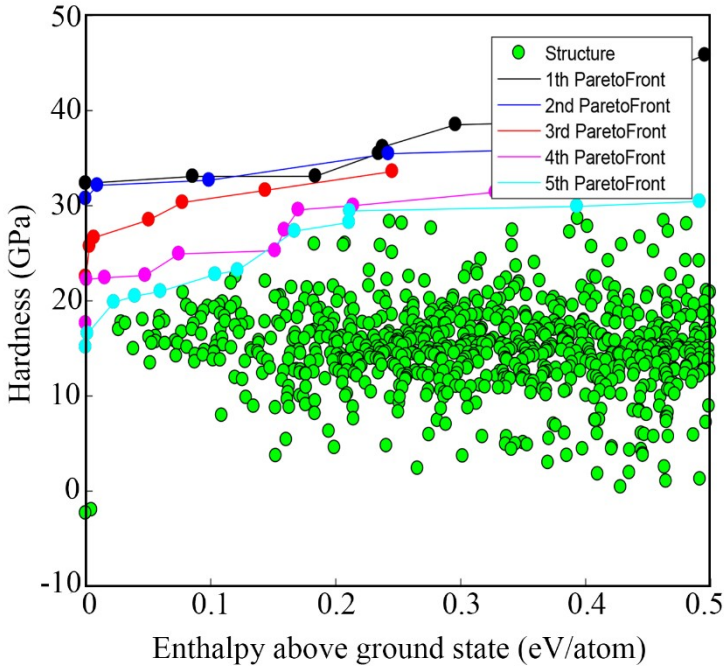


Implemention of mulit-objective Pareto method and its test on Mo_xN_y

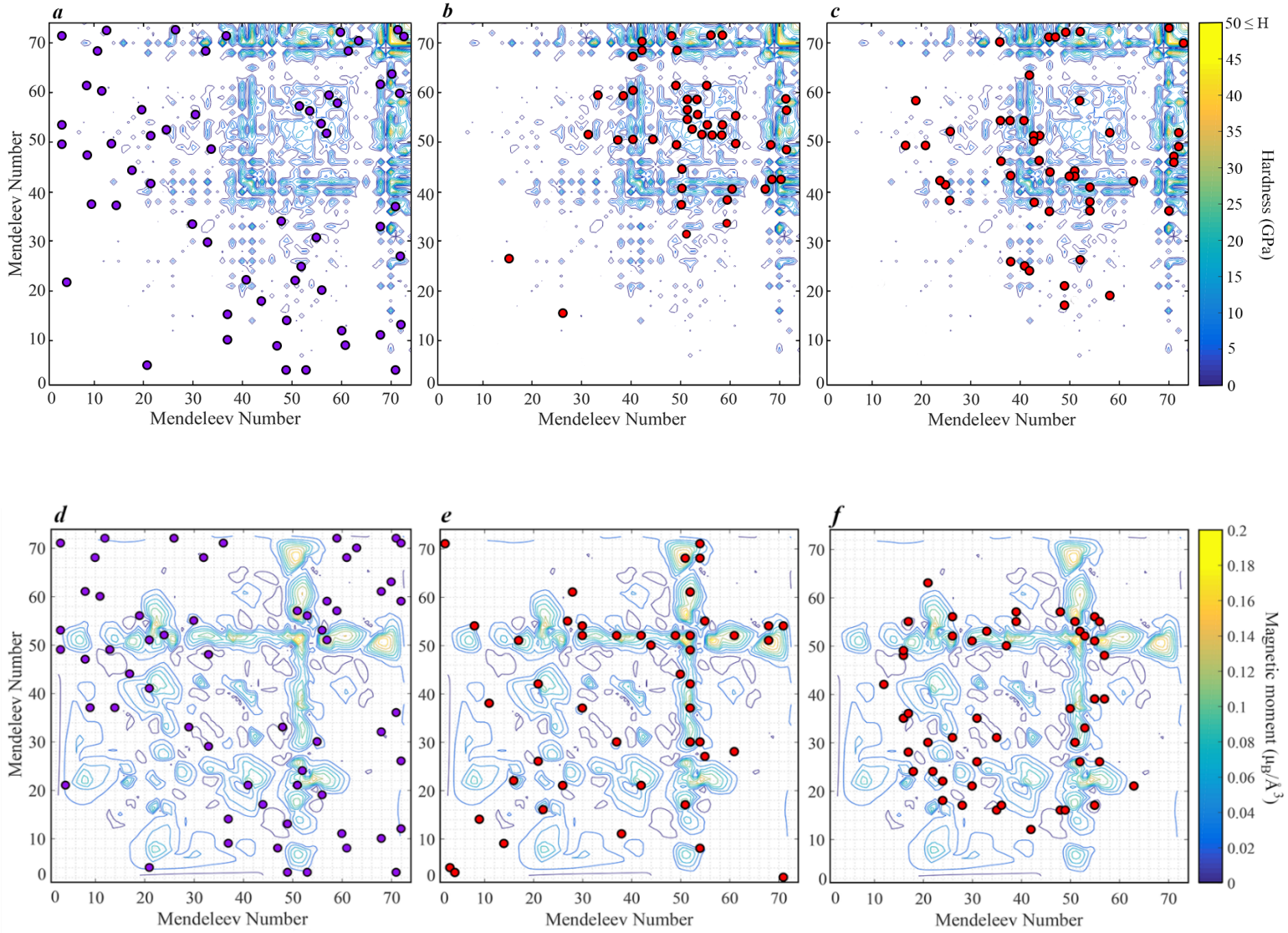


