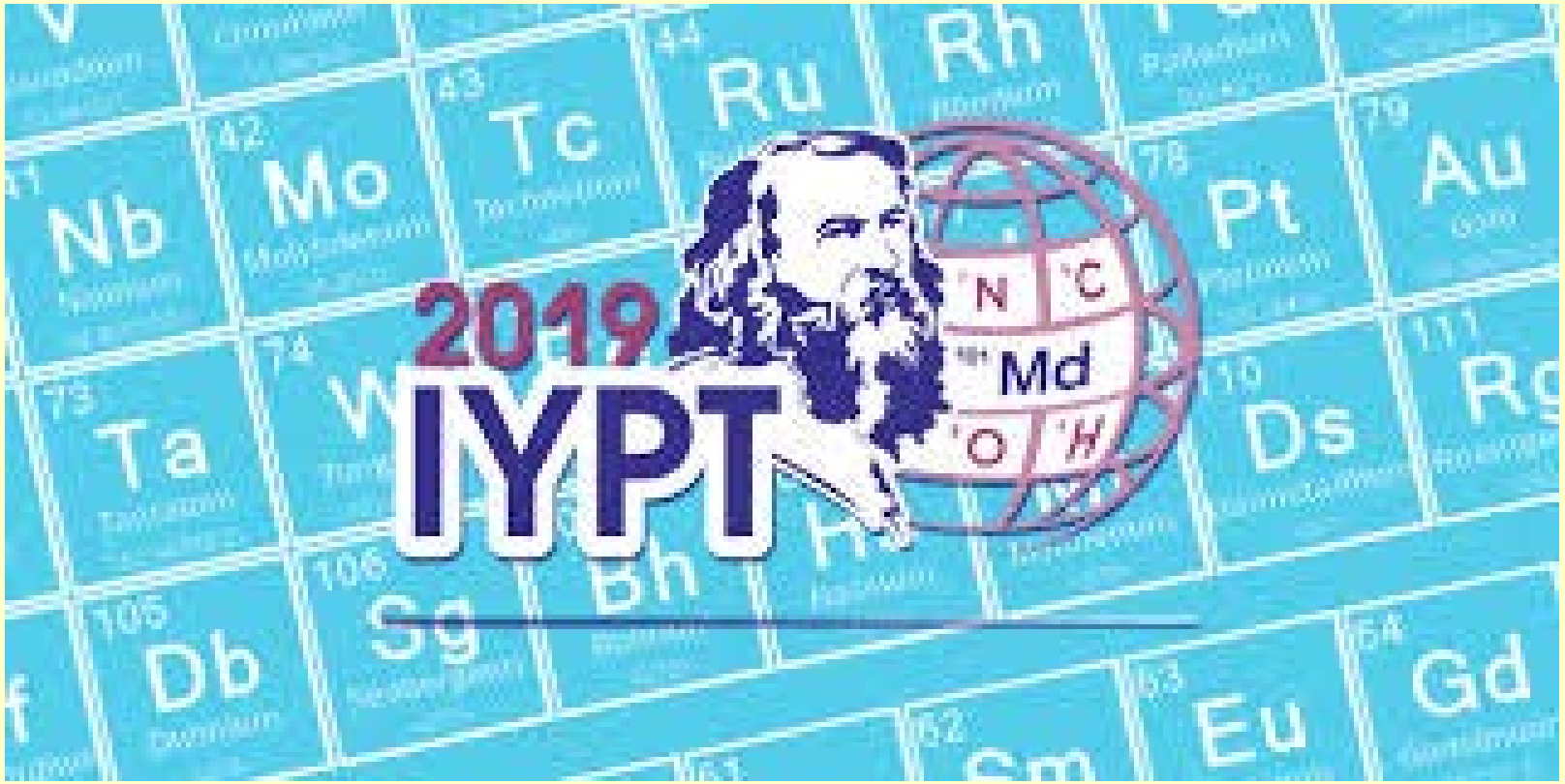
Computational Materials Discovery Using the USPEX Code

Artem R. Oganov

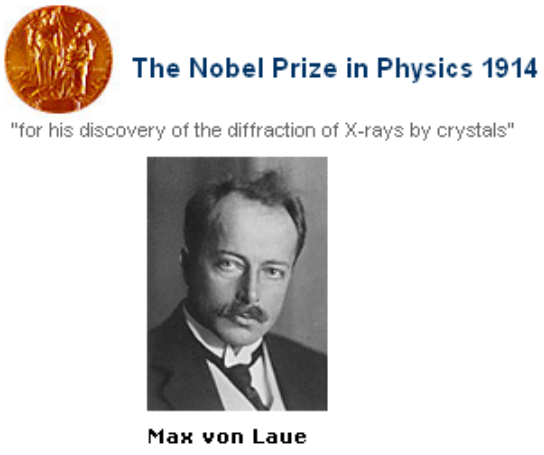
Skolkovo Institute of Science and Technology, Russia

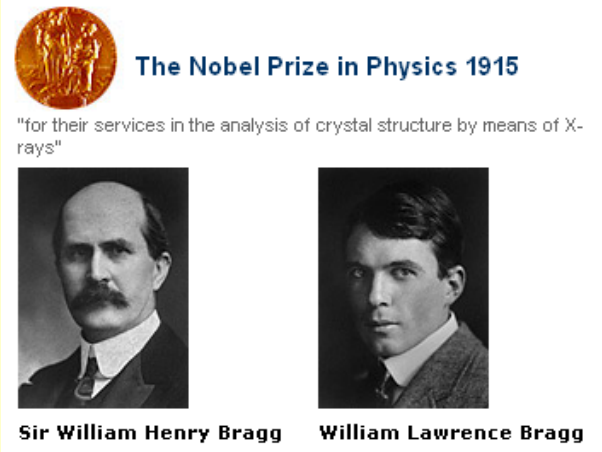
First Event of
International Year of Mendeleev's Periodic Table

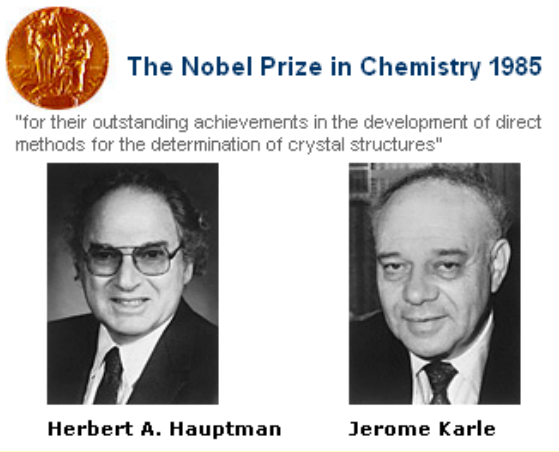


+ tradition of USPEX workshops
+ tradition of ICTP workshops

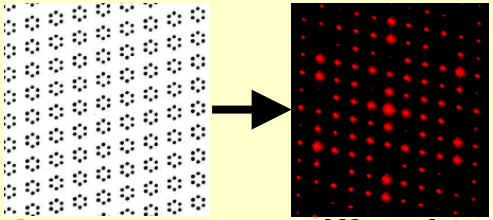
Crystal structure determines physical properties.
Crystal structure determination was a major breakthrough.





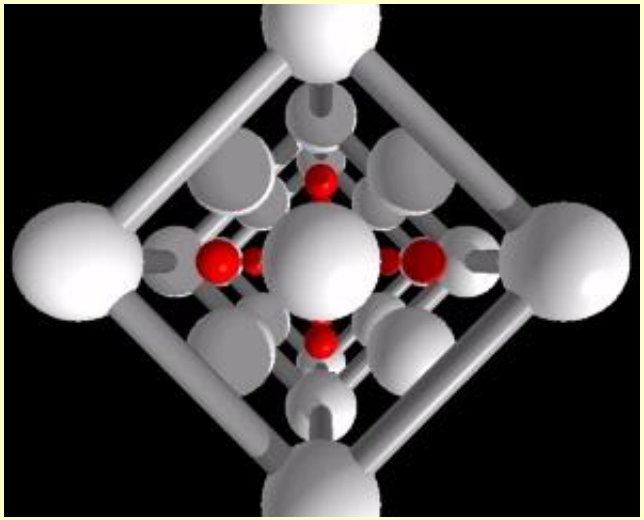


(from http://nobelprize.org)

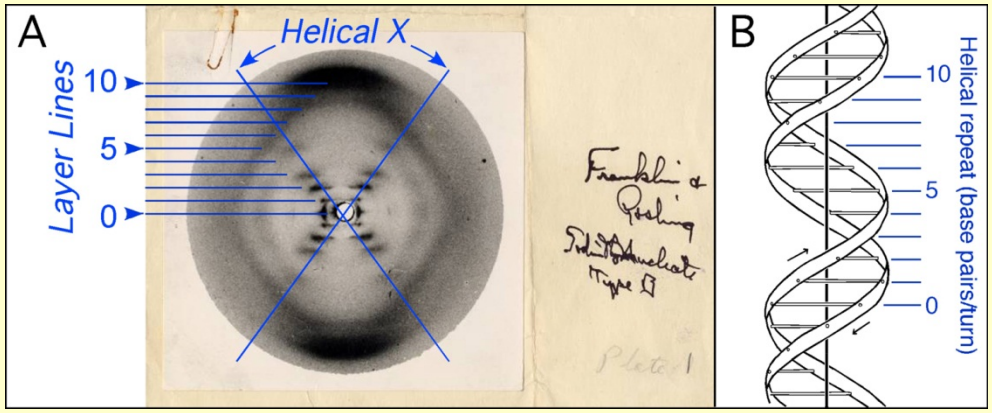


Zincblende ZnS.

One of the first solved structures (1912-1913)



X-ray diffraction: window into the structure of matter



Determination of the structure of DNA (Watson, Crick, 1953)

Some of Nobel prizes based on X-ray diffraction

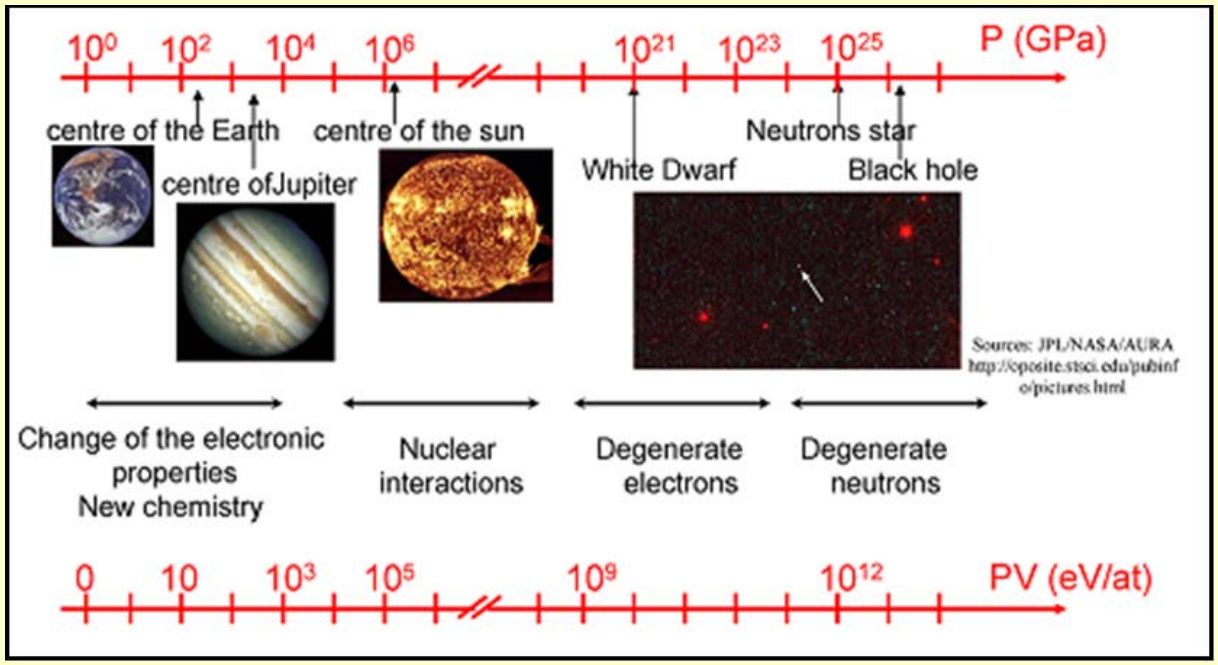
Nobel Prizes for X-ray Crystallography [edit]

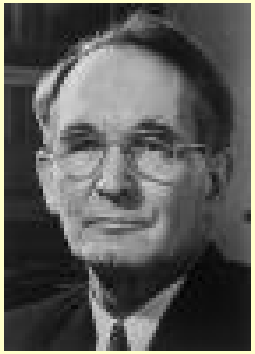
Year [hide]	Laureate	Prize	Rationale
1914	Max von Laue	Physics	"For his discovery of the diffraction of X-rays by crystals",[118] an important step in the development of X-ray spectroscopy.
1915	William Henry Bragg	Physics	"For their services in the analysis of crystal structure by means of X-rays",[119]
1915	William Lawrence Bragg	Physics	"For their services in the analysis of crystal structure by means of X-rays",[119]
1962	Max F. Perutz	Chemistry	"for their studies of the structures of globular proteins"[120]
1962	John C. Kendrew	Chemistry	"for their studies of the structures of globular proteins"[120]
1962	James Dewey Watson	Medicine	"For their discoveries concerning the molecular structure of nucleic acids and its significance for information transfer in living material"[121]
1962	Francis Harry Compton Crick	Medicine	"For their discoveries concerning the molecular structure of nucleic acids and its significance for information transfer in living material"[121]
1962	Maurice Hugh Frederick Wilkins	Medicine	"For their discoveries concerning the molecular structure of nucleic acids and its significance for information transfer in living material"[121]
1964	Dorothy Hodgkin	Chemistry	"For her determinations by X-ray techniques of the structures of important biochemical substances"[122]
1972	Stanford Moore	Chemistry	"For their contribution to the understanding of the connection between chemical structure and catalytic activity of the active centre of the ribonuclease molecule"[123]
1972	William H. Stein	Chemistry	"For their contribution to the understanding of the connection between chemical structure and catalytic activity of the active centre of the ribonuclease molecule"[123]
1976	William N. Lipscomb	Chemistry	"For his studies on the structure of boranes illuminating problems of chemical bonding"[124]
1985	Jerome Karle	Chemistry	"For their outstanding achievements in developing direct methods for the determination of crystal structures"[125]
1985	Herbert A. Hauptman	Chemistry	"For their outstanding achievements in developing direct methods for the determination of crystal structures"[125]
1988	Johann Deisenhofer	Chemistry	"For their determination of the three-dimensional structure of a photosynthetic reaction centre"[126]
1988	Hartmut Michel	Chemistry	"For their determination of the three-dimensional structure of a photosynthetic reaction centre"[126]
1988	Robert Huber	Chemistry	"For their determination of the three-dimensional structure of a photosynthetic reaction centre"[126]
1997	John E. Walker	Chemistry	"For their elucidation of the enzymatic mechanism underlying the synthesis of adenosine triphosphate (ATP)"[127]
2003	Roderick MacKinnon	Chemistry	"For discoveries concerning channels in cell membranes [...] for structural and mechanistic studies of ion channels"[128]
2003	Peter Agre	Chemistry	"For discoveries concerning channels in cell membranes [...] for the discovery of water channels"[128]
2006	Roger D. Kornberg	Chemistry	"For his studies of the molecular basis of eukaryotic transcription"[129]
2009	Ada E. Yonath	Chemistry	"For studies of the structure and function of the ribosome"[130]
2009	Thomas A. Steitz	Chemistry	"For studies of the structure and function of the ribosome"[130]
2009	Venkatraman Ramakrishnan	Chemistry	"For studies of the structure and function of the ribosome"[130]
2012	Brian Kobilka	Chemistry	"For studies of G-protein-coupled receptors"[131]

We work at:

(1) high pressures – because of fundamental importance;

(2) zero pressure – for practical applications.





