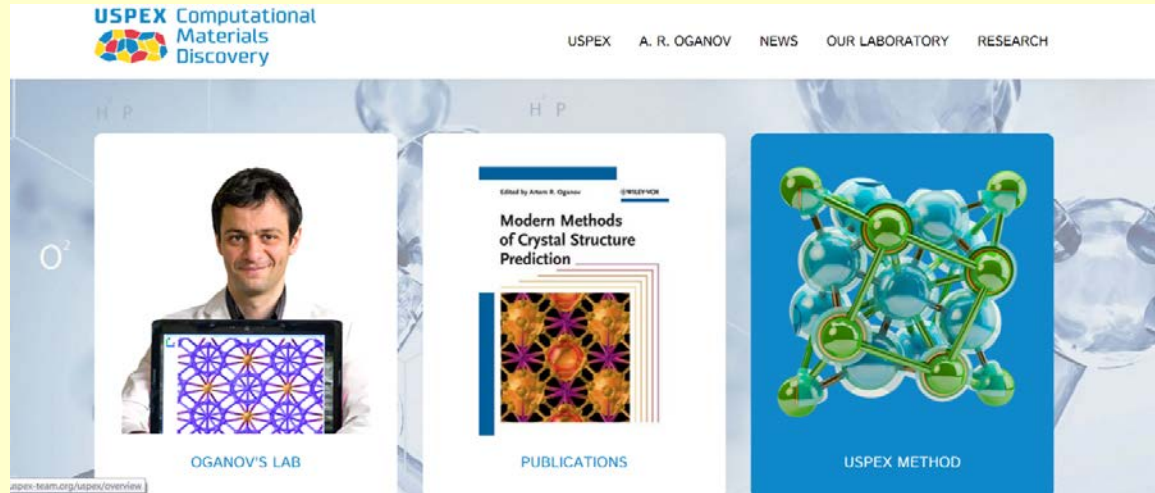




**The workshop is supported by Russian Science Foundation grant No. 19072-30043
“Computational materials discovery laboratory”**

The USPEX (Universal Structure Prediction: Evolutionary Xtallography) project

<http://uspex-team.org>



- The most popular code for computational materials design in the world (>7000 users from 83 countries).
- Effort of ~100 man-years.
- >1000 publications, 5 patents.

- Universal:
 - prediction of stable structure AND composition, 3D, 2D, 1D, 0D – systems.
 - optimization of physical properties,
 - prediction of phase transition mechanisms

Basic Facts on USPEX

- The most popular structure prediction code in the world (>7000 users).
- The largest and the most versatile code in this field. Many capabilities are unique.
- The fastest and the most reliable structure prediction code today.
- THE CODE IS FREE, but you have to agree to certain conditions of fair use **(register now!)**.

- Every year ~2 USPEX workshops.
- USPEX mailing list **(join it!)**. USPEX Forum **(use it!)**.
- USPEX Facebook page **(join it!)**.
- USPEX QQ group (group number 326701679 – **join it!**)
- ~10 visiting scholars every year in the Oganov laboratory.

- Support for citizen science: <http://uspex-at-home.ru>

***“USPEX” (“oo-spe-kh”) means “success” in Russian**

Features of the USPEX code:

Algorithm:

- Evolutionary optimization (USPEX algorithm). Options to use random sampling, minima-hopping-like, particle-swarm optimization, metadynamics.
- Initialization using fully random, symmetric random structures, topological random, or user-fed structures.
- Fingerprint niching technique, local order parameter (ARO&Valle, 2009).

Types of runs:

- Global optimization of either the energy or properties (density, hardness, band gap, etc.)
- Pareto optimization of several properties simultaneously.
- Fixed-cell or variable-cell, fixed-composition or variable-composition runs are possible.
- For molecular crystals, can operate with ready-made molecules.
- Low-dimensional systems.
- Harvesting metastable states is possible.
- Phase transition pathways.

Software aspects:

- Interfaced with VASP, SIESTA, CP2k, QuantumEspresso, DMACRYS, GULP, ATK,...
- Excellent scaling on up to 10^{3-4} cores.

Analysis:

- Automatic detection of space groups.
- Benefits from powerful analysis and visualization code STM4.

Distribution:

- **USPEX code is freely available at: <http://uspex-team.org>**
- Distributed with a >130-page manual and >30 examples.

Statistics

- >7000 users from 83 countries.
- 1607 USA
- >>662 China
- 206 Russia
- 202 India
- 101 Japan
- 96 France
- 97 U.K.
- 82 Germany
- 65 S. Korea
- 50 Italy

Funding of USPEX



Российский научный фонд



National Science Foundation
WHERE DISCOVERIES BEGIN



NSFC

National Natural Science Foundation of China



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RECRUITMENT
PROGRAM OF GLOBAL EXPERTS

欢迎海外高层次人才回国（来华）创新创业



- Industrial partners: Intel, Samsung, Toyota, Fujitsu, APC.

People behind USPEX

Main contributors:

Artem R. Oganov

Zahed Allahyari

Pavel Bushlanov

Andriy Lyakhov

Colin Glass

Sergey Lepeshkin

Guangrui Qian

Salah-Eddine Boulfelfel

Vladan Stevanovic

Artem Samtsevich

Harold Stokes

Evgeny Tikhonov

Maxim Rakin

Vladislav Blatov

Ivan Kruglov

Xiao Dong

Computational Materials Discovery with the USPEX code

Artem R. Oganov

Skolkovo Institute of Science and Technology, Russia



The workshop is supported by Russian Science Foundation grant No. 19072-30043 “Computational materials discovery laboratory”

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



The Nobel Prize in Physics 1914

"for his discovery of the diffraction of X-rays by crystals"



Max von Laue



The Nobel Prize in Physics 1915

"for their services in the analysis of crystal structure by means of X-rays"



Sir William Henry Bragg



William Lawrence Bragg



The Nobel Prize in Chemistry 1985

"for their outstanding achievements in the development of direct methods for the determination of crystal structures"

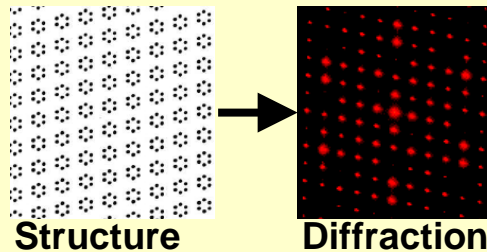


Herbert A. Hauptman



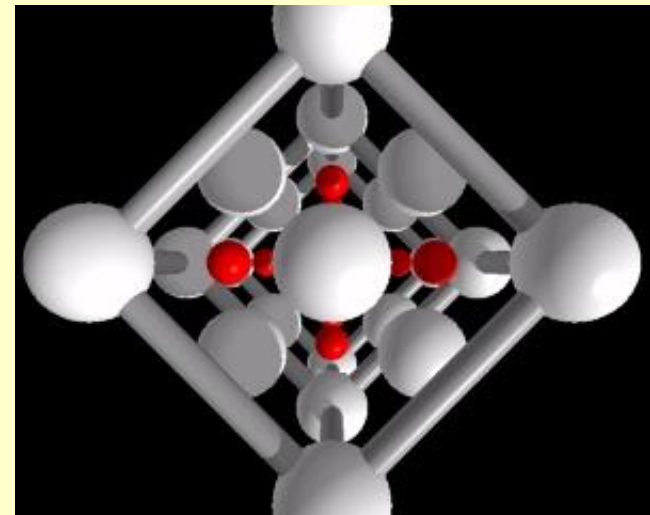
Jerome Karle

(from <http://nobelprize.org>)