J. Phys. Chem. C, *120* (20), pp 11060–11067 **(2016)**.





Efficiency of the algorithm in system selection and improving the Pareto front



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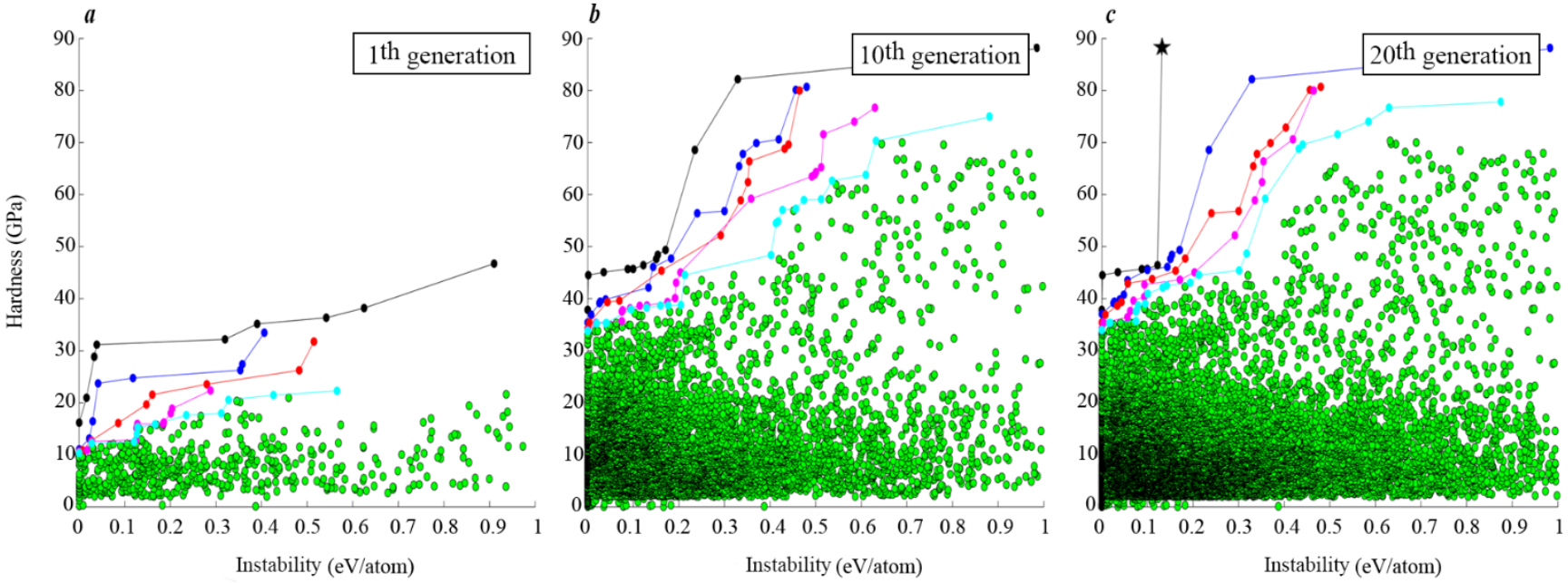
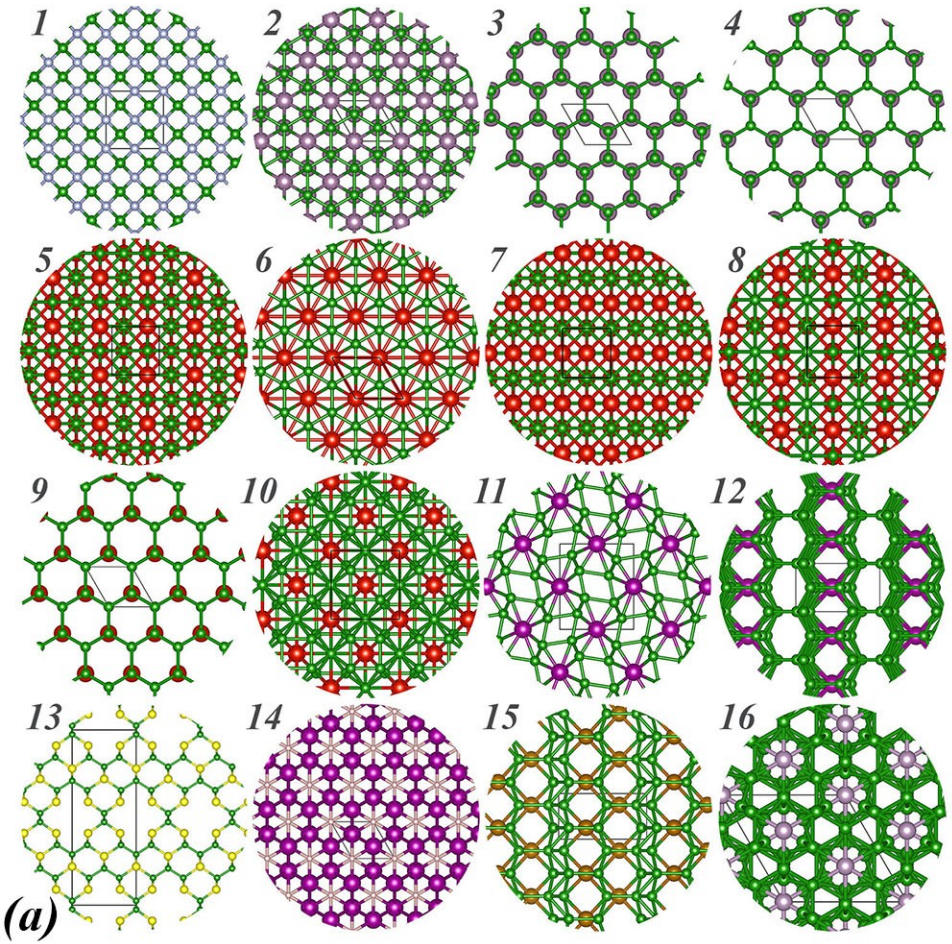
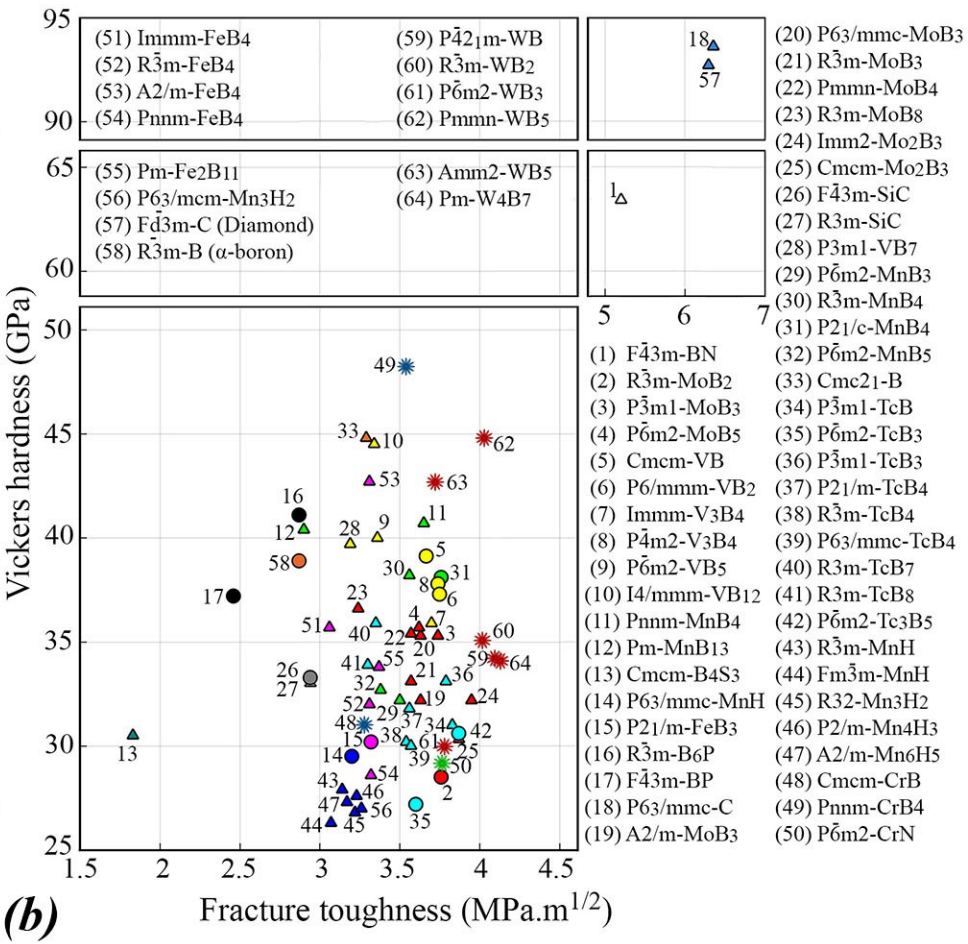