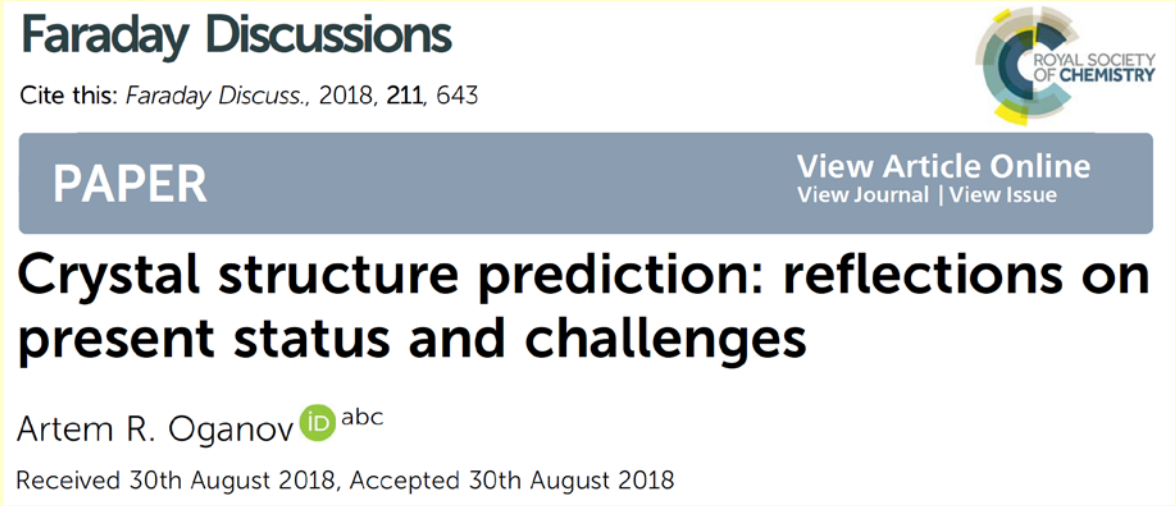
P.W. Bridgman

1946 Nobel laureate (Physics)

Scale: 100 GPa = 1 Mbar =

200x

Are crystal structures predictable?



Faraday Discussions

Cite this: *Faraday Discuss.*, 2018, **211**, 643

ROYAL SOCIETY OF CHEMISTRY

PAPER

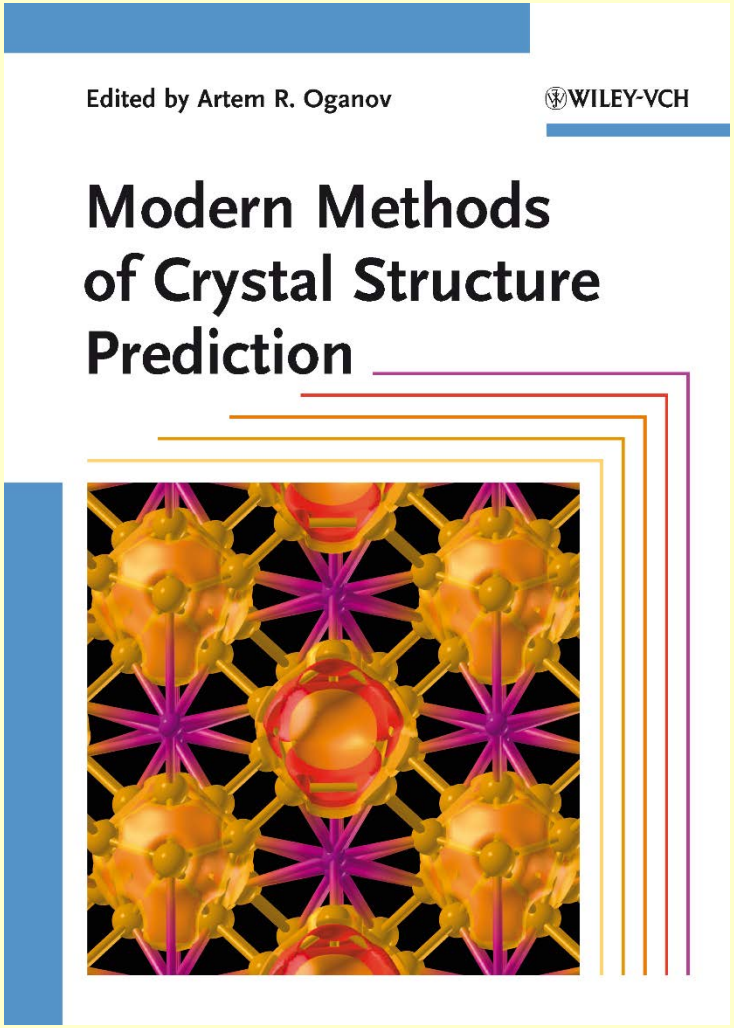
View Article Online
View Journal | View Issue

Crystal structure prediction: reflections on present status and challenges

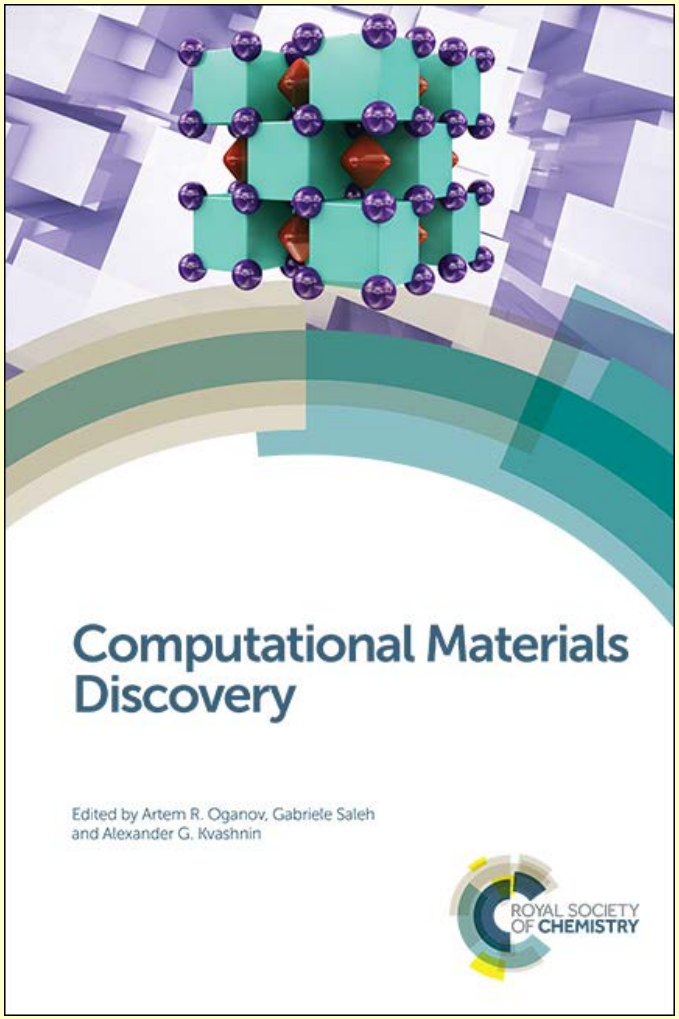
Artem R. Oganov [abc]

Received 30th August 2018, Accepted 30th August 2018

Useful books



2010



2018

Acc. Chem. Res. **1994,** *27,* 309−314

Are Crystal Structures Predictable?

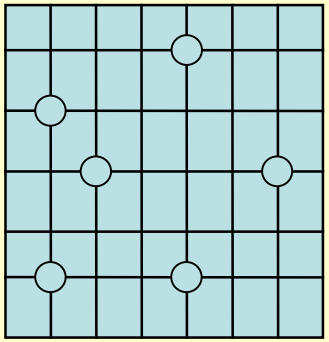
ANGELO GAVEZZOTTI*

"No": by just writing down this concise statement, in what would be the first one-word paper in the chemical literature, one could safely summarize the present state of affairs

Need to find GLOBAL energy minimum.

Trying all structures is impossible:

$$C = \frac{1}{(V/\delta^3)} \frac{(V/\delta^3)!}{[(V/\delta^3) - N]!N!}$$



N_{atoms}	Variants	CPU time
1	**1**	**1 sec.**
10	**10^{11}**	**10^{3} yrs.**
20	**10^{25}**	**10^{17} yrs.**
30	**10^{39}**	**10^{31} yrs.**

RESEARCH NEWS

Crystal structure prediction – evolutionary or revolutionary crystallography?

S. L. Chaplot and K. R. Rao CURRENT SCIENCE, VOL. 91, NO. 11, 10 DECEMBER 2006

Overview of USPEX (Oganov & Glass, *J.Chem.Phys.* 2006)

The USPEX project
(Universal Structure Prediction: Evolutionary Xtallography)

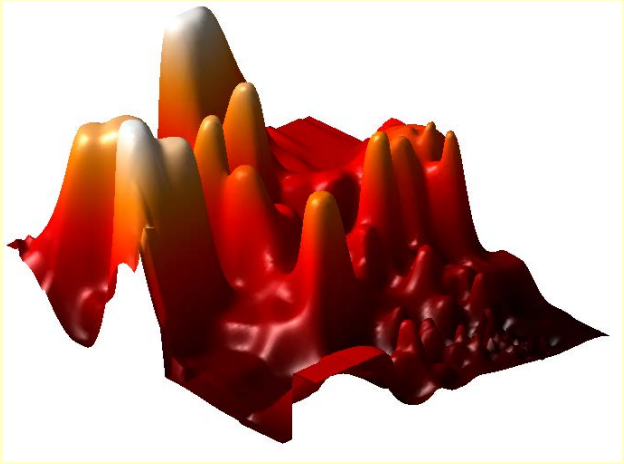
http://uspex-team.org

[Oganov A.R., Glass C.W., *J.Chem.Phys.* 124, 244704 (2006)]

- **Combination of evolutionary algorithm and quantum-mechanical calculations.**
- **>4500 users.**

- **Solves «intractable» problem of structure prediction**
  -3D, 2D, 1D, 0D –systems,
  -prediction of phase transition mechanisms.

- **Interfaced with: VASP, Quantum Espresso, CASTEP, FHI-aims, ABINIT, Siesta, Gaussian, ORCA, ATK, DFTB, MOPAC, GULP, LAMMPS, Tinker, DMACRYS**



Energy landscape of Au_8Pd

W. Kohn

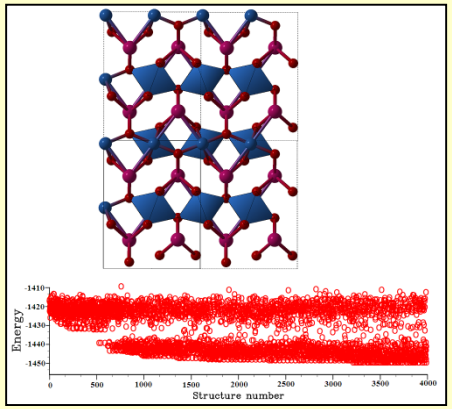
J. P. Perdew

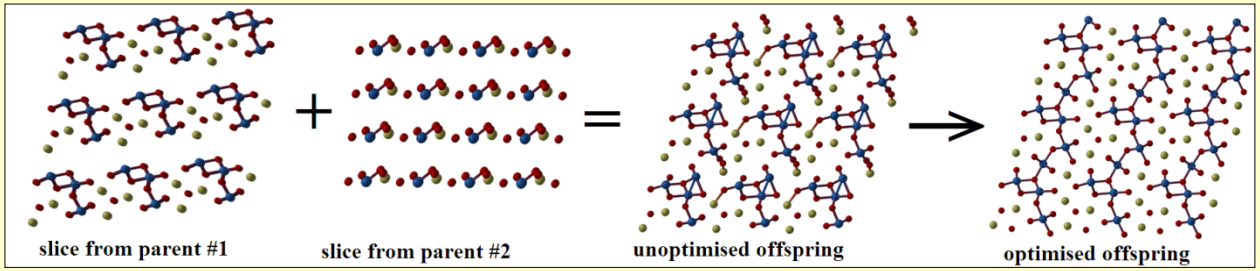
$$(-\frac{\nabla^2}{2}+v_{e-n}[\rho(\mathbf{r})]+v_H[\rho(\mathbf{r})]+v_{xc}[\rho(\mathbf{r})])\phi_i(\mathbf{r})=\varepsilon_i\phi_i(\mathbf{r})$$

$$E_{GGA,\mathrm{xc}}=\int \mathrm{d}\mathbf{r}\, F_{\mathrm{xc}}(\rho,\frac{|\nabla\rho|}{2k_{\mathrm{F}}\rho(\mathbf{r})})\rho(\mathbf{r})e_{\mathrm{x}}[\rho(\mathbf{r})]$$

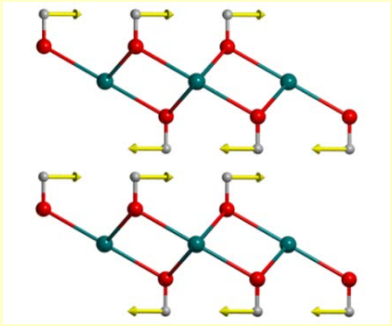
USPEX
(Universal Structure Predictor: Evolutionary Xtallography)

- (Random) initial population: fully random or using randomly selected space groups
- Evaluate structures by relaxed (free) energy
- Select lowest-energy structures as parents for new generation
- Standard variation operators:

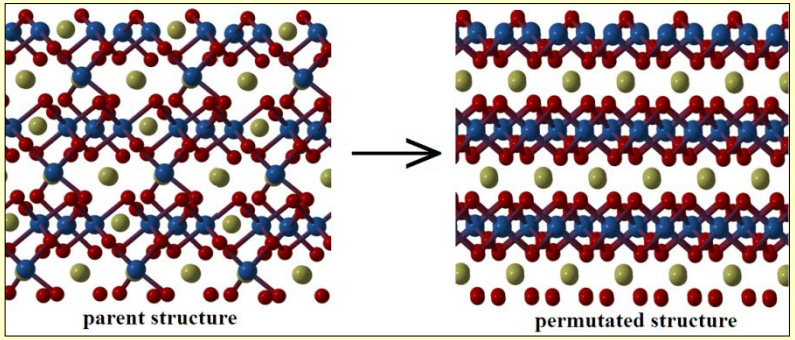




(1) Heredity (crossover)