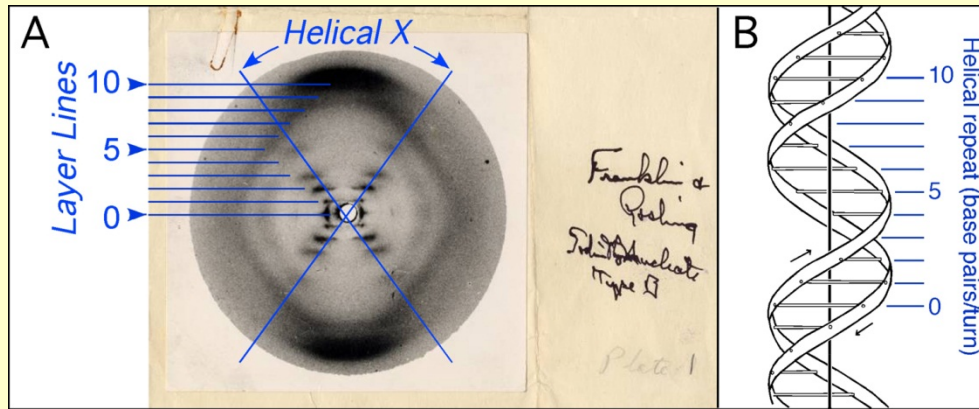


Zincblende ZnS.

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 Drenth	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]

Briefly about crystal structure prediction

Faraday Discussions

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




PAPER

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Crystal structure prediction: reflections on present status and challenges

Artem R. Oganov  abc

Received 30th August 2018, Accepted 30th August 2018

Useful reviews and books

Faraday Discussions

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



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Crystal structure prediction: reflections on present status and challenges

Artem R. Oganov ^{abc}

Received 30th August 2018, Accepted 30th August 2018

***Faraday Discussions* (2018)**

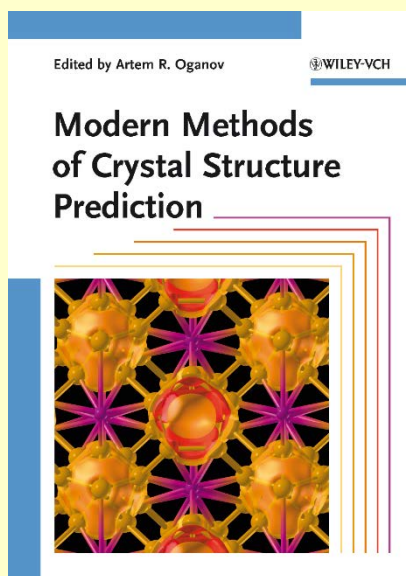
REVIEWS

Structure prediction drives materials discovery

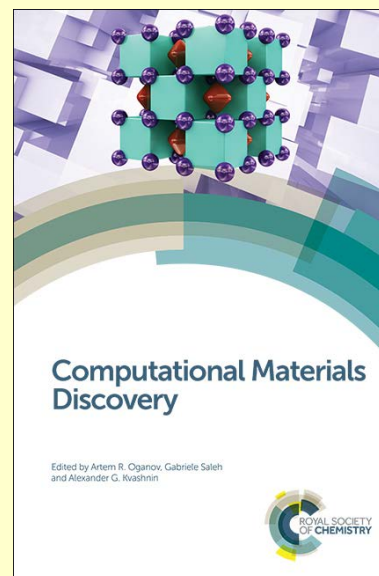
Artem R. Oganov^{1,2,3*}, Chris J. Pickard^{4,5*}, Qiang Zhu⁶ and Richard J. Needs⁷

Abstract | Progress in the discovery of new materials has been accelerated by the development of reliable quantum-mechanical approaches to crystal structure prediction. The properties of a material depend very sensitively on its structure; therefore, structure prediction is the key to computational materials discovery. Structure prediction was considered to be a formidable problem, but the development of new computational tools has allowed the structures of many new and increasingly complex materials to be anticipated. These widely applicable methods, based on global optimization and relying on little or no empirical knowledge, have been used to study crystalline structures, point defects, surfaces and interfaces. In this Review, we discuss structure prediction methods, examining their potential for the study of different materials systems, and present examples of computationally driven discoveries of new materials — including superhard materials, superconductors and organic materials — that will enable new technologies. Advances in first-principle structure predictions also lead to a better understanding of physical and chemical phenomena in materials.

***Nature Reviews Materials* (2019)**



2011



2018

Are Crystal Structures Predictable?

ANGELO GAVEZZOTTI*

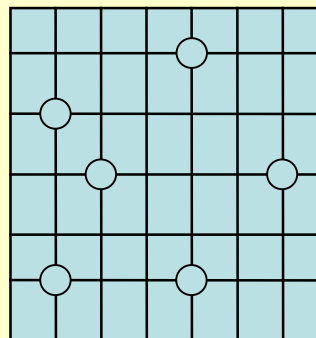


“No”: by just writing down this concise statement, in what would be the first one-word paper in the chemical literature, one could safely summarize the present state of affairs

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 Predictor: Evolutionary Xtallography)

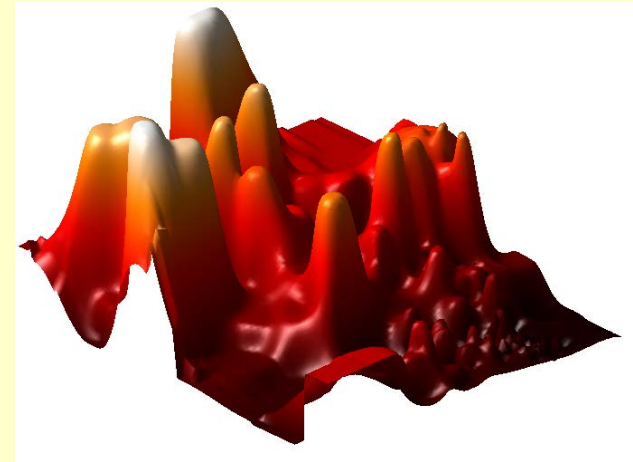
<http://uspex-team.org>

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

- Combination of evolutionary algorithm and quantum-mechanical calculations.
- >7000 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 Au₈Pd