	Compounds	H_v (GPa)	K_{1C} (MPa.m$^{1/2}$)	Instability (eV/atom)	Space group		Compounds	H_v (GPa)	K_{1C} (MPa.m$^{1/2}$)	Instability (eV/atom)	Space group
Carbon	C	**92.7**	6.33	0.13	$Fd\bar{3}m$	**Boron**	B	38.9	2.87	0	$R\bar{3}m$
	C	**93.6**	6.36	0.139	$P6_3/mmc$		B	**44.8**	3.29	0.136	$Cmc2_1$
B-S	B_4S_3	30.5	1.83	0.102	$Cmcm$	**B-N**	BN	**63.4**,(**62.8**)[25],[**46-80**][20]	5.1	0.075	$F\bar{4}3m$
	MoB_2	28.5,(33.1)[44],[24.2][53]	3.76	0	$R\bar{3}m$		TcB	31,(30.3)[54]	3.83	0.013	$P\bar{3}m1$
	MoB_3	35.3	3.74	0.035	$P\bar{3}m1$		TcB_3	27.2,(29)[55]	3.6	0	$P\bar{6}m2$
	MoB_3	32.2	3.63	0.077	$A2/m$		TcB_3	33.1	3.79	0.003	$P\bar{3}m1$
		35.3,(37.3)[44]	3.63	0.017	$P6_3/mmc$		TcB_4	31.8	3.56	0.069	$P2_1/m$
		33.1,(31.8)[43]	3.57	0.011	$R\bar{3}m$		TcB_4	30.2	3.54	0.069	$R\bar{3}m$
Mo-B	MoB_4	35.4	3.57	0.099	$Pmmn$	**Tc-B**		30,(32)[55]	3.57	0.027	$P6_3/mmc$
	MoB_5	35.7	3.62	0.054	$P\bar{6}m2$		TcB_7	35.9	3.35	0.084	$R3m$
	MoB_8	36.6	3.24	0.118	$R3m$		TcB_8	33.9	3.3	0.113	$R3m$
	Mo_2B_3	32.2	3.95	0.029	$Imm2$		Tc_3B_5	30.6	3.87	0	$P\bar{6}m2$
	Mo_2B_3	30.4	3.87	0.043	$Cmcm$						
Si-C	SiC	33.3,(33.1)[31],[28][31]	2.94	0	$F\bar{4}3m$	**B-P**	BP	37.2,(29.3)[31],[33][31]	2.46	0	$F\bar{4}3m$
	SiC	33.1	2.94	0.001	$R3m$		B_6P	**41.1**	2.87	0	$R\bar{3}m$
	VB	39.1,(38.3)[49]	3.66	0	$Cmcm$		MnH	29.5	3.2	0	$P6_3/mmc$
	VB_2	37.3,(39.5)[49],[27.2][50]	3.75	0	$P6/mmm$		MnH	27.9	3.14	0.013	$R\bar{3}m$
	VB_5	**40**	3.36	0.158	$P\bar{6}m2$		MnH	26.3	3.07	0.044	$Fm\bar{3}m$
V-B	VB_7	39.7	3.19	0.143	$P3m1$	**Mn-H**	Mn_3H_2	26.8	3.22	0.017	$R32$
	VB_{12}	**44.5**	3.34	0.125	$I4/mmm$		Mn_3H_2	27	3.26	0.019	$P6_3/mcm$
	V_3B_4	37.8	3.74	0	$P\bar{4}m2$		Mn_4H_3	27.6	3.23	0.002	$P2/m$
	V_3B_4	35.9,(38.2)[49]	3.7	0.006	$Immm$		Mn_6H_5	27.3	3.17	0.011	$A2/m$
	MnB_3	32.2	3.5	0.029	$P\bar{6}m2$		FeB_3	30.2	3.32	0	$P2_1/m$
	MnB_4†	**40.7**	3.65	0.009	$Pnnm$		FeB_4	35.7	3.06	0.021	$Immm$
Mn-B	MnB_4	38.2	3.56	0.1	$R\bar{3}m$	**Fe-B**	FeB_4‡	32	3.31	0.039	$R\bar{3}m$
		38.1,(**40.5**)[51],[37.4][52]	3.76	0	$P2_1/c$		FeB_4	**42.7**	3.31	0.063	$A2/m$
	MnB_5	32.7	3.38	0.097	$P\bar{6}m2$			28.6,(24.4)[61][**62**][59]	3.32	0.002	$Pnnm$
	MnB_{13}	**40.4**	2.9	0.181	Pm		Fe_2B_{11}	33.8	3.37	0.081	Pm