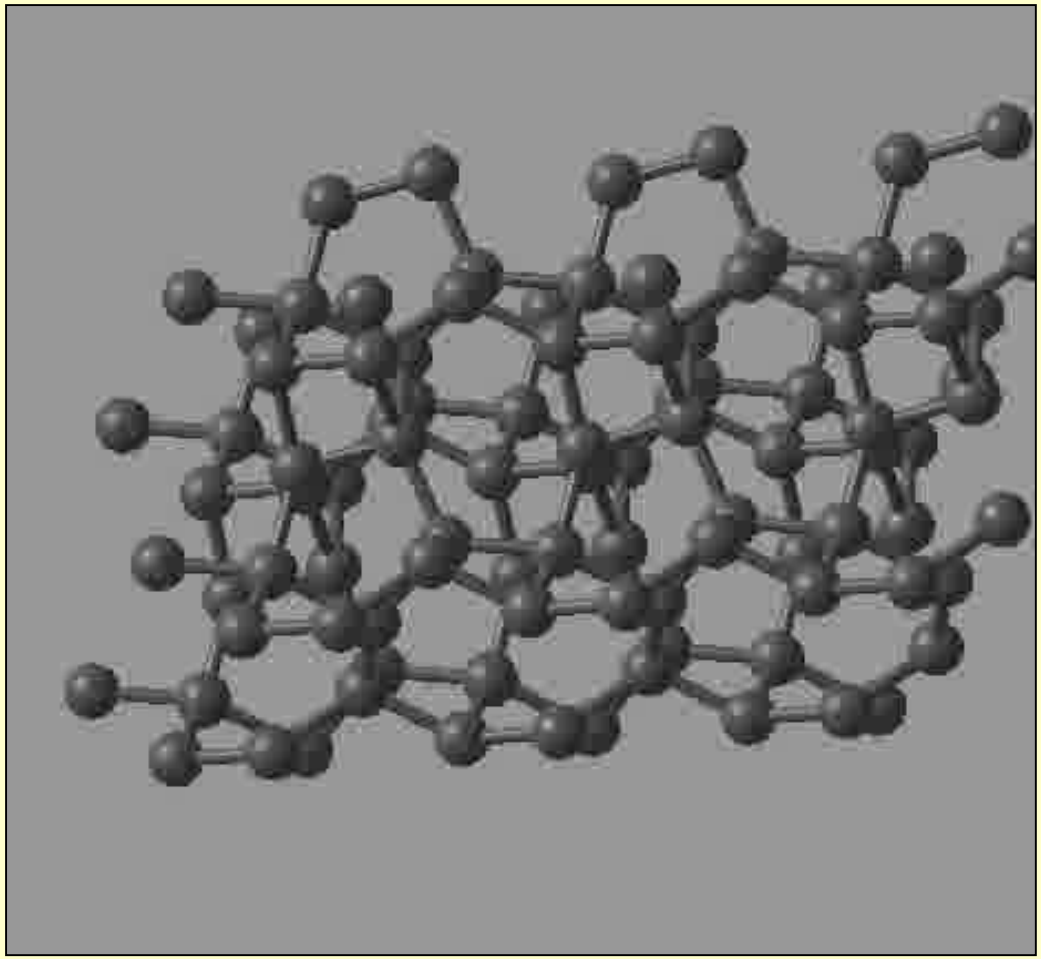
(2) Soft-mode mutation



(3) Permutation

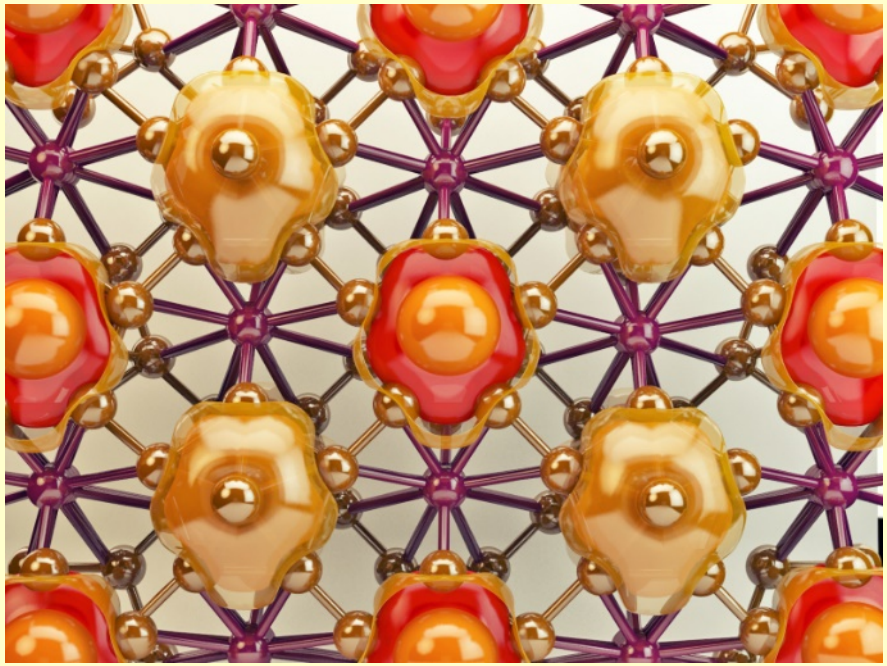
+(4) Transmutation, +(5) Rotational mutation, +(6) Lattice mutation, +...

Without any empirical information, method reliably predicts materials

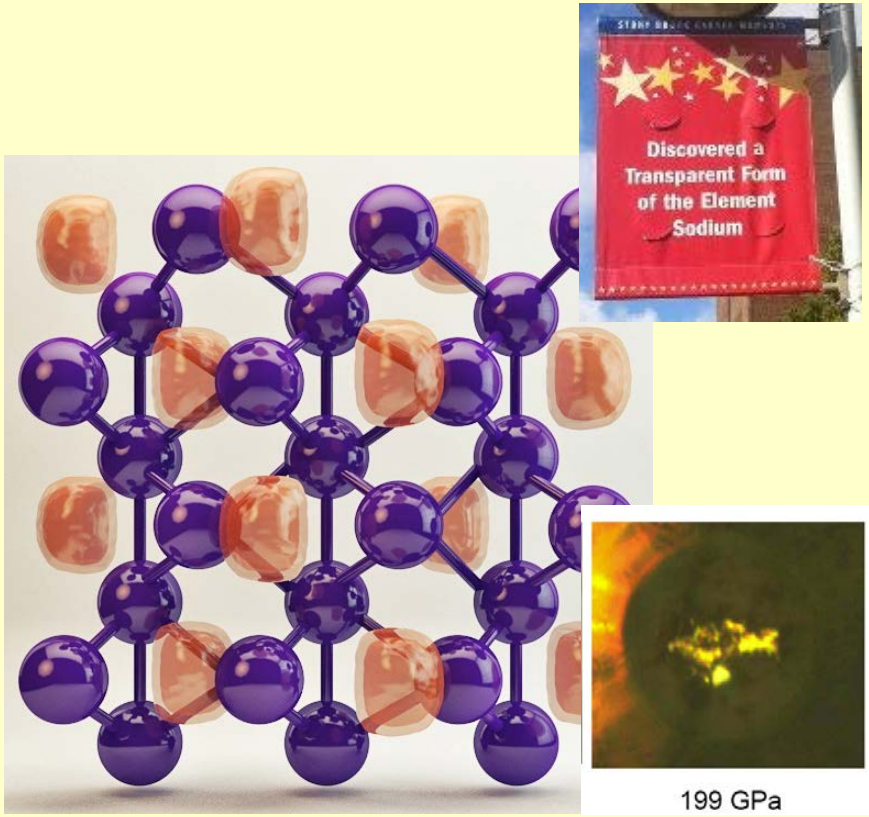


Carbon at 100 GPa – diamond structure is stable

Predicting new crystal structures without empirical information



New superhard structure of boron
(Oganov et al., *Nature*, 2009)

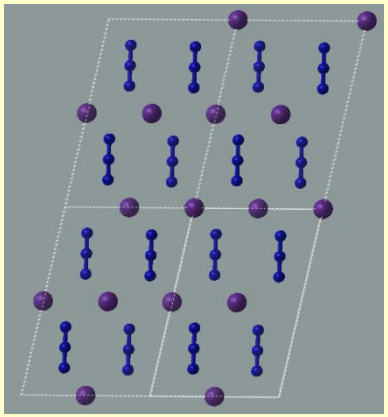


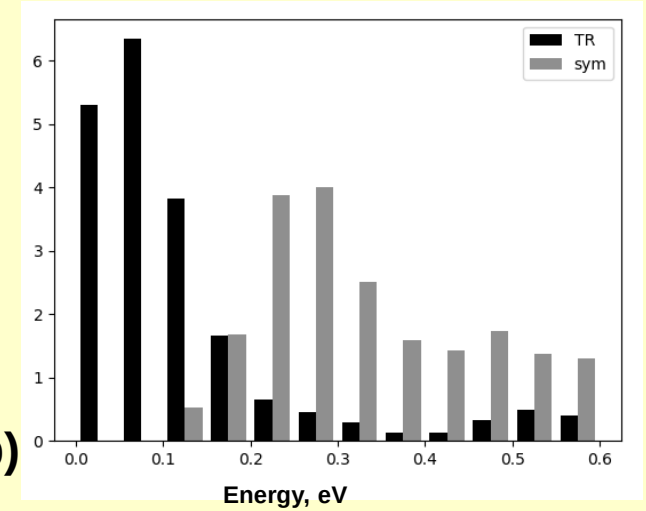
High-pressure transparent
allotrope of sodium
(Ma, Eremets, Oganov, *Nature*, 2009)

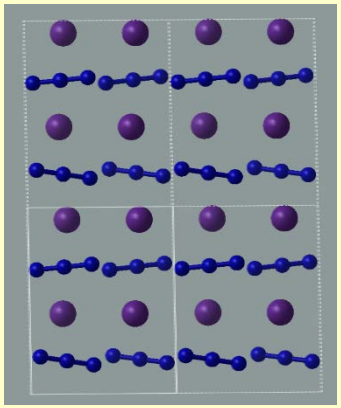
Topological structure generator: major development

[Bushlanov, Blatov, Oganov, *Comp. Phys. Comm.*, 2019]

Speedup ~3 times

(a) 

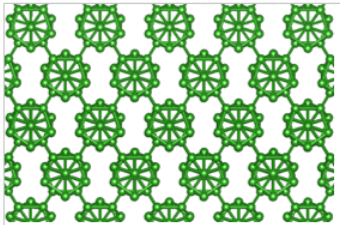
(b) 

(c) 

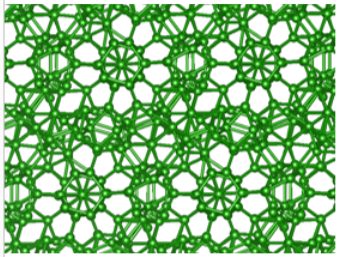
Example of KN_3: (a) topological structure, (c) random symmetric structure, (c) energy distribution of topological (TR) and random symmetric structures

Statistics (100 runs) of USPEX performance on $MgAl_2O_4$ (28 atoms/cell) at 100 GPa

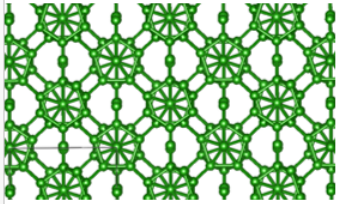
	Old USPEX	On-the-fly adaptation	Adaptation +topology
<#structures>	1307	1069	368
Success rate	100%	100%	100%



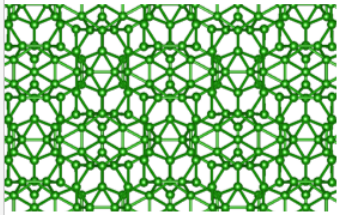
α-boron
E^{DFT} = –6.706 eV/atom
Atoms: 12,
Space group: *R*-3*m*,
Core-hours: 10^3 AL-MTP vs. $3 \cdot 10^3$ DFT
$|E^{DFT} - E^{MTP}|$ = 28.6 meV/atom



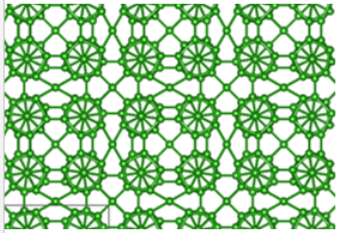
β-boron approximant
E^{DFT} = –6.704 eV/atom,
Atoms: 106,
Space group: *P*1,
Core-hours: $7 \cdot 10^3$ AL-MTP vs. $6.6 \cdot 10^7$ DFT
$|E^{DFT} - E^{MTP}|$ = 10.1 meV/atom



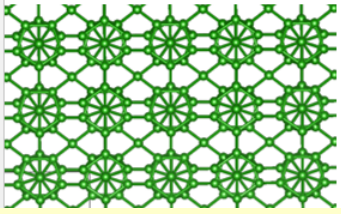
γ-boron
E^{DFT} = –6.678 eV/atom
Atoms: 28,
Space group: *Pnnm*,
Core-hours: $2 \cdot 10^3$ AL-MTP vs. $2.5 \cdot 10^4$ DFT
$|E^{DFT} - E^{MTP}|$ = 58.1 meV/atom



E^{DFT} = –6.667 eV/atom,
Atoms: 54,
Space group: *Im*-3,
Core-hours: $3 \cdot 10^3$ AL-MTP vs. $3.5 \cdot 10^5$ DFT
$|E^{DFT} - E^{MTP}|$ = 7.3 meV/atom



E^{DFT} = –6.667 eV/atom,
Atoms: 52,
Space group: *P*-42*m*,
Core-hours: $3 \cdot 10^3$ AL-MTP vs. $3.2 \cdot 10^5$ DFT
$|E^{DFT} - E^{MTP}|$ = 37.3 meV/atom



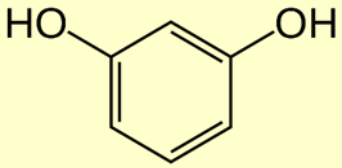
E^{DFT} = –6.665 eV/atom,
Atoms: 26,
Space group: *Cccm*,
Core-hours: $2 \cdot 10^3$ AL-MTP vs. $2.1 \cdot 10^4$ DFT
$|E^{DFT} - E^{MTP}|$ = 13.6 meV/atom

Handling complexity with machine learning: boron allotropes

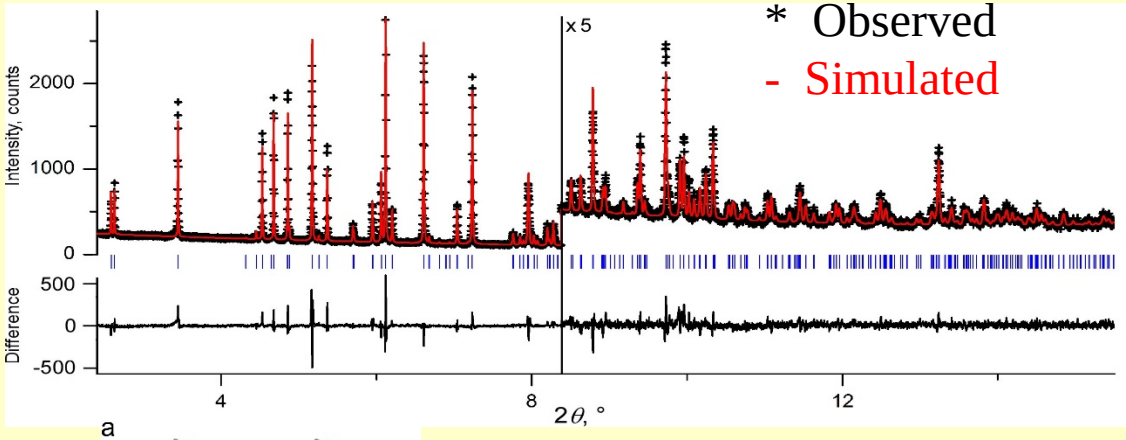
(E.Podryabinkin, E. Tikhonov, A. Shapeev, A.R. Oganov, arXiv:1802.07605)

- **ML potential with active learning (Shapeev, 2018). 800 parameters.**
- **MAE = 11 meV/atom.**
- **Reproduced α-, β-, γ-, T52 phases of boron.**
- **Predicted low-energy metastable cubic cI54 phase.**
- **Speedup by >100 times.**

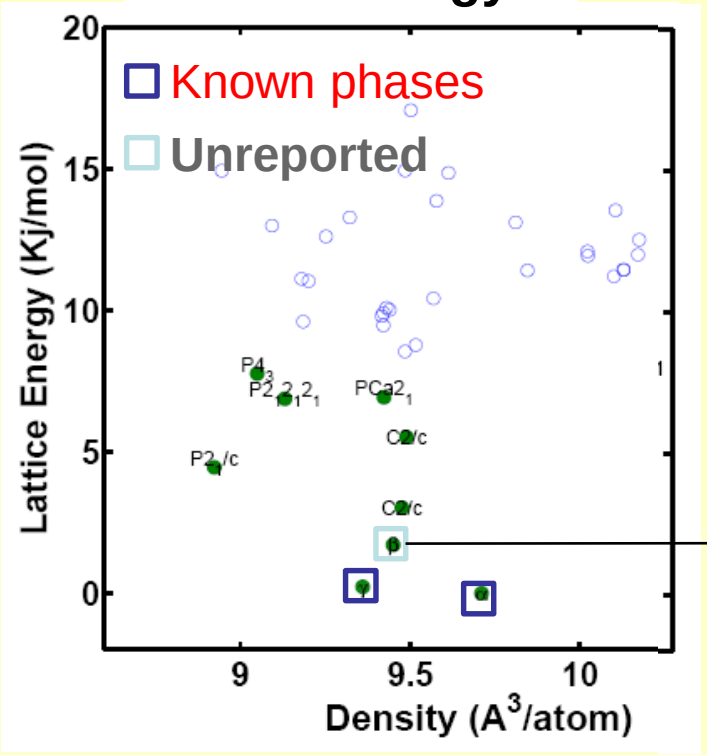
USPEX can handle molecular crystals: solved γ-resorcinol