W. Kohn



J. P. Perdew

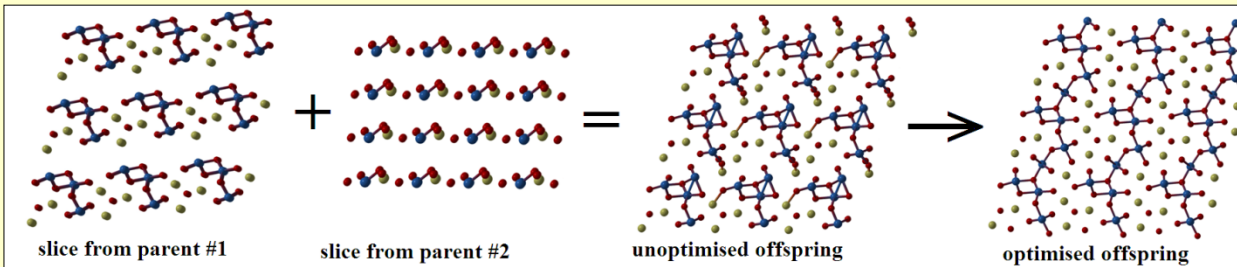
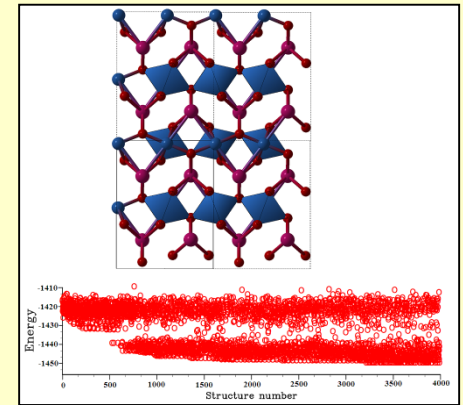
$$\left(-\frac{\nabla^2}{2} + v_{e-n}[\rho(\mathbf{r})] + v_H[\rho(\mathbf{r})] + v_{xc}[\rho(\mathbf{r})]\right)\phi_i(\mathbf{r}) = \varepsilon_i\phi_i(\mathbf{r})$$

$$E_{GGA,xc} = \int d\mathbf{r} F_{xc}(\rho, \frac{|\nabla\rho|}{2k_f\rho(\mathbf{r})})\rho(\mathbf{r})e_x[\rho(\mathbf{r})]$$

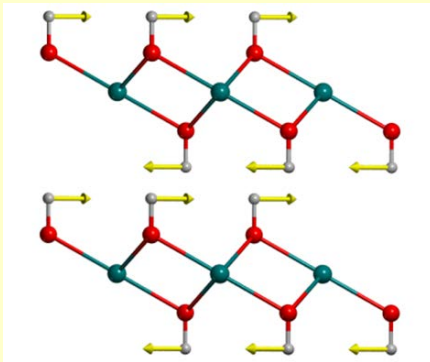
USPEX

(Universal Structure Predictor: Evolutionary Xtallography)

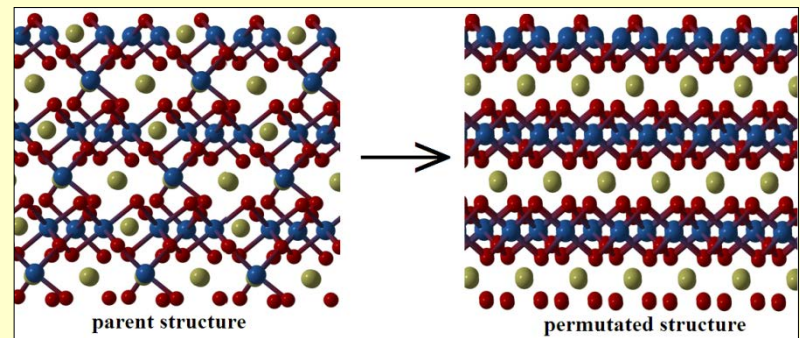
- (Random) initial population
- Evaluate structures by relaxed (free) energy
- Select lowest-energy structures as parents for new generation
- Standard variation operators:



(1) Heredity (crossover)