Ashby plot of hardness vs. toughness for predicted phases

- *J. Phys. Chem. Lett.*, *8* (4), pp 755–764 **(2017)**.
- *J. Phys. Chem. Lett.*, *9* (12), pp 3470–3477 **(2018)**.



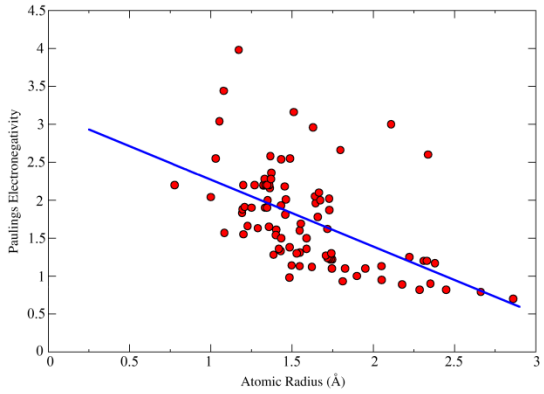


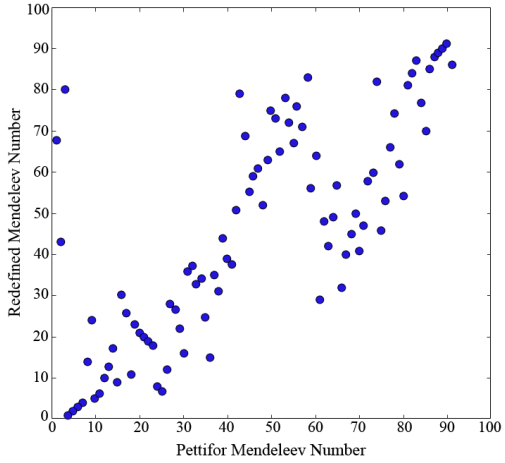
Conclusion

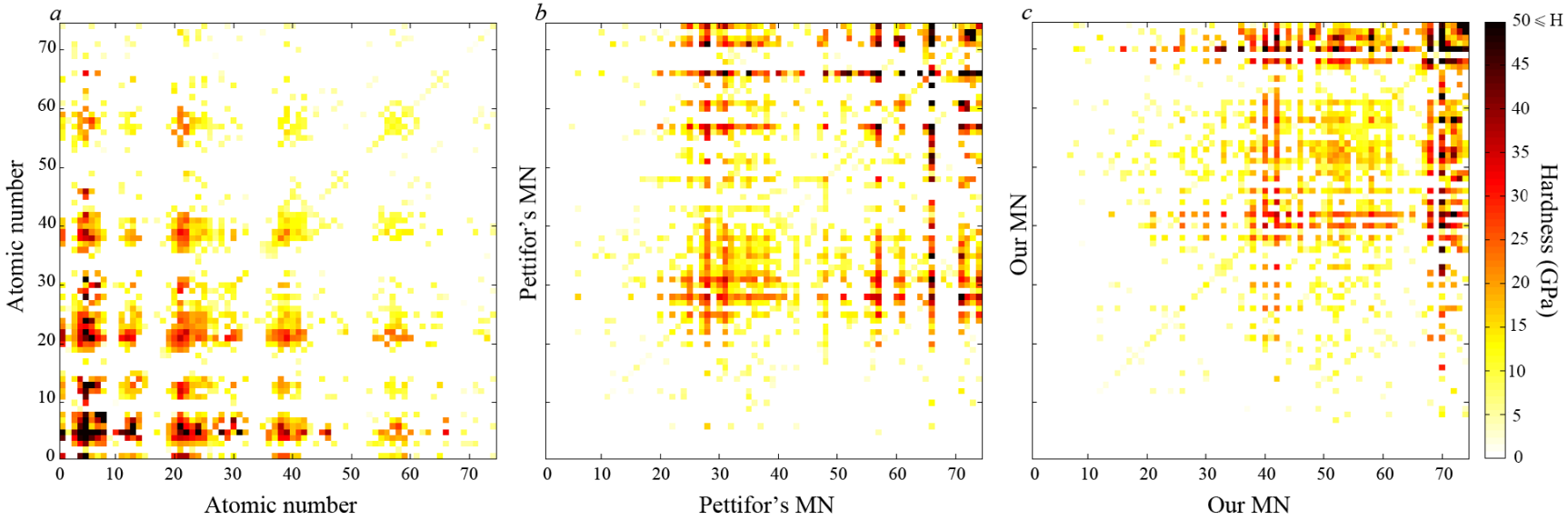
- Well defined chemical space can be obtained using the most significant properties of materials (electronegativity and atomic size) at any arbitrary pressure and binary systems are nearby in this space.
- Multi-objective Pareto technique makes it possible to search for materials optimal in more than one property.
- Combination of MendS, MO Pareto technique and well structed chemical space works efficiently in searching for materials optimal in multi target properties.
- MendS works at arbitrary pressure and for binary, ternary systems.

Thank you for your attention!

Our redefined MN, and it's comparison with the Pettifor's MN.

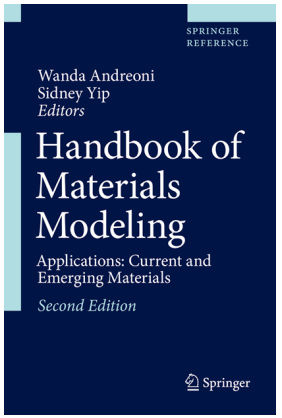






Grants

- Russian Science Foundation project **№ 17-73-20038**. “Computational design for new materials with optimal hardness and fracture toughness”, (2017).
- Russian Science Foundation project **№ 16-13-10459**. “New methods for search of materials with optimal properties”, (2016).



Publications

- **“Multi-objective optimization as a tool for materials design”,** Handbook of Materials Modeling. Volume 2 applications: Current and Emerging materials. *Springer Verlag*. *in Press*, **(2018)**.
- “**New candidates for the global minimum of medium-sized silicon clusters: A hybrid DFTB/DFT genetic algorithm applied to** Si_n**,** n **= 8 – 80**”, *J. Chem. Phys.*, 149, 074313 **(2018)**.
- “**Efficient technique for computational design of thermoelectric materials**”, *Comput. Phys. Commun.*, 222, 152-157 **(2018)**.
- “**Computational Search for Novel Hard Chromium-Based Materials**”, *J. Phys. Chem. Lett.*, *8* (4), pp 755–764 **(2017)**.
- **“Coevolutionary search for optimal materials in the space of all possible compounds”,** Under submission.
- **“Computational prediction of new magnetic materials”,** Under submission.
- **“Construction of a Coherent chemical space”,** Under preparation.