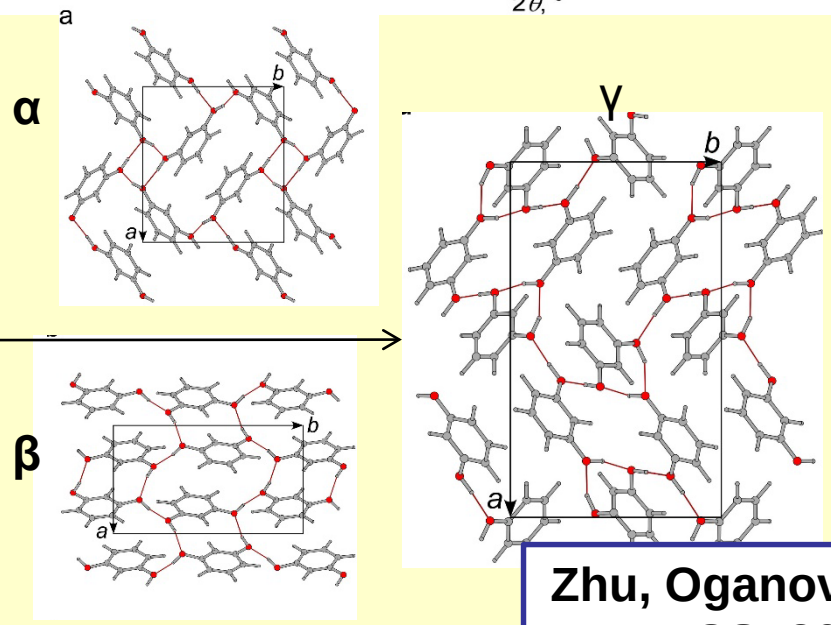


Powder XRD comparison



Lattice Energy Plot





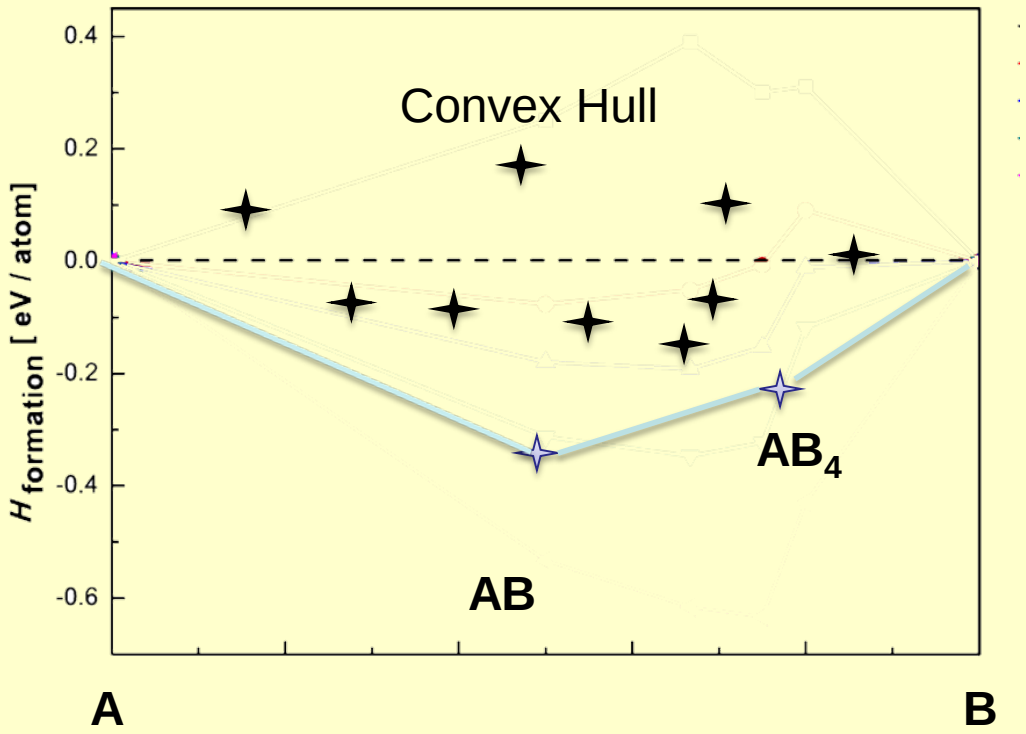
Zhu, Oganov, et al, JACS, 2016

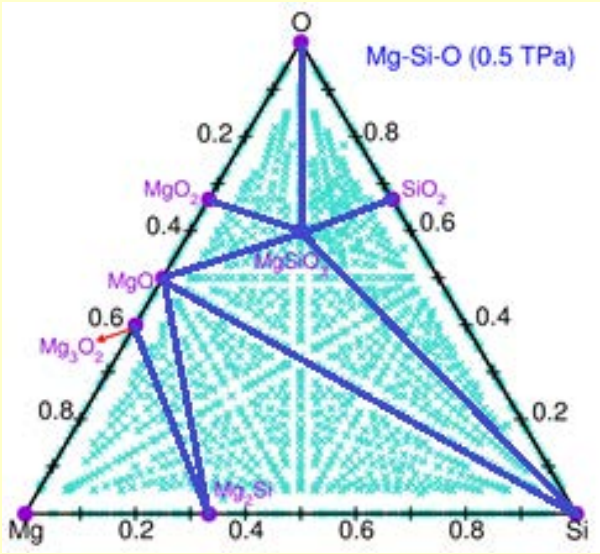
Prediction of stable structure for a given chemical composition is possible.

Now, let’s predict the chemical composition!

USPEX can automatically find all stable compounds in a multicomponent system.

Thermodynamic stability in variable-composition systems





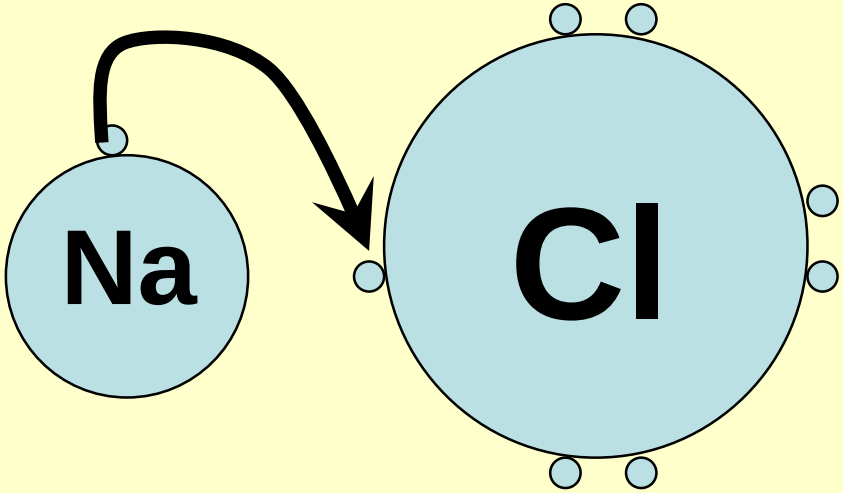
3-component convex hull: Mg-Si-O system at 500 GPa (Niu & Oganov, *Sci. Rep.* 2015)

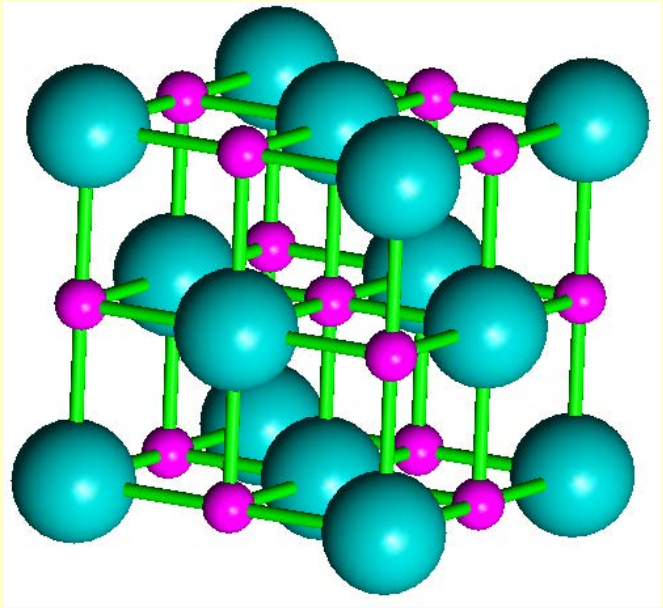
Stable structure must be below all the possible decomposition lines !!

Na-Cl

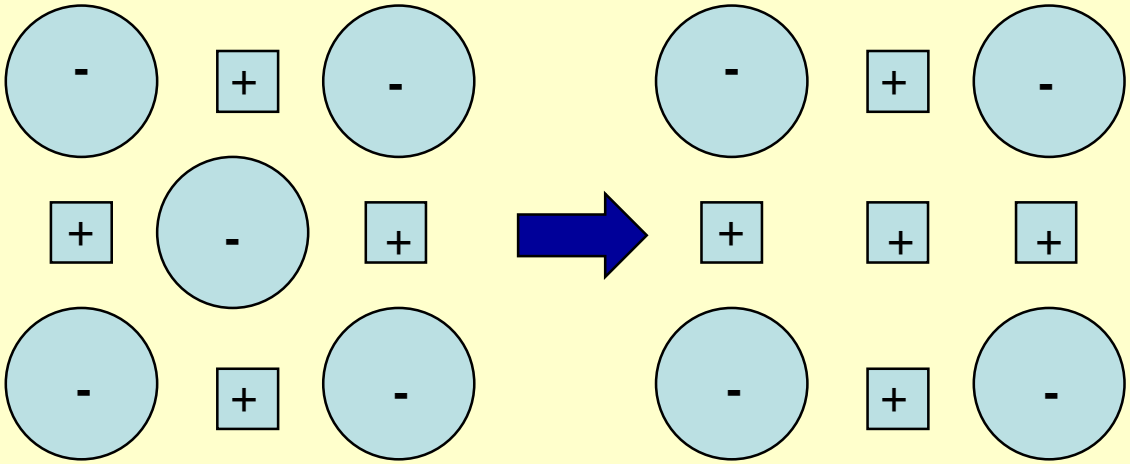
A question from my childhood

- Na and Cl: large electronegativity difference ⇒ ionic bonding, Na^+ and Cl^-. Charge balance requires NaCl stoichiometry.





Structure of NaCl

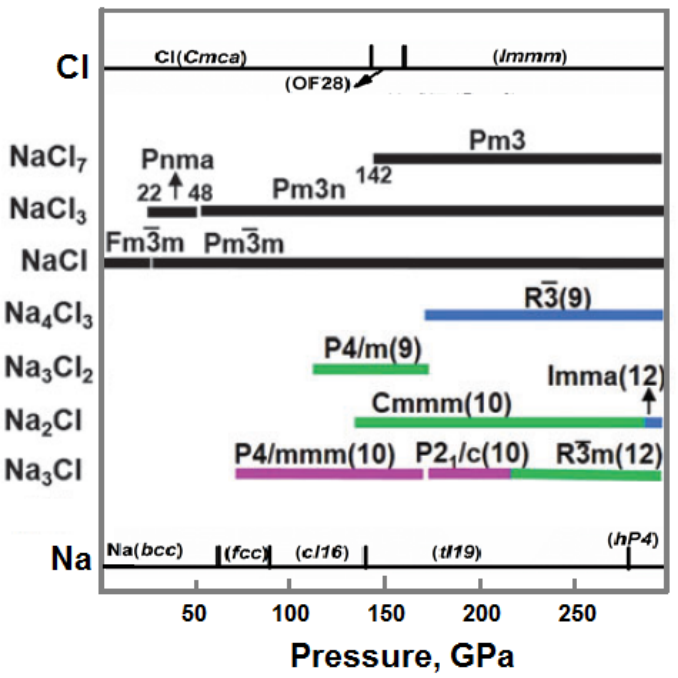


What would happen if you give the computer a "forbidden" compound, e.g. Na_2Cl?

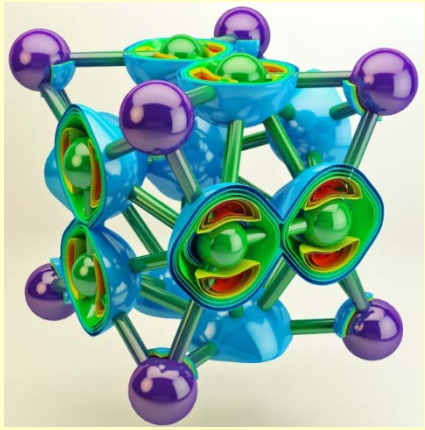
Na-Cl

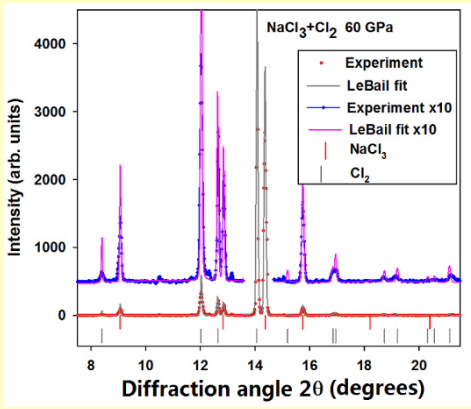
Predictive power of modern methods:

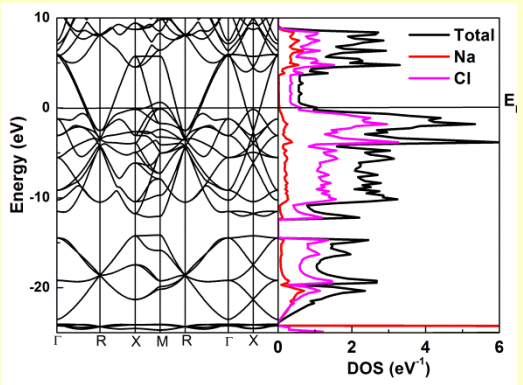
Na_3Cl, Na_2Cl, Na_3Cl_2, NaCl, $NaCl_3$, $NaCl_7$ are stable under pressure [Zhang, Oganov, et al. *Science*, 2013].

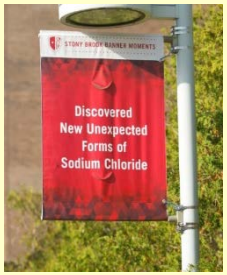


Stability fields of sodium chlorides









$NaCl_3$: atomic and electronic structure, and experimental XRD pattern

Chemical anomalies:

-Divalent Cl in Na_2Cl!
-Coexistence of metallic and ionic blocks in Na_3Cl!
-Positively charged Cl in $NaCl_7$!

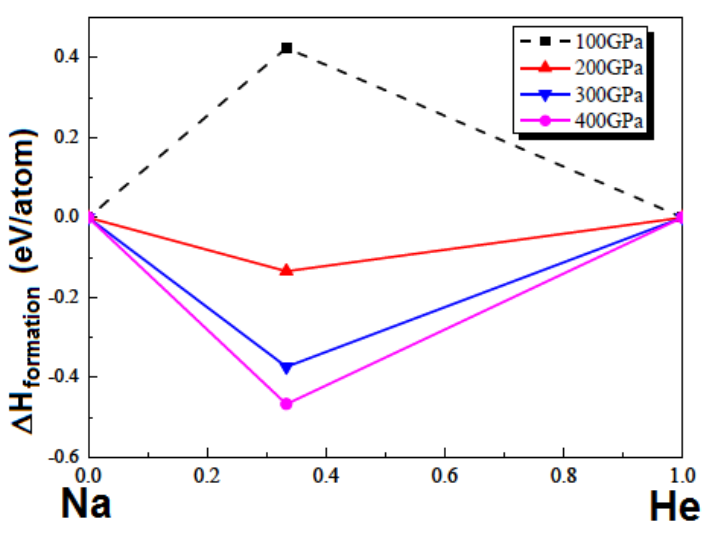
[Zhang, Oganov, et al., *Science* (2013)]
[Saleh & Oganov, *PCCP* (2015)]

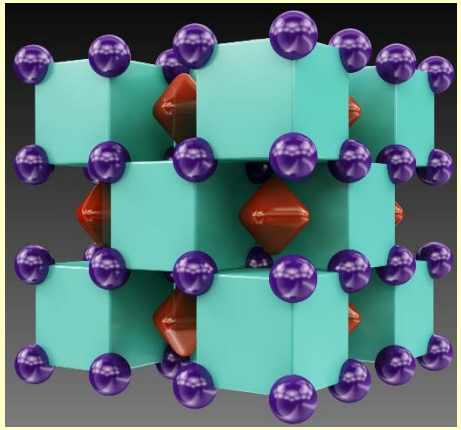
Helium chemistry? Yes!