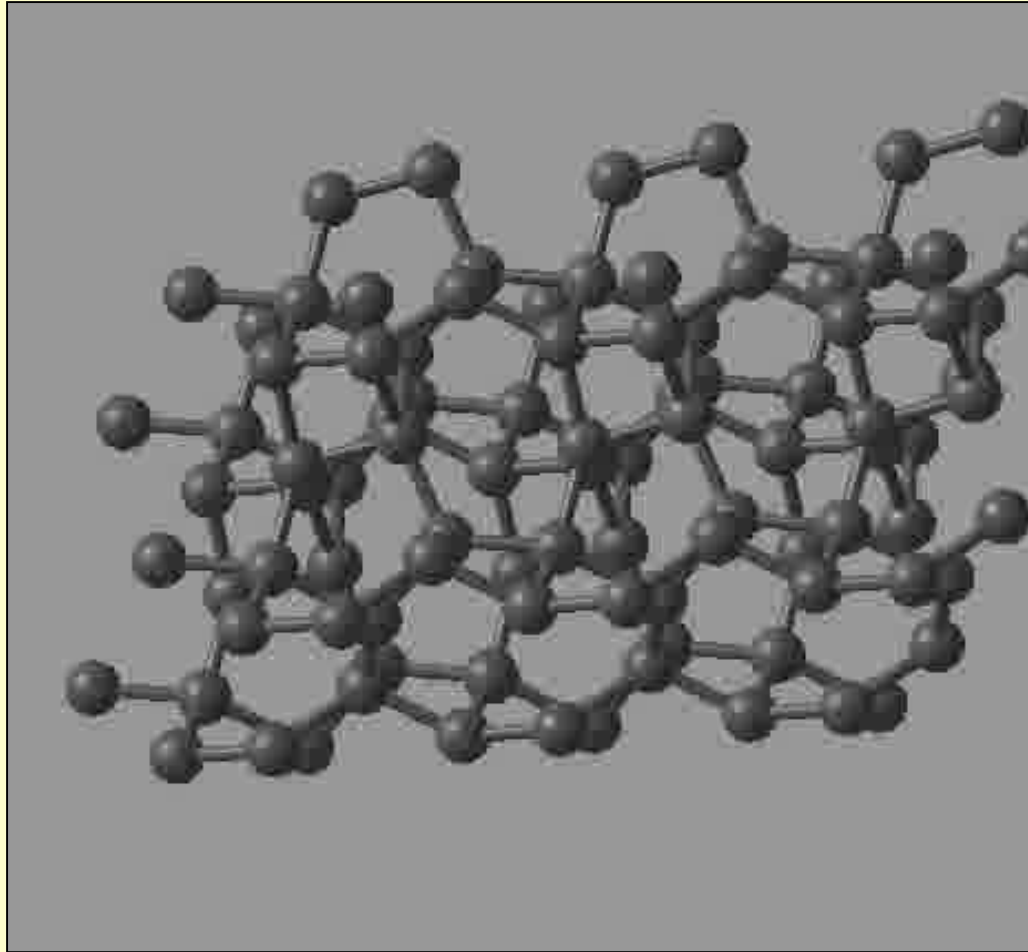
(2) Soft mode mutation



(3) Permutation

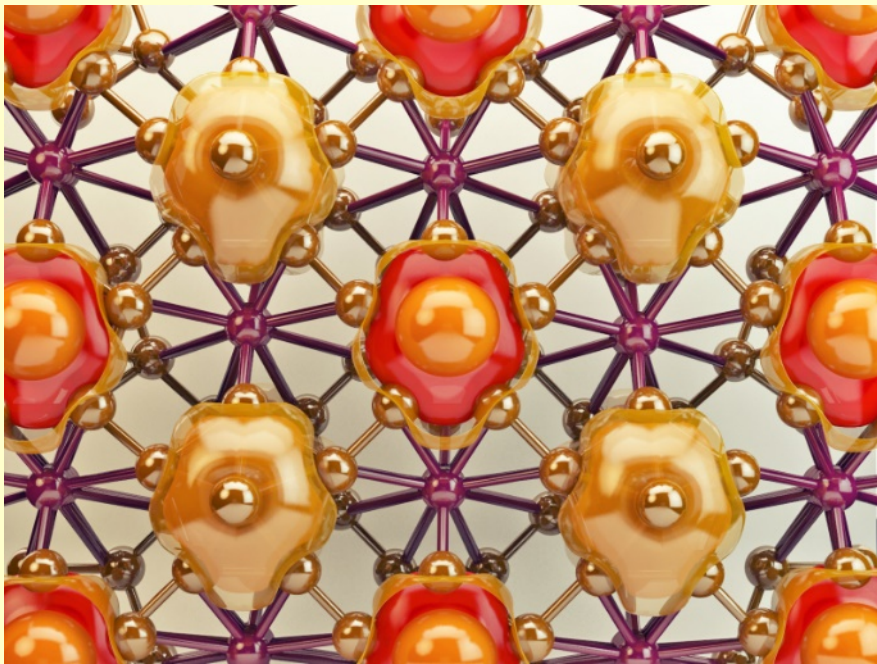
+ (4) Transmutation, + (5) Rotational mutation, + (6) Soft-mode mutation, + ...

**Without any empirical information,
method reliably predicts materials**



Carbon at 100 GPa – diamond structure is stable

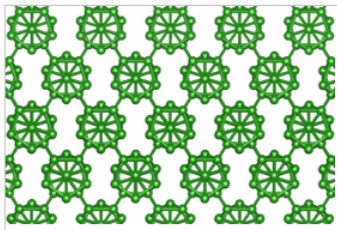
Predicting new crystal structures without empirical information



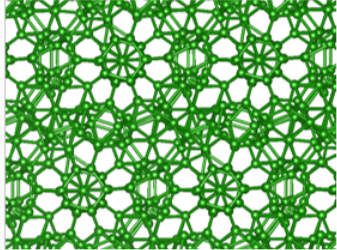
New superhard structure of boron
(Oganov et al., *Nature*, 2009)



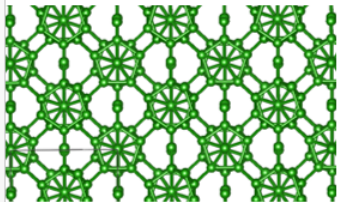
High-pressure **transparent**
allotrope of sodium
(Ma, Eremets, Oganov, *Nature*, 2009)



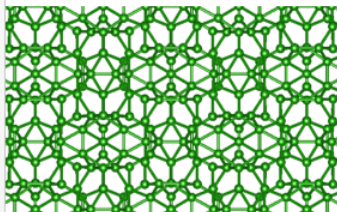
α -boron
 $E^{\text{DFT}} = -6.706$ eV/atom
Atoms: 12,
Space group: $R\bar{3}m$,
Core-hours: 10^3 AL-MTP vs. $3 \cdot 10^3$ DFT
 $|E^{\text{DFT}} - E^{\text{MTP}}| = 28.6$ meV/atom



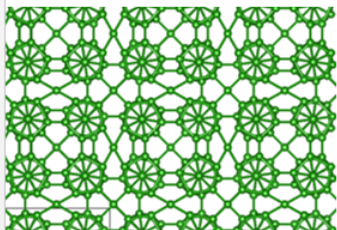
β -boron approximat
 $E^{\text{DFT}} = -6.704$ eV/atom,
Atoms: 106,
Space group: $P1$,
Core-hours: $7 \cdot 10^3$ AL-MTP vs. $6.6 \cdot 10^7$ DFT
 $|E^{\text{DFT}} - E^{\text{MTP}}| = 10.1$ meV/atom



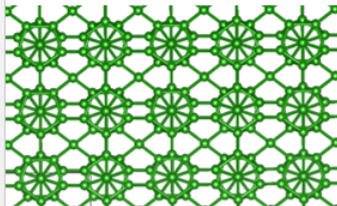
γ -boron
 $E^{\text{DFT}} = -6.678$ eV/atom
Atoms: 28,
Space group: $Pnnm$,
Core-hours: $2 \cdot 10^3$ AL-MTP vs. $2.5 \cdot 10^4$ DFT
 $|E^{\text{DFT}} - E^{\text{MTP}}| = 58.1$ meV/atom



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



$E^{\text{DFT}} = -6.667$ eV/atom,
Atoms: 52,
Space group: $P\bar{4}2m$,
Core-hours: $3 \cdot 10^3$ AL-MTP vs. $3.2 \cdot 10^5$ DFT
 $|E^{\text{DFT}} - E^{\text{MTP}}| = 37.3$ meV/atom



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

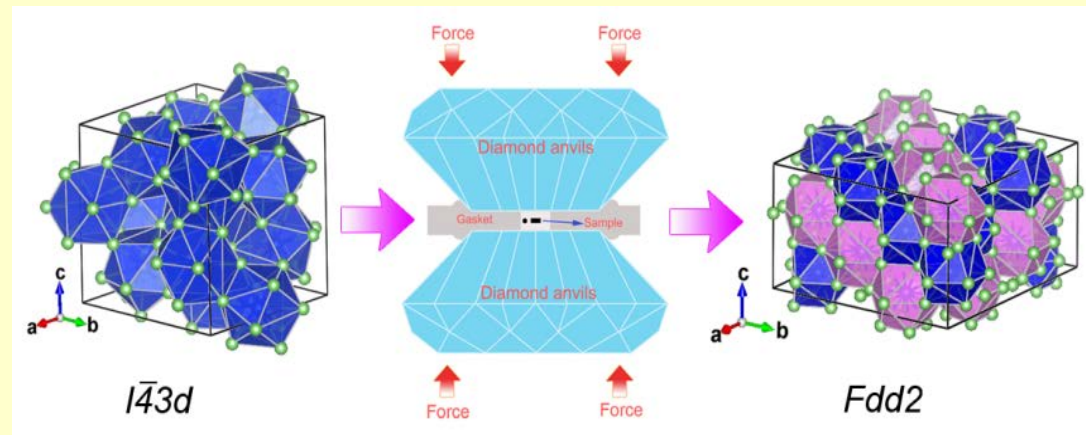
Handling complexity with machine learning: boron allotropes

(E.Podryabinkin, E. Tikhonov, A. Shapeev, A.R. Oganov, PRB, 2019)

- 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.

Structure of $\text{Li}_{15}\text{Si}_4$ with 152 atoms/cell: record complexity, promise for Li-batteries

Li-Si

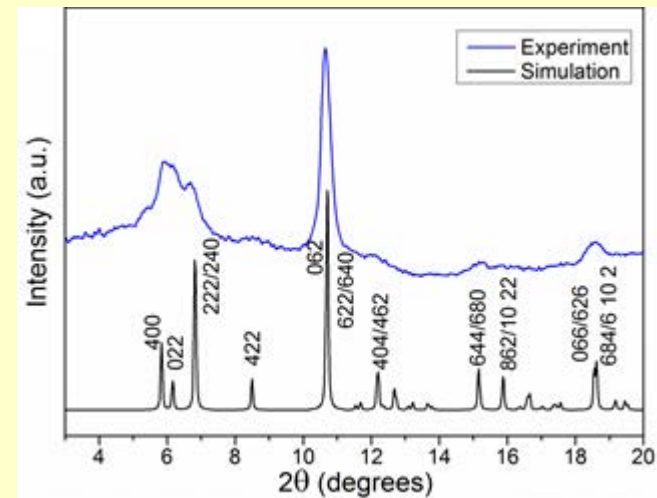


Structural transformation of $\text{Li}_{15}\text{Si}_4$ at 7 GPa. New phase has more attractive properties for use in Li-batteries.

Evolutionary metadynamics is a hybrid of:

- Metadynamics (Martonak, Laio, Parrinello, PRL 2003)
- Evolutionary algorithm USPEX (Oganov & Glass, JCP 2006)

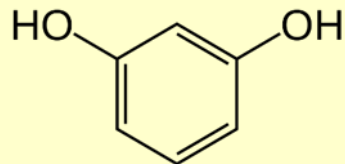
It includes *q*-vectors and allows system size to change spontaneously



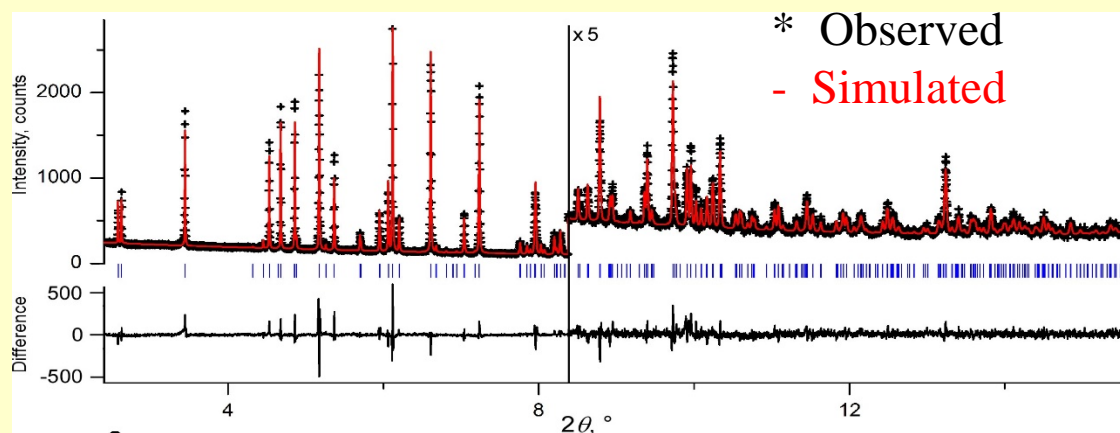
XRD of $Fdd2\text{-Li}_{15}\text{Si}_4$ at 18 GPa

[Zeng & Oganov, *Adv. Energy Mat.*, 2015]

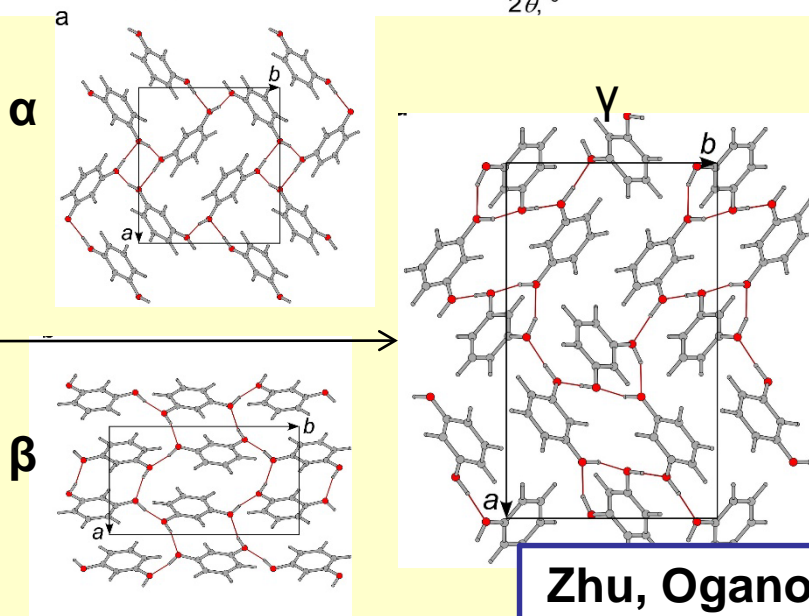
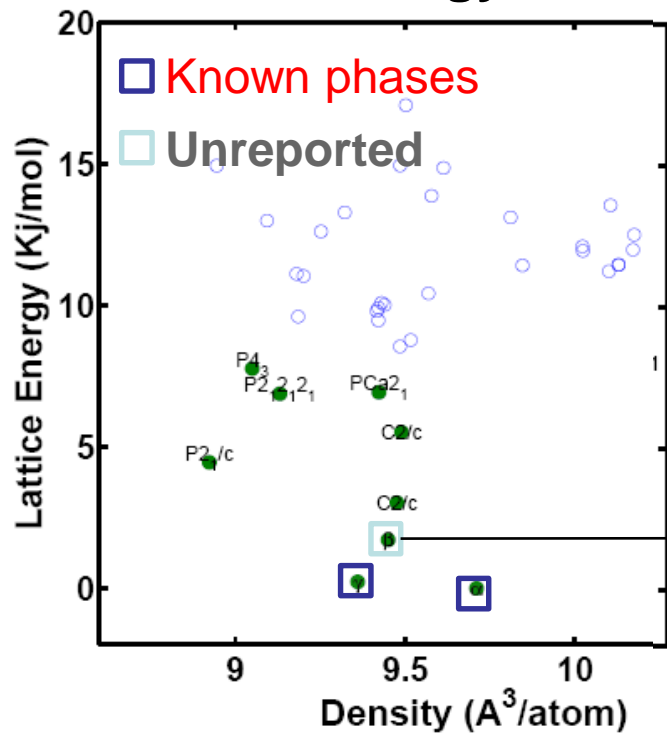
USPEX can handle molecular crystals: solved γ -resorcinol