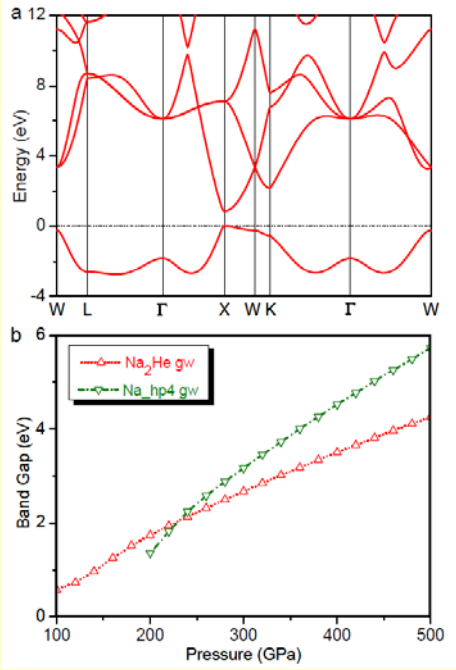
[Dong, Oganov, Goncharov, *Nature Chemistry* 2017]

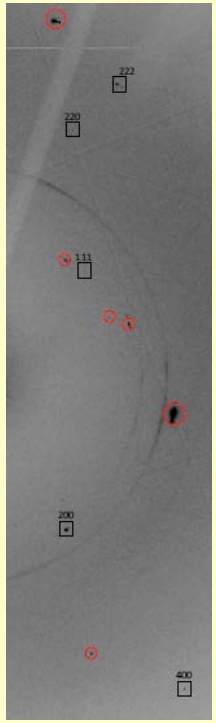
Na-He

- **Helium is the 2nd most abundant element in the Universe (24 wt.%).**
- **No stable compounds are known at normal conditions. Under pressure: van der Waals compound $NeHe_2$ (Loubeyre et al., 1993).**





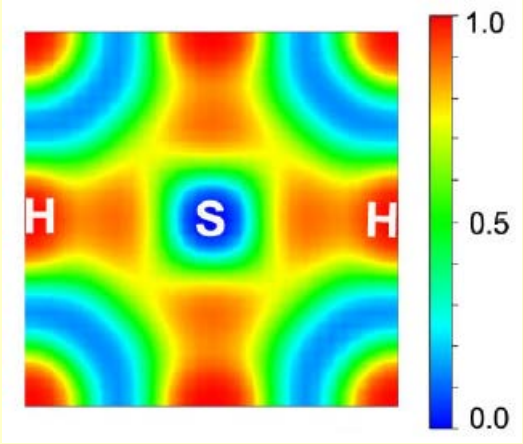




1. **Na_2He is stable at >113 GPa, at least up to 1000 GPa.**
2. **New stable helium compounds: Na_2HeO (Dong & Oganov, 2017); CaF_2He, MgF_2He (Liu, 2018).**

Highest-Tc superconductivity: new record, 203 Kelvin (Duan et al., *Sci. Rep.* 4, 6968 (2014))

H-S



OPEN

SUBJECT AREAS:
THEORY AND COMPUTATION
CONDENSED MATTER PHYSICS

Received
7 July 2014

Accepted
29 September 2014

Published
10 November 2014

Correspondence and requests for materials should be addressed to T.C. (cuitian@jlu.edu.cn)

Pressure-induced metallization of dense $(H_2S)_2H_2$ with high-T_c superconductivity

Defang Duan[1,2], Yunxian Liu[1], Fubo Tian[1], Da Li[1], Xiaoli Huang[1], Zhonglong Zhao[1], Hongyu Yu[1], Bingbing Liu[1], Wenjing Tian[2] & Tian Cui[1]

[1]State Key Laboratory of Superhard Materials, College of physics, Jilin University, Changchun, 130012, P. R. China, [2]State Key Laboratory of Supramolecular Structure and Materials, Jilin University, Changchun, 130012, P. R. China.

The high pressure structures, metallization, and superconductivity of recently synthesized H_3-containing compounds $(H_2S)_2H_2$ are elucidated by *ab initio* calculations. The ordered crystal structure with *P*1 symmetry is determined, supported by the good agreement between theoretical and experimental X-ray diffraction data, equation of states, and Raman spectra. The *Cccm* structure is favorable with partial hydrogen bond symmetrization above 37 GPa. Upon further compression, H_2 molecules disappear and two intriguing metallic structures with *R*3*m* and *Im*-3*m* symmetries are reconstructive above 111 and 180 GPa, respectively. The predicted metallization pressure is 111 GPa, which is approximately one-third of the currently suggested metallization pressure of bulk molecular hydrogen. Application of the Allen-Dynes-modified McMillan equation for the *Im*-3*m* structure yields high T_c values of 191 K to 204 K at 200 GPa, which is among the highest values reported for H_2-rich van der Waals compounds and MH_3 type hydride thus far.

Conventional superconductivity at 203 kelvin at high pressures in the sulfur hydride system

A. P. Drozdov, M. I. Eremets, I. A. Troyan, V. Ksenofontov & S. I. Shylin

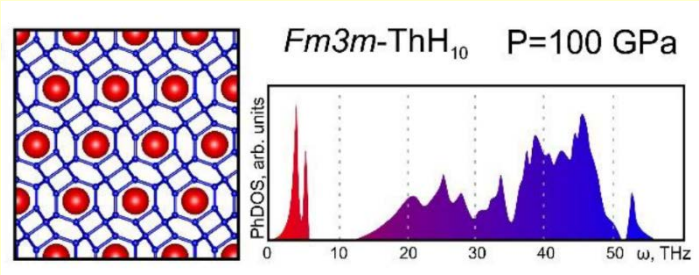
Nature (2015) | doi:10.1038/nature14964
Received 25 June 2015 | Accepted 22 July 2015 | Published online 17 August 2015

A superconductor is a material that can conduct electricity without resistance below a superconducting transition temperature, T_c. The highest T_c that has been achieved to date is in the copper oxide system[1]: 133 kelvin at ambient pressure[2] and 164 kelvin at high pressures[3]. As the nature of superconductivity in these materials is still not fully understood (they are not conventional superconductors), the prospects for achieving still higher transition temperatures by this route are not clear. In contrast, the Bardeen–Cooper–Schrieffer theory of conventional superconductivity gives a guide for achieving high T_c with no theoretical upper bound—all that is needed is a favourable combination of high-frequency phonons, strong electron–phonon coupling, and a high density of states[4]. These conditions can in principle be fulfilled for metallic hydrogen and covalent compounds dominated by hydrogen[5, 6], as hydrogen atoms provide the necessary high-frequency phonon modes as well as the strong electron–phonon coupling. Numerous calculations support this idea and have predicted transition temperatures in the range 50–235 kelvin for many hydrides[7], but only a moderate T_c of 17 kelvin has been observed experimentally[8]. Here we investigate sulfur hydride[9], where a T_c of 80 kelvin has been predicted[10]. We find that this system transforms to a metal at a pressure of approximately 90 gigapascals. On cooling, we see signatures of superconductivity: a sharp drop of the resistivity to zero and a decrease of the transition temperature with magnetic field, with magnetic susceptibility measurements confirming a T_c of 203 kelvin. Moreover, a pronounced isotope shift of T_c in sulfur deuteride is suggestive of an electron–phonon mechanism of superconductivity that is consistent with the Bardeen–Cooper–Schrieffer scenario. We argue that the phase responsible for high-T_c superconductivity in this system is likely to be H_3S, formed from H_2S by decomposition under pressure. These findings raise hope for the prospects for achieving room-temperature superconductivity in other hydrogen-based materials.

- **Old record Tc=135 K (Schilling, 1993) is broken: theorists (T. Cui, 2014) predicted new compound H_3S with Tc~200 K.**
- **Confirmed by A. Drozdov et al. (*Nature* 525, 73 (2015)).**

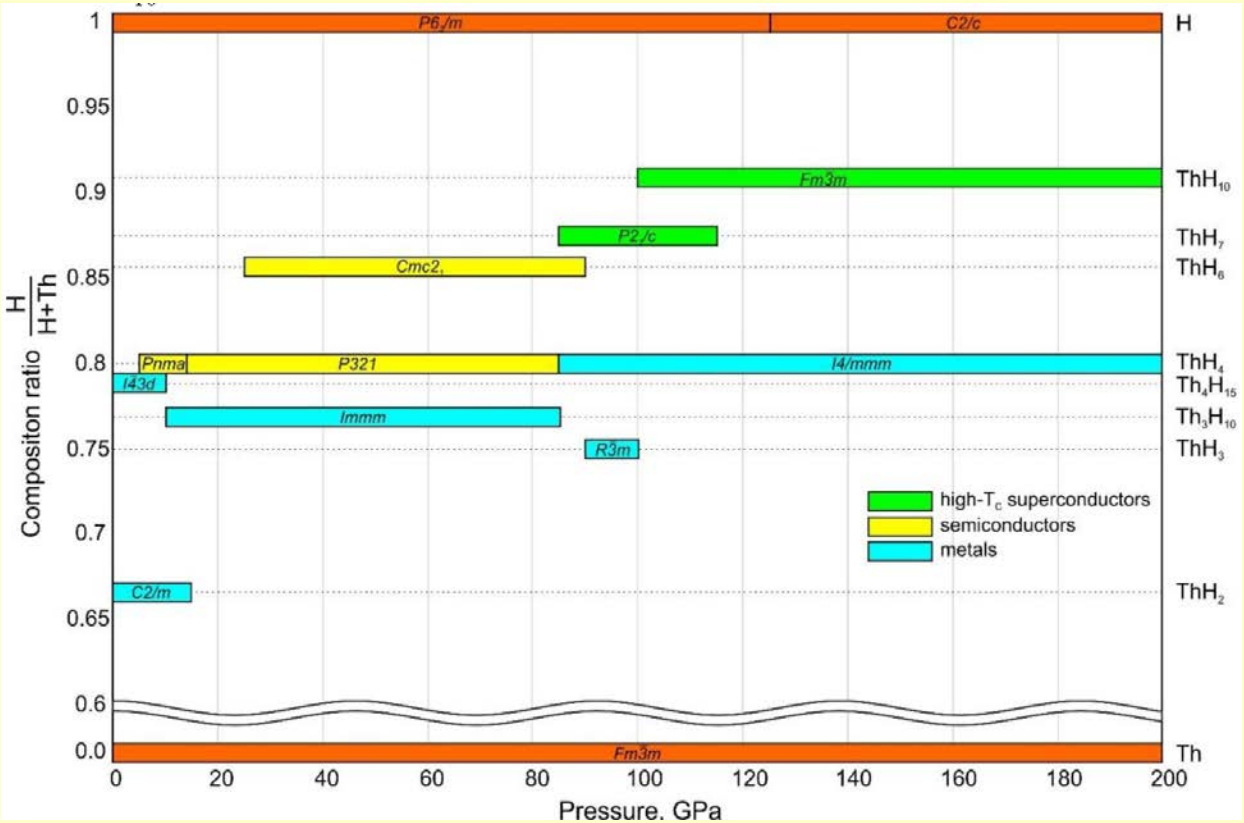
ThH_{10}: new unique superconductor

Th-H



Tc at 100 GPa: 241 K

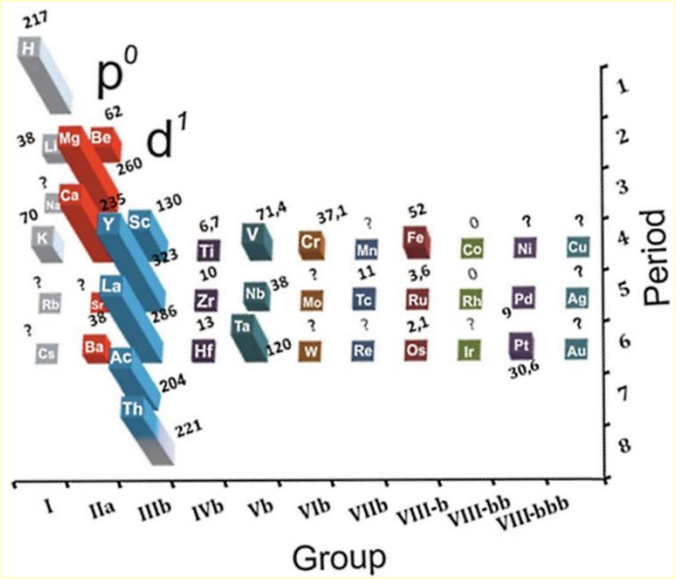
For LaH_{10} and YH_{10} even higher Tc predicted, but at much higher pressures (Liu et al., 2017).



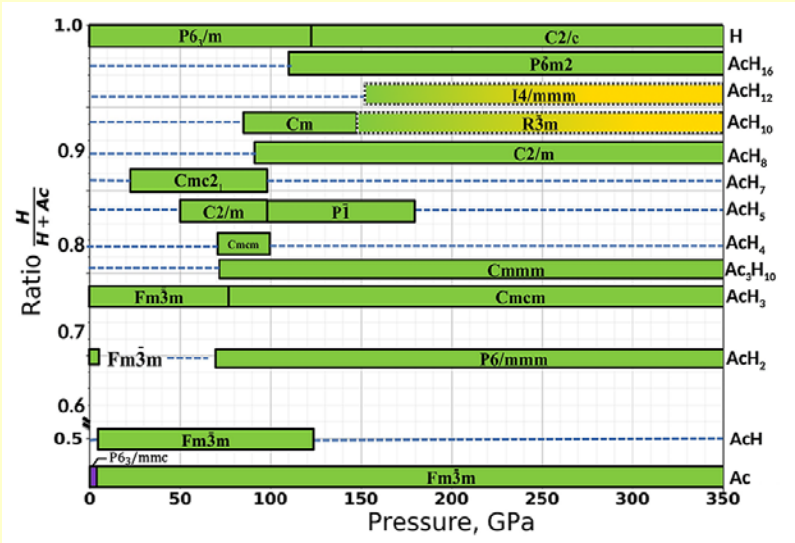
Th-H phase diagram

[Kvashnin & Oganov, ACS Appl. Mater. Interf. 2018]

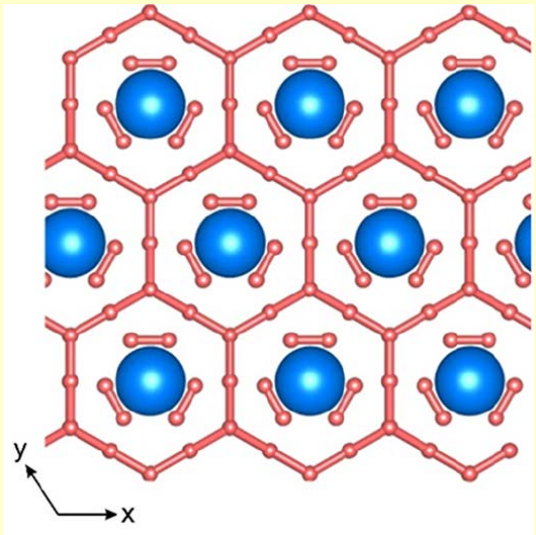
Metals forming high-Tc superconducting hydrides form a “II-III belt” in Mendeleev’s Table: test on Ac-H [Semenok & Oganov, JPCL, 2018]