Powder XRD comparison



Lattice Energy Plot

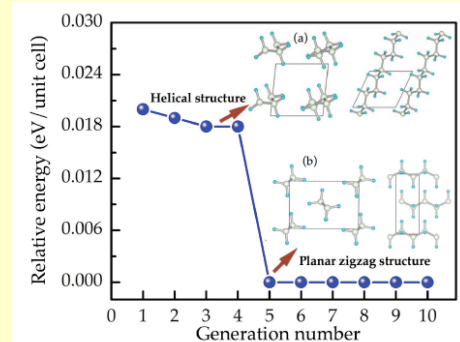
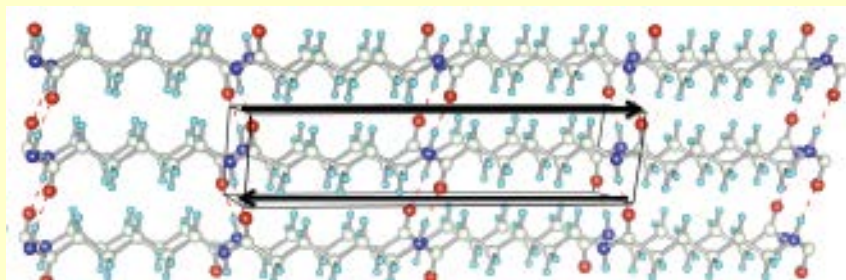


Zhu, Oganov, et al,
JACS, 2016

Prediction of new polymers for flexible capacitors

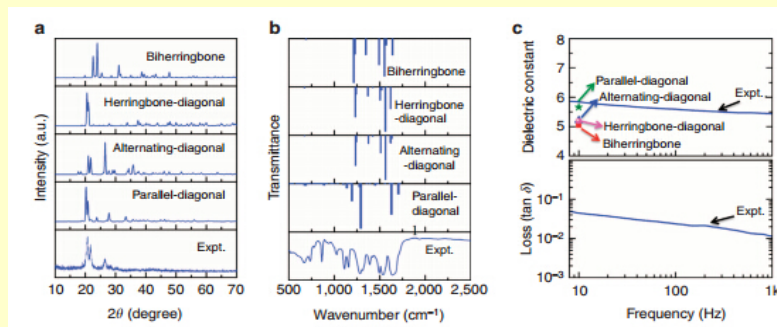
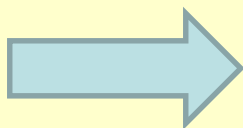
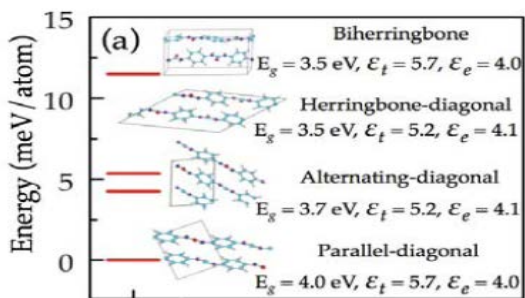
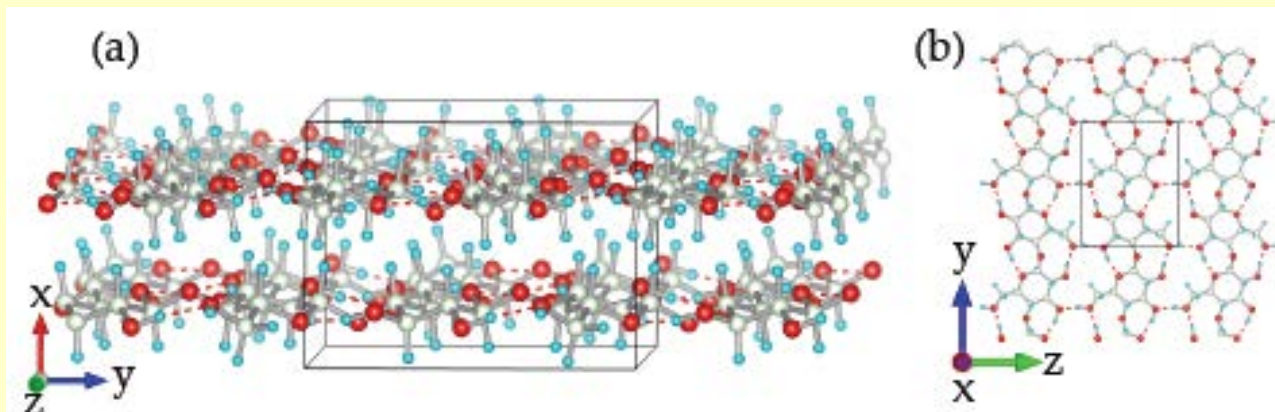
(Zhu, Sharma, Oganov: *J.Chem.Phys.* 2014, *Nature Commun.* 2014)

**Nylon-6
test**



Test on polyethylene

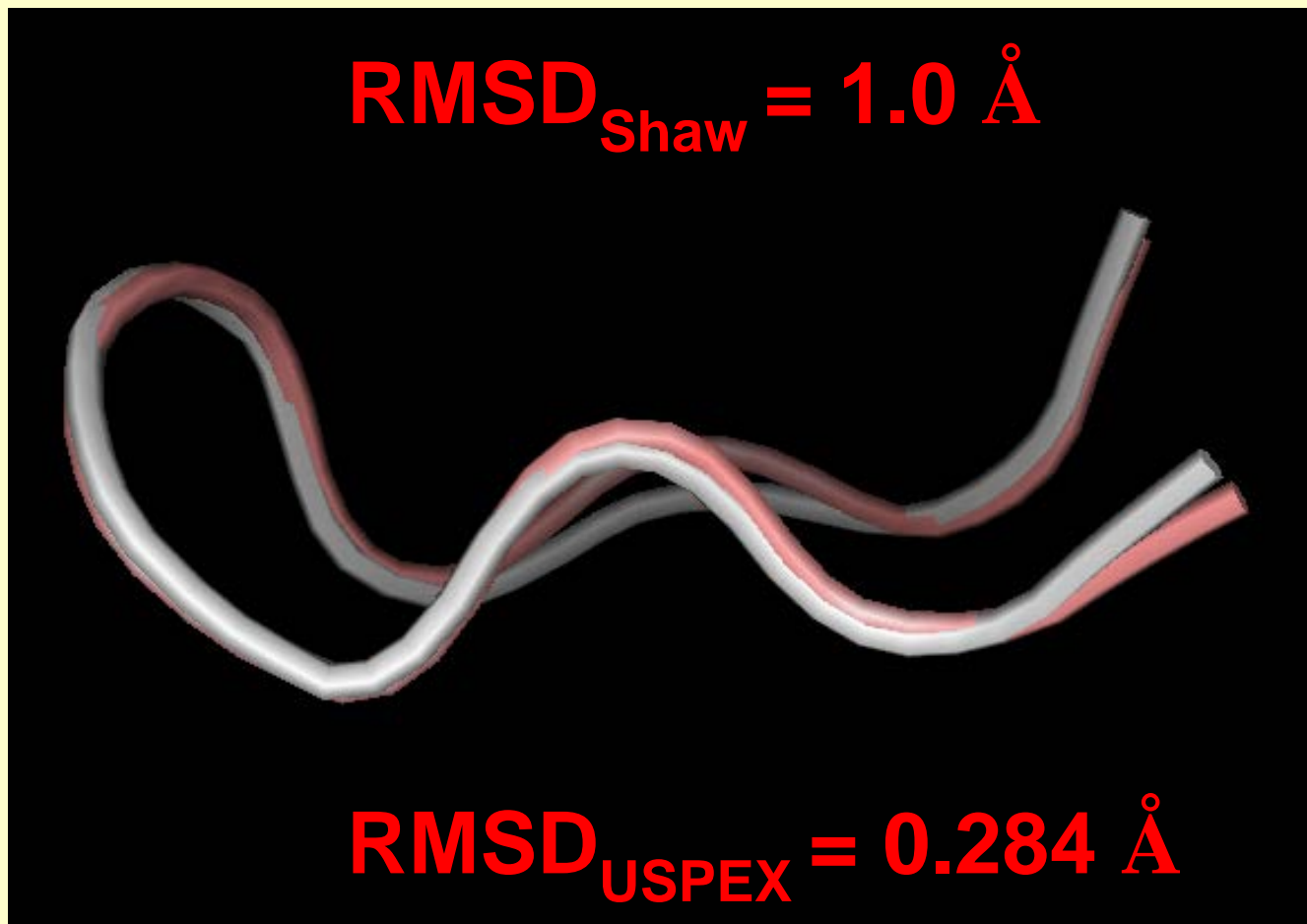
**Cellulose
test**



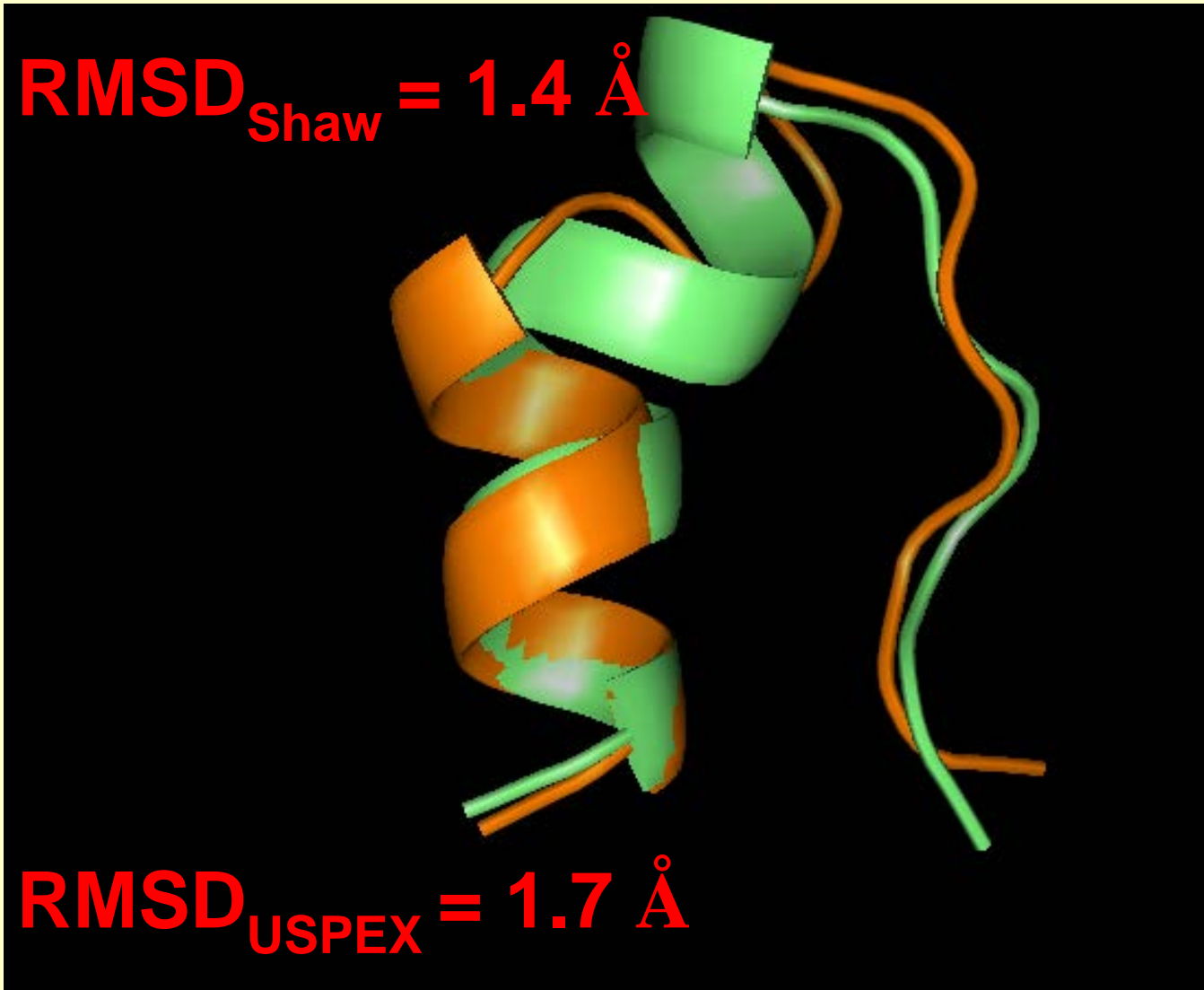
Prediction of 3 new high-k polymers

Experimental proof

First steps to protein structure prediction with USPEX: chignolin (I. Kruglov, 2018)