Distribution of Tc for metal hydrides



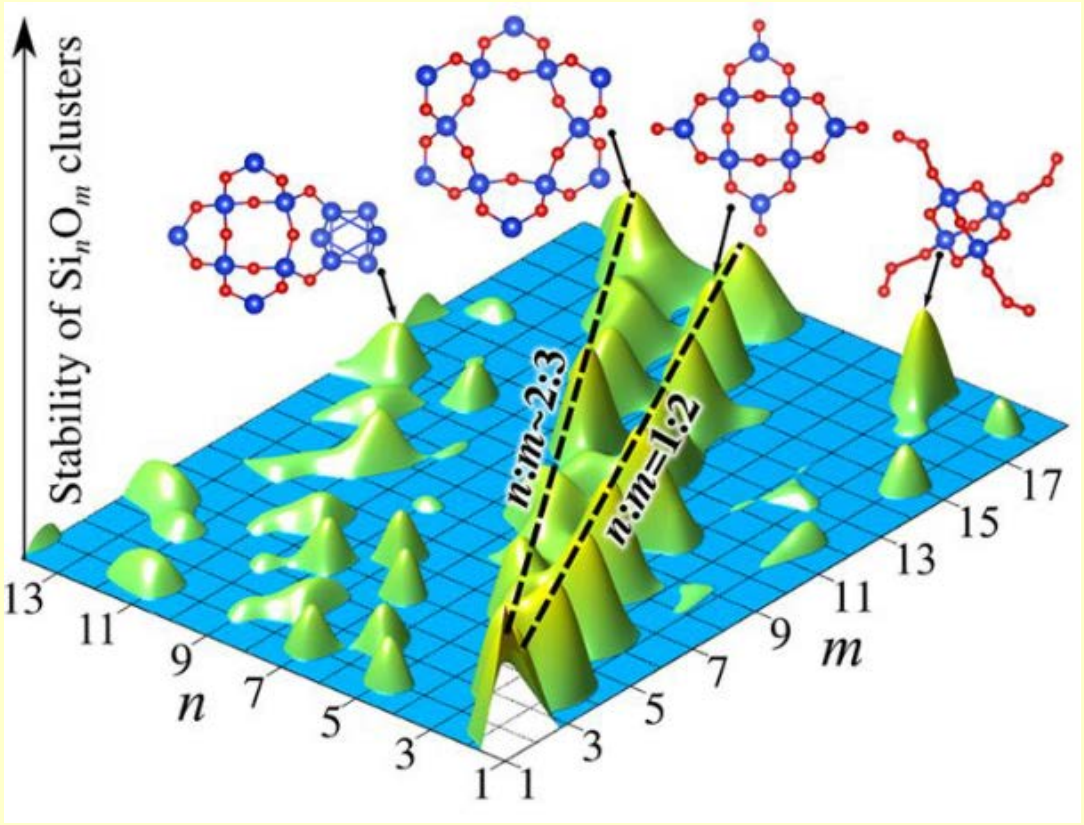
Ac-H phase diagram



AcH_{16}. Tc ~ 230 K at 150 GPa

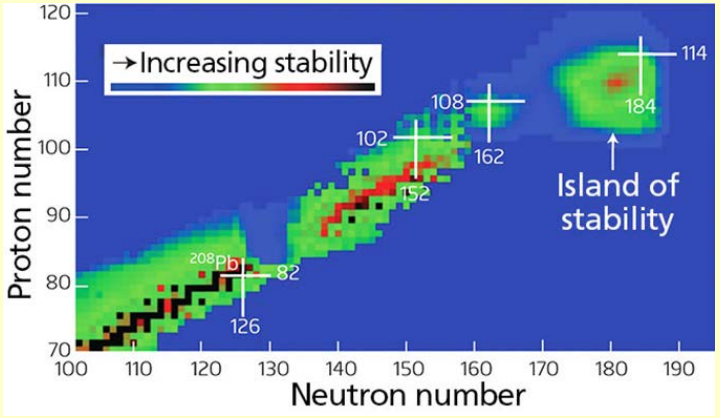
Map of stability of Si-O clusters
[Lepeshkin & Oganov, *J. Phys. Chem. Lett.* 2019]

Si-O

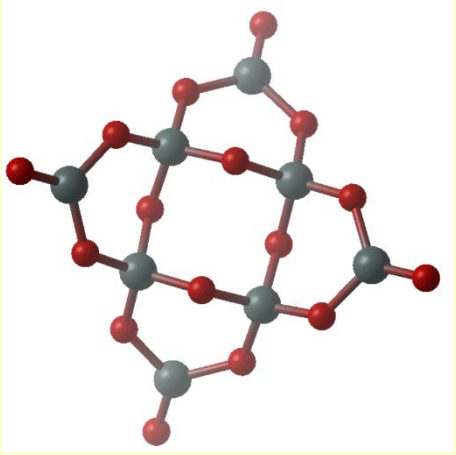


Ridges of stability: SiO_2, Si_2O_3
Islands of stability: e.g., Si_4O_{18}

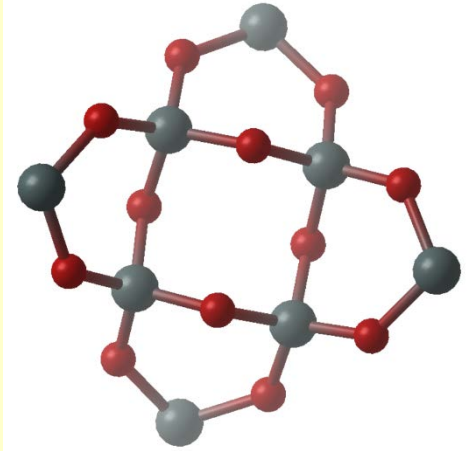
Analogy with magic atomic nuclei



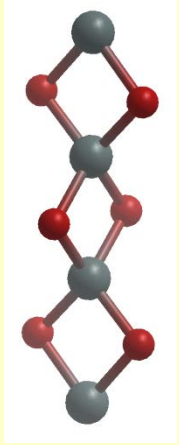
Si-O



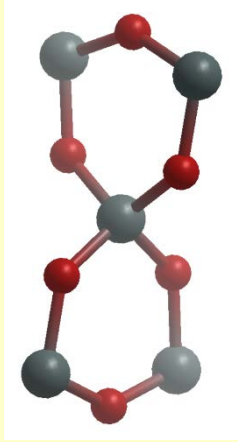
Si_8O_{16}



Si_8O_{12}

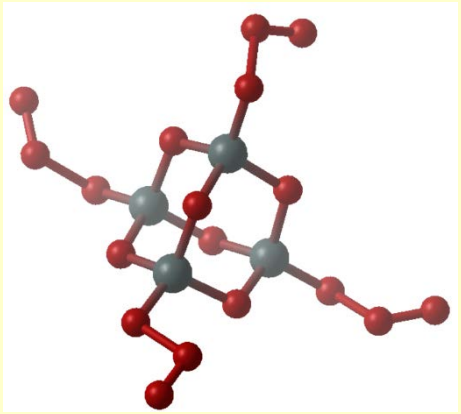


Si_4O_6

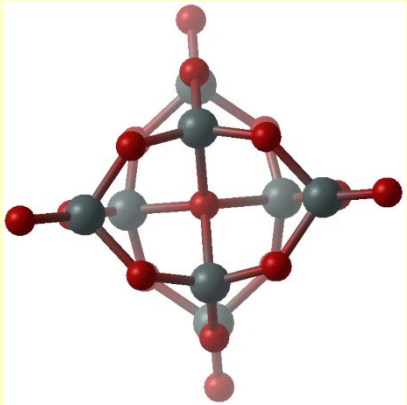


Si_5O_6

Magic clusters. Non-magnetic

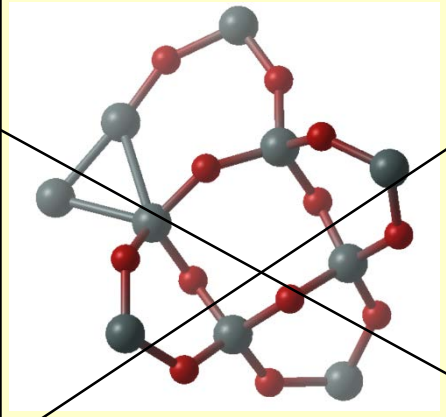


Si_4O_{18}



Si_8O_{17}

Magic magnetic(!) clusters. Excess of O

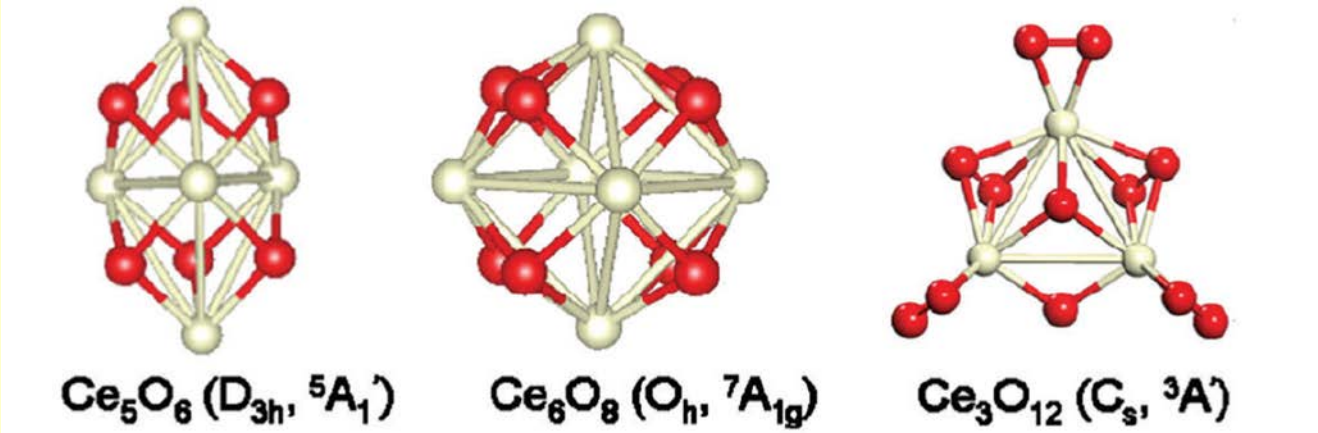


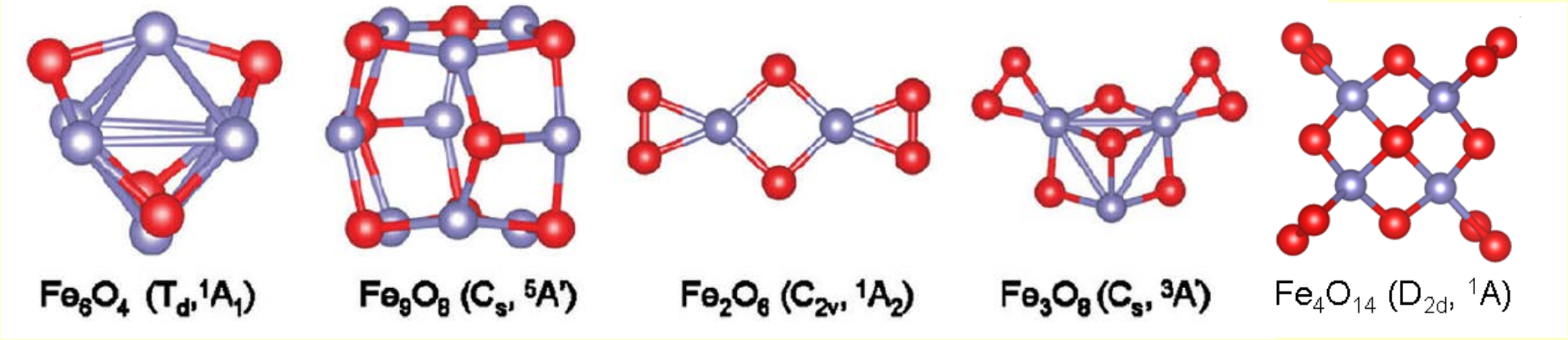
$Si_{10}O_{12}$

Unstable

Unusual compositions of transition metal oxide clusters

[Yu & Oganov, *Phys. Chem. Chem. Phys.*, 2018]





Do crystals grow from such particles?

Prediction of stable structure AND composition is possible.

Now, let’s predict materials with the best properties.

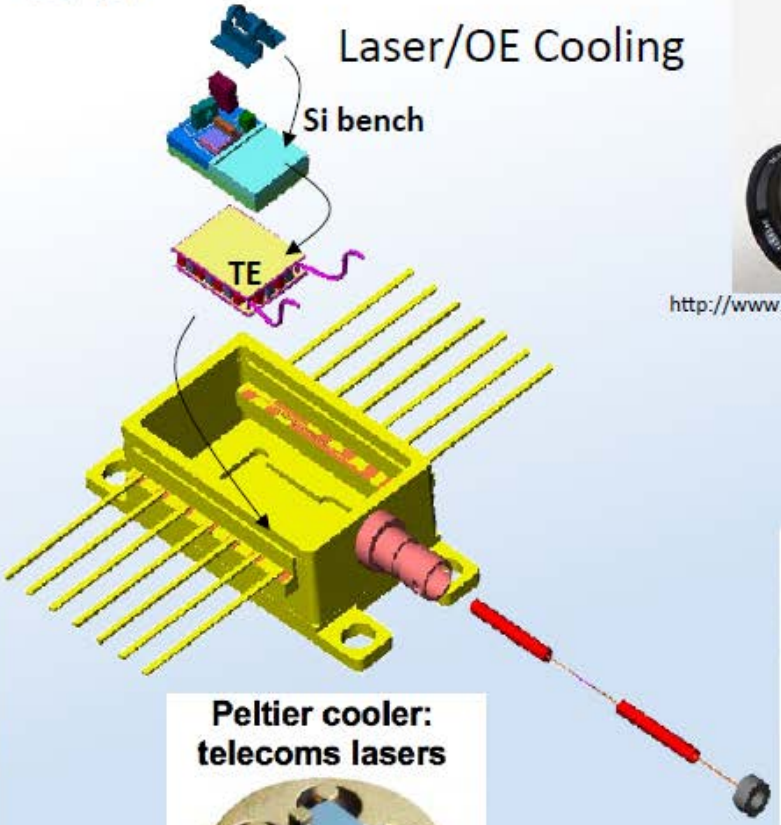
Towards materials design: example of thermoelectrics

Applications

Water/Beer/Wine Cooler

www.kingsbottle.com

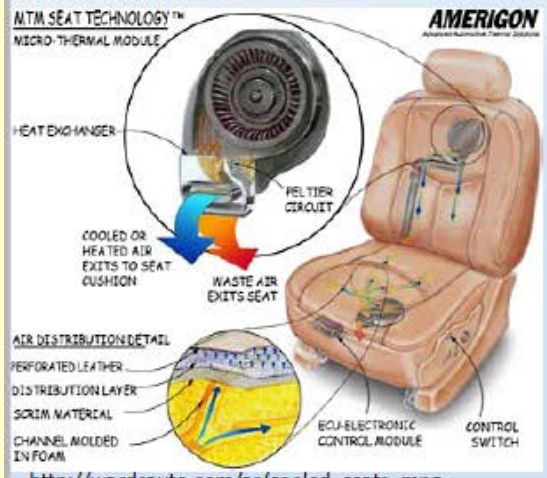
Laser/OE Cooling



Cryogenic IR Night Vision

http://www.x20.org/products/pv400-used-night-vision-scope/

Cooled Car Seat

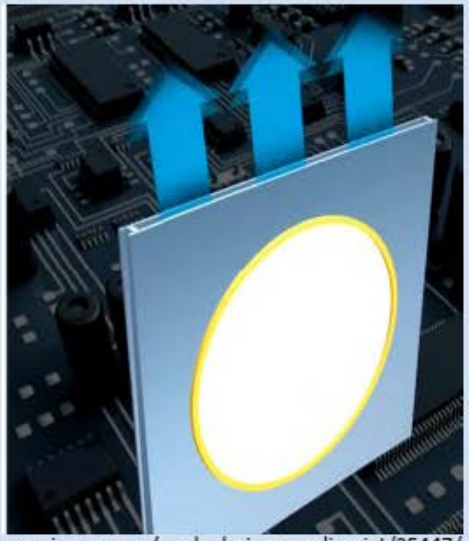


http://wardsauto.com/ar/cooled_seats_mpg

Peltier cooler: telecoms lasers

Copyright Micropelt

Electronic Cooling

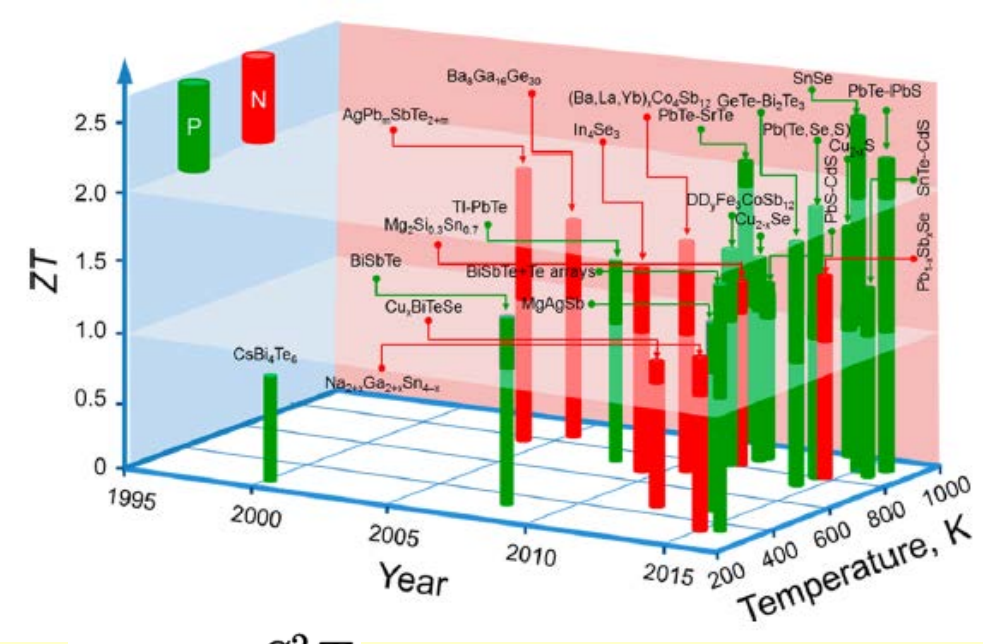


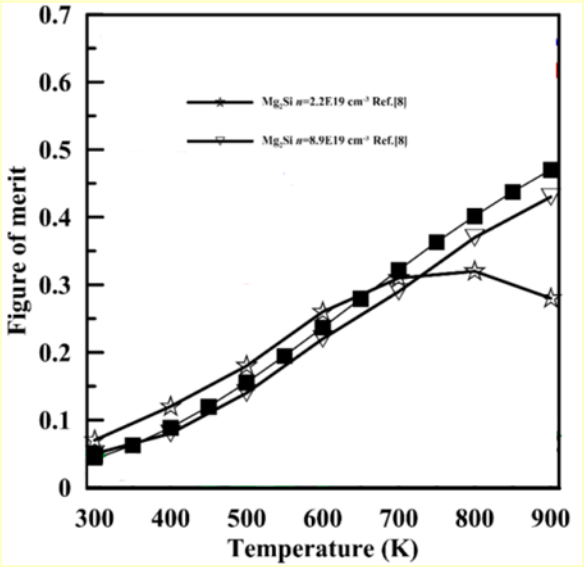
http://www.gizmag.com/ge-dual-piezo-cooling-jet/25447/

How to improve efficiency of thermoelectric devices?

"One shouldn't work on semiconductors, that is a filthy mess; who knows whether any semiconductors exist"

-W. Pauli, letter to R. Peierls (1931)





[Fan & Oganov (2018)]

$$ZT = \frac{\sigma S^2 T}{\kappa}$$

$$S = \frac{8\pi^2 k_B^2}{3eh^2} m^* T \left(\frac{\pi}{3n}\right)^{2/3}$$

$$\eta = \frac{\Delta T}{T_H} \frac{\sqrt{1+zT}-1}{\sqrt{1+zT}+\frac{T_C}{T_H}}$$

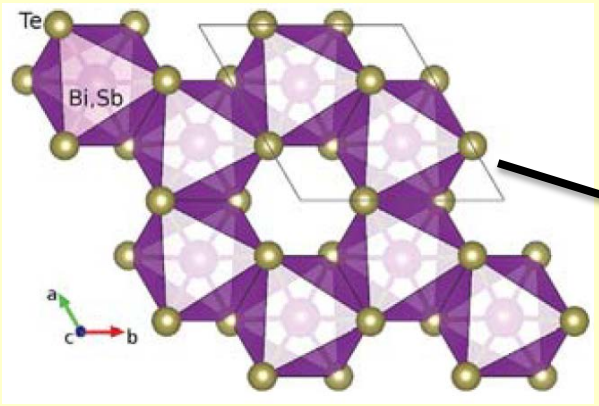
- efficiency

Multiobjective (Pareto) optimization finds a new thermoelectric polymorph of Bi_2Te_3

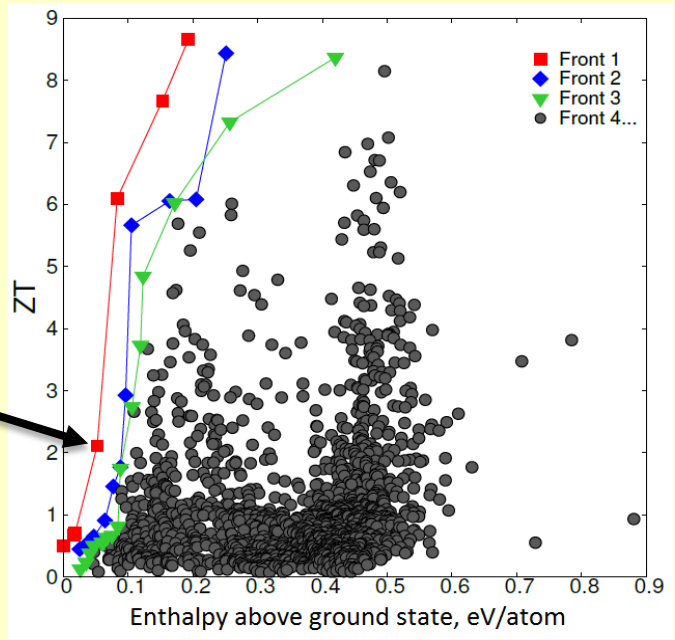
Computer Physics Communications 222 (2018) 152–157

Efficient technique for computational design of thermoelectric materials

Maribel Núñez-Valdez , Zahed Allahyari , Tao Fan , Artem R. Oganov



Predicted *P*6_3*cm* structure of Bi_2Te_3



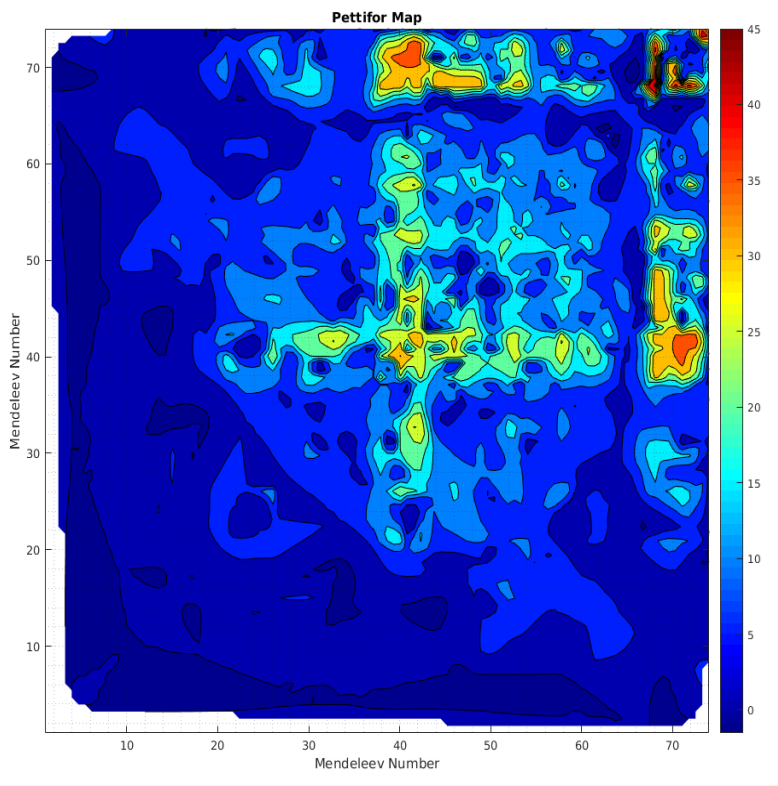
Pareto optimization of ZT and stability in the Bi-Te system

We can simultaneously optimize composition, structure, stability and other properties for a given chemical system.

Now, let’s predict the best material(s) among all possible chemical systems!

Mendelevian Search – breakthrough method for discovering best materials among all possible compounds

[Allahyari & Oganov, 2018]



- **118 elements**
- **7021 binary systems**
- **273937 ternaries**
- **In each system - ∞ possible structures**

Mendeleev Number – a way to arrange elements and compounds by properties

[Pettifor, 1984; Allahyari & Oganov, 2018]

Mendeleev Number	Atom	Mendeleev Number	Atom	Mendeleev Number	Atom
1	Fr	32	Tl	62	Po
2	Cs	33	U	63	Fe
3	Rb	34	Pa	64	Cu
4	K	35	Zr	65	Co
5	Ra	36	Pu	66	As
6	Ba	37	Np	67	Ni
7	Sm	38	Nb	68	Kr
8	Gd	39	Ta	69	Mo
9	Eu	40	In	70	I
10	Sr	41	Pb	71	Pd
11	Tm	42	Cd	72	Ir
12	Pm	43	Xe	73	Os
13	Ca	44	Ti	74	P
14	Na	45	Al	75	Ru
15	Ac	46	Bi	76	Pt
16	La	47	Sn	77	At
17	Yb	48	Hg	78	Rh
18	Tb	49	Zn	79	W
19	Y	50	Ga	80	Rn
20	Dy	51	V	81	Se
21	Ho	52	Mn	82	B
22	Ce	53	Sb	83	Au
23	Er	54	Te	84	S
24	Li	55	Cr	85	Br
25	Th	56	Ag	86	H
26	Lu	57	Be	87	C
27	Pr	58	Ge	88	Cl
28	Nd	59	Re	89	N
29	Mg	60	Si	90	O
30	Sc	61	Tc	91	F
31	Hf				

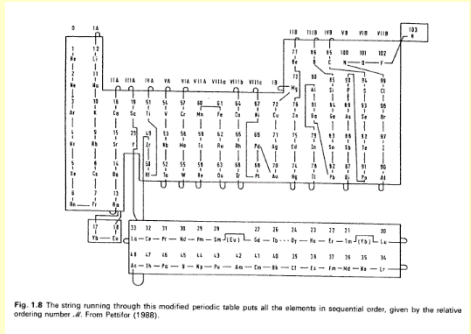
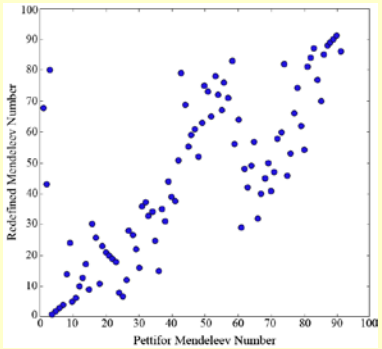
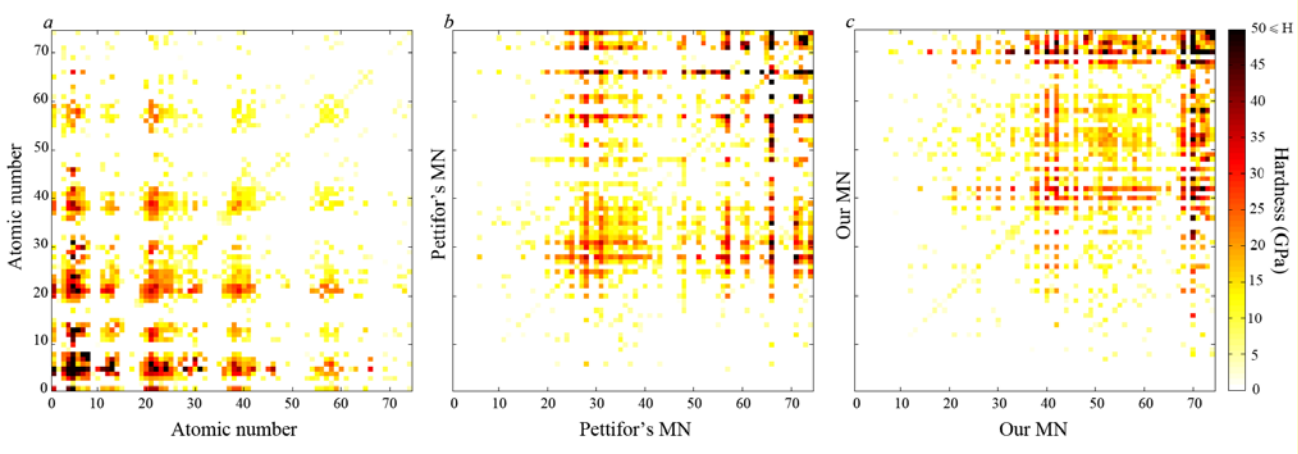


Fig. 1.8 The string running through this modified periodic table puts all the elements in sequential order, given by the relative ordering number, A'. From Pettifor (1988).

Pettifor's construction



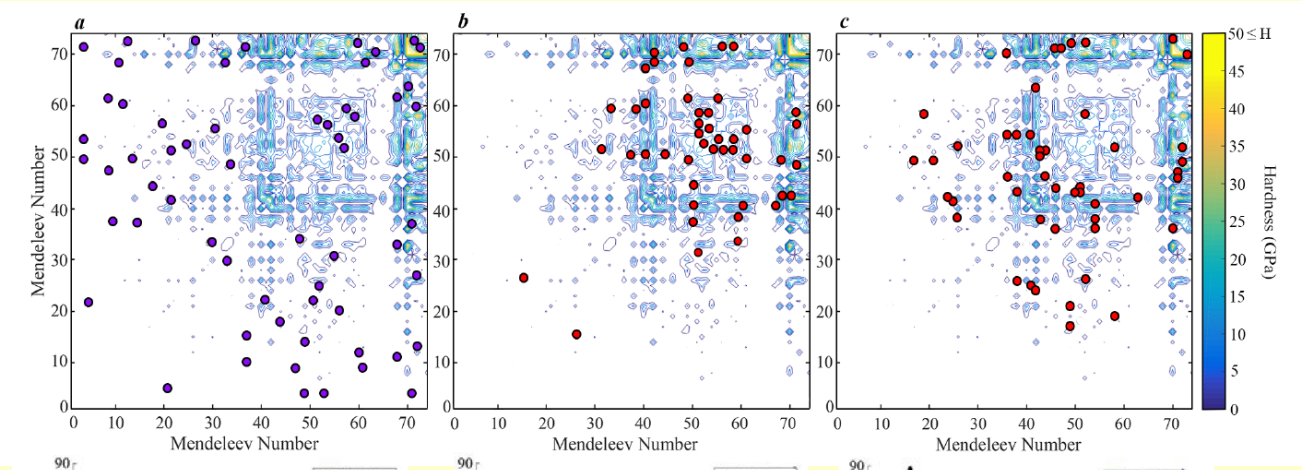
Comparison with Pettifor's numbers

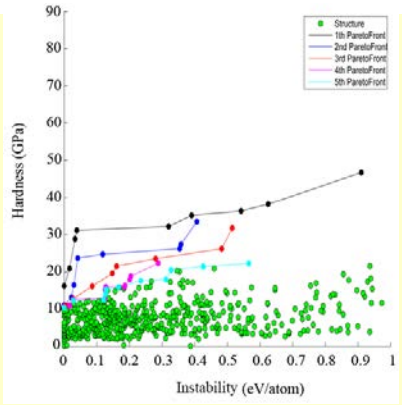


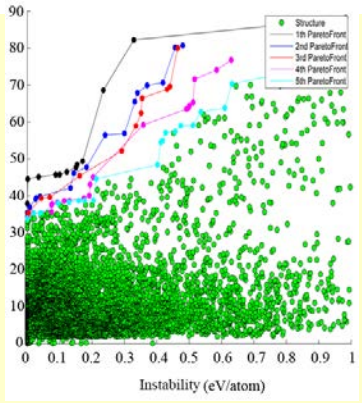
Grouping of hardness by (a) sequential number, (b) Pettifor's Mendeleev number, (c) our Mendeleev number

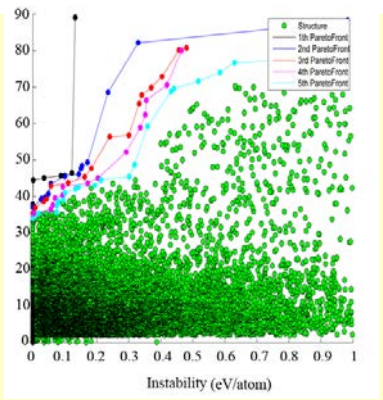
Mendelevian search for the hardest possible material: diamond and lonsdaleite are found!

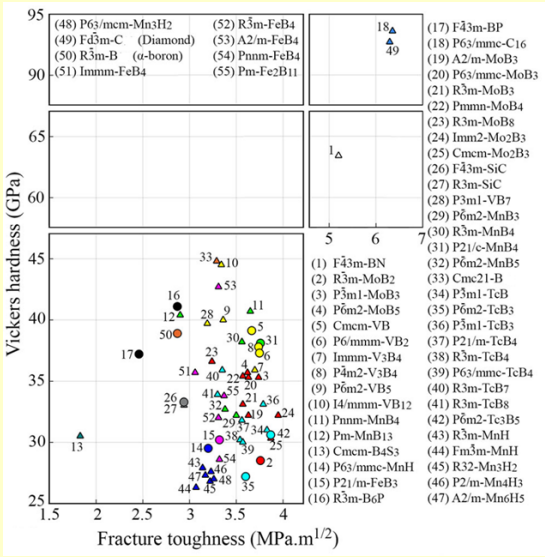
1st generation **5th generation** **10th generation**





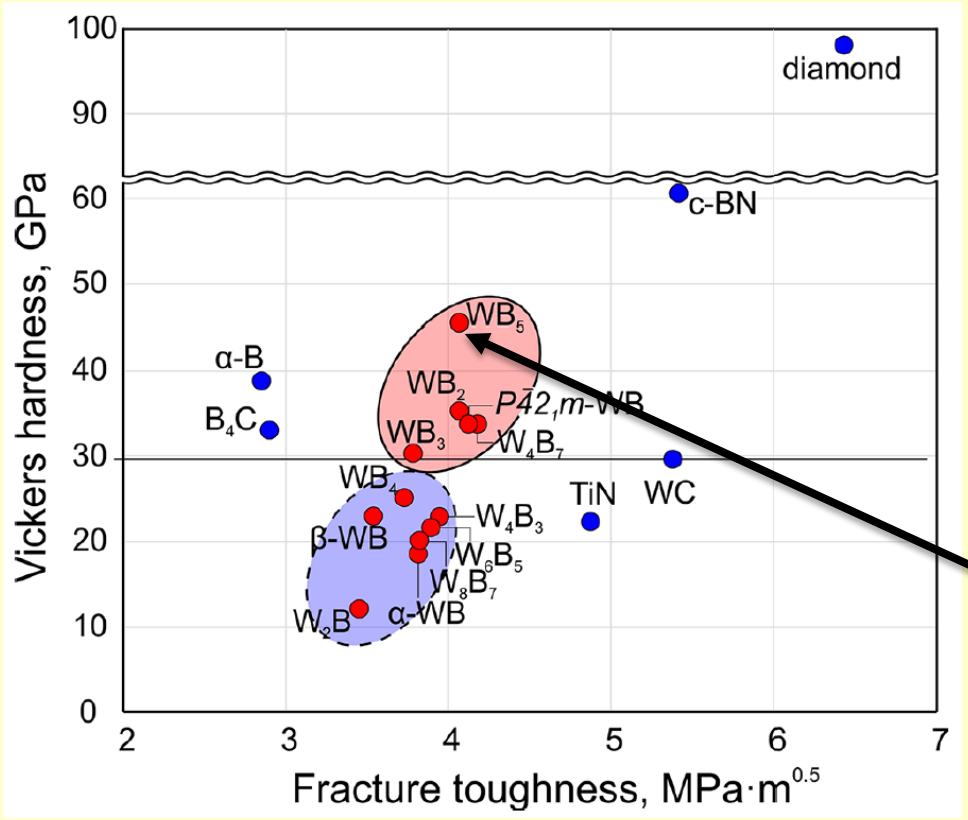


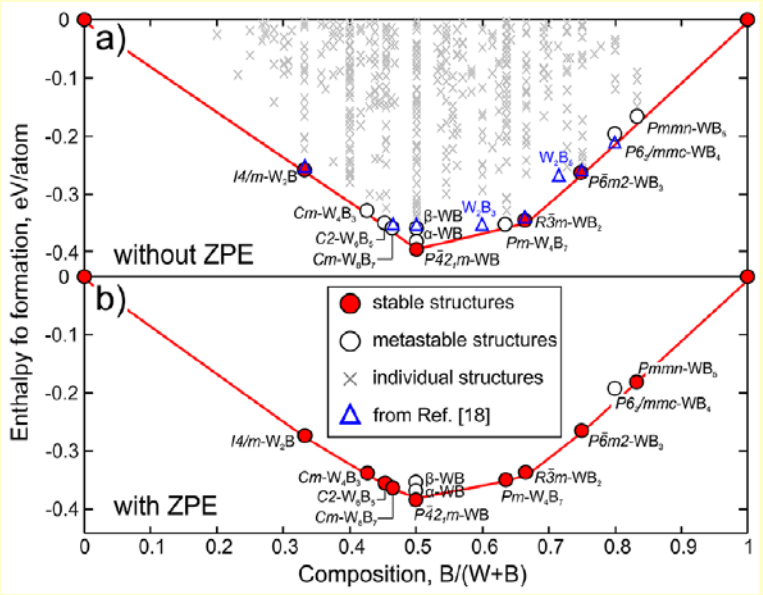


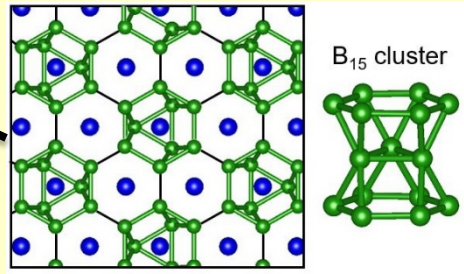


WB_5: new supermaterial

[Kvashnin & Oganov, J. Phys. Chem. Lett., 2018]





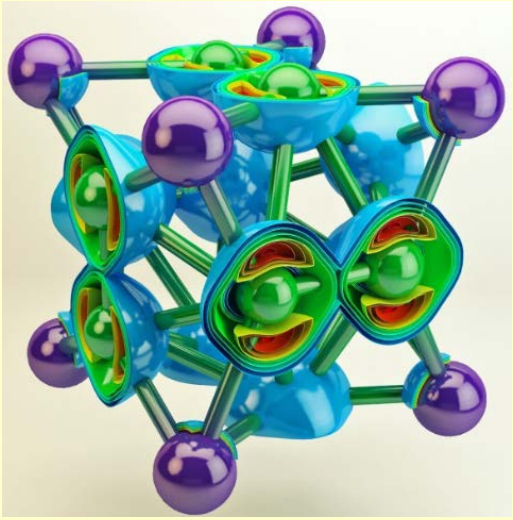


New material WB_5

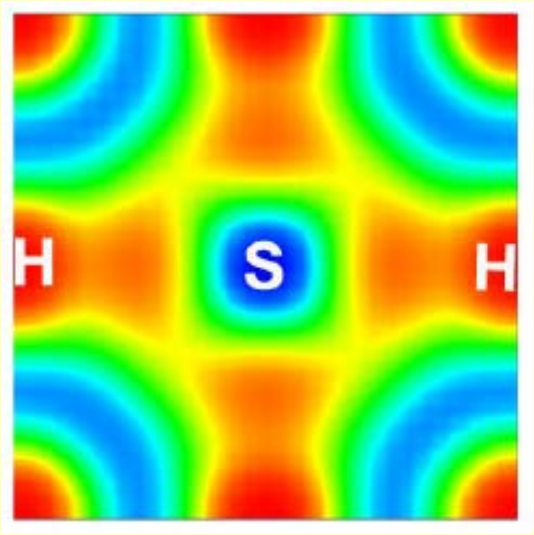
Tungsten carbide WC - standard

Synthesized by V. Filonenko

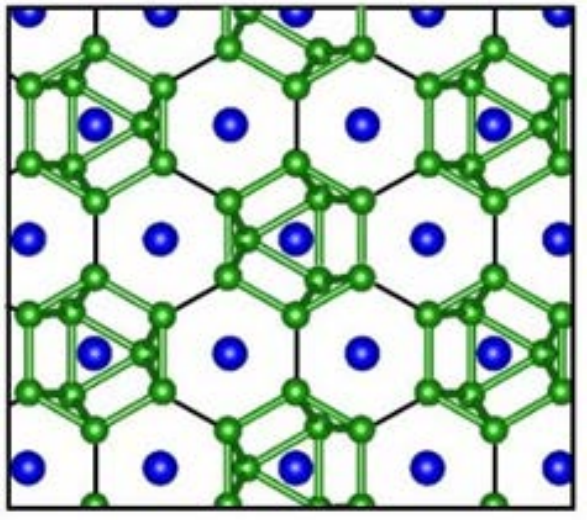
Advanced algorithms predict new supermaterials and help us understand nature



Unusual chemistry at extreme conditions



New record of high-Tc superconductivity



New superhard materials

Our team. Where great minds do NOT think alike

Q. Zhu

X. Dong

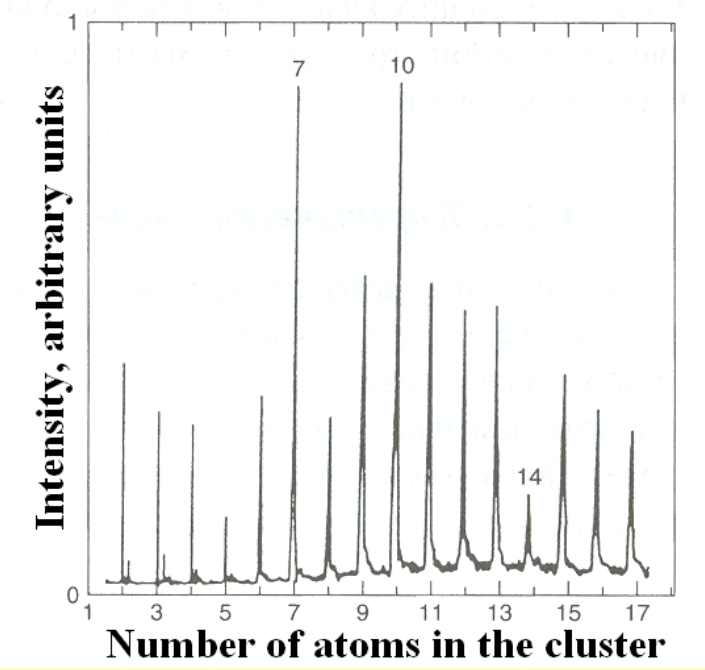
A. Goncharov

V.A. Blatov

USPEX Computational Materials Discovery

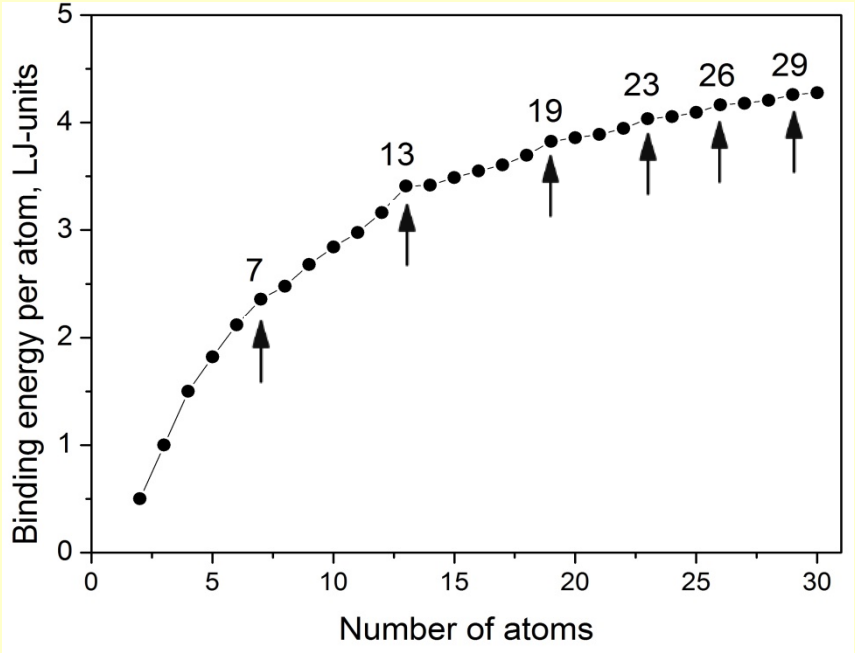
Stability of clusters

Real system: Pb clusters



Mass-spectrum of Pb_n clusters (from Poole & Owens, 2003)

Model system: Lennard-Jones clusters

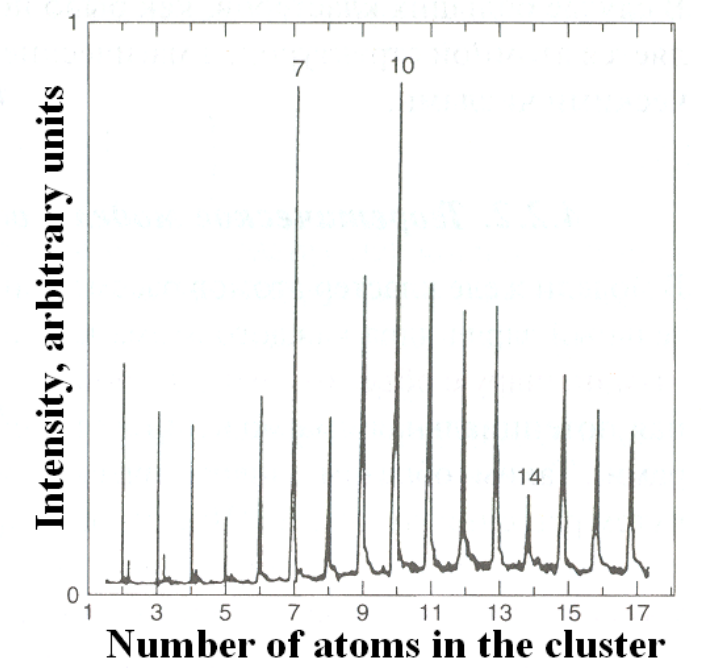


↑ – magic clusters.

Larger clusters are generally more thermodynamically stable. The most stable state is crystal.
For nanoparticles, stability is measured relative to neighboring nanoparticles.

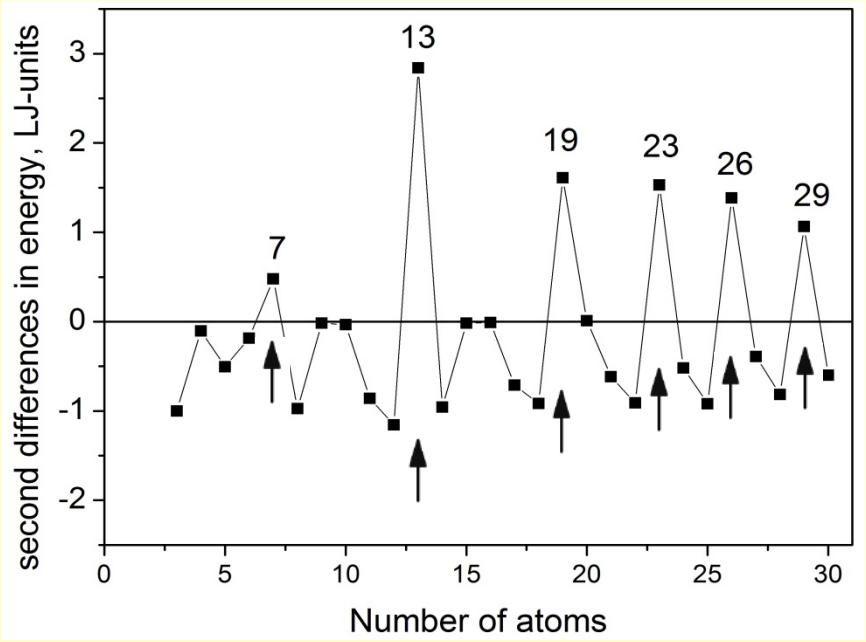
Stability of clusters

Real system: Pb clusters



Mass-spectrum of Pb_n clusters (from Poole & Owens, 2003)

Model system: Lennard-Jones clusters



– magic clusters.

Criterion of local stability (magic clusters):

$$\Delta^2 \mathrm{E} = \mathrm{E}(n+1) + \mathrm{E}(n-1) - 2\mathrm{E}(n) > 0$$

For binary clusters (A_mB_n):

$$\Delta_x^2 \mathrm{E} = \mathrm{E}(m,n+1) + \mathrm{E}(m,n-1) - 2\mathrm{E}(m,n) > 0$$

$$\Delta_y^2 \mathrm{E} = \mathrm{E}(m+1,n) + \mathrm{E}(m-1,n) - 2\mathrm{E}(m,n) > 0$$