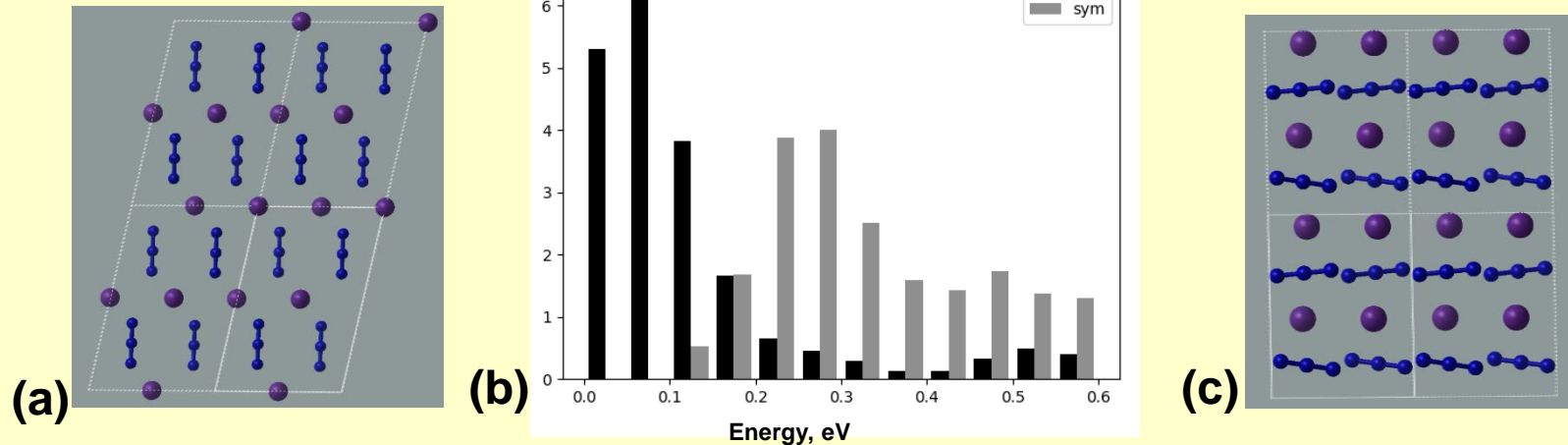


**Towards protein structure prediction:
test on Trp-cage (I. Kruglov, 2018)**



New methodological development: topological structure generator (Bushlanov, Blatov, Oganov, 2019)

Speedup ~3 times



Example of KN_3 : (a) topological structure, (c) random symmetric structure, (b) 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

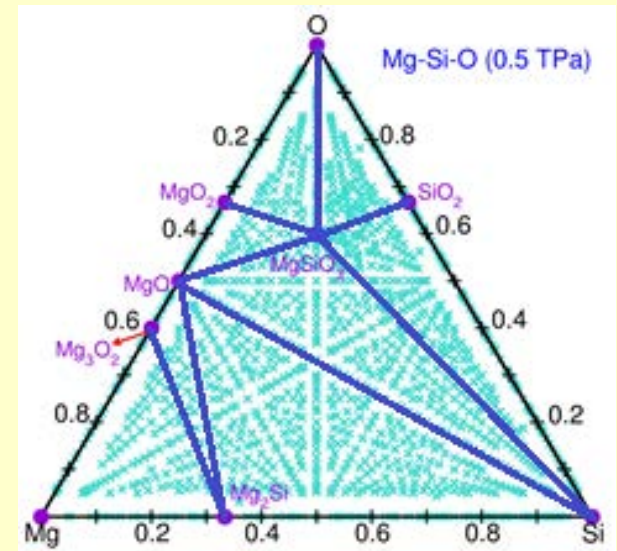
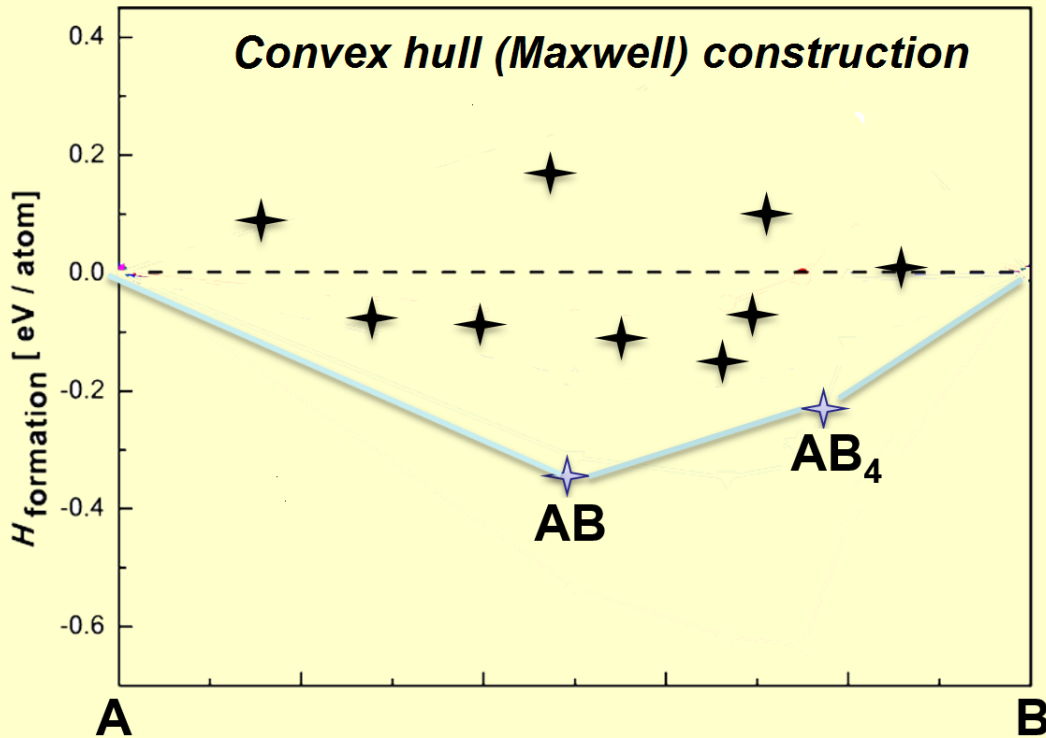
	Original	On-the-fly adaptation	On-the-fly adaptation AND topology
<No. of structures>	1307	1069	368
Success rate	100%	100%	100%

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

Now, let's predict the chemical composition!

To predict thermodynamic stability, we must use the Maxwell construction (the **convex hull**)

Thermodynamic stability in variable-composition systems

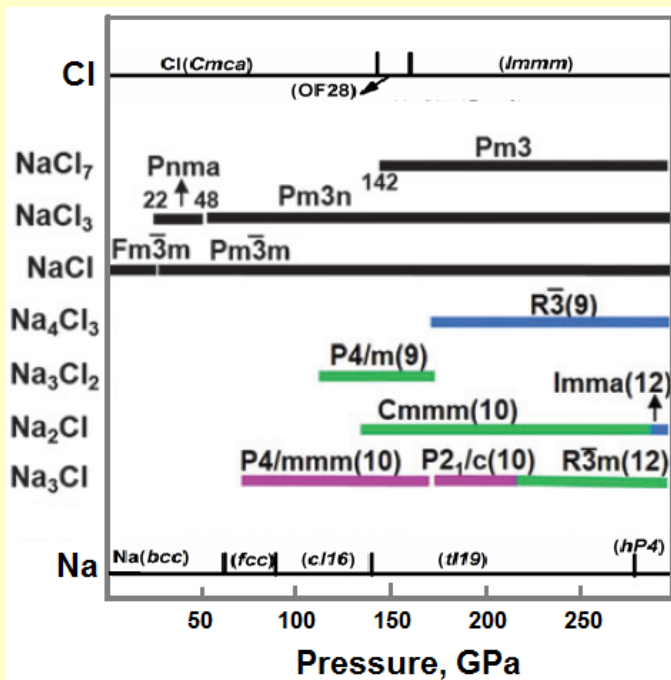


**3-component convex hull:
Mg-Si-O system at 500 GPa
(Niu & Oganov, *Sci. Rep.* 2015)**

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

Predictive power of modern methods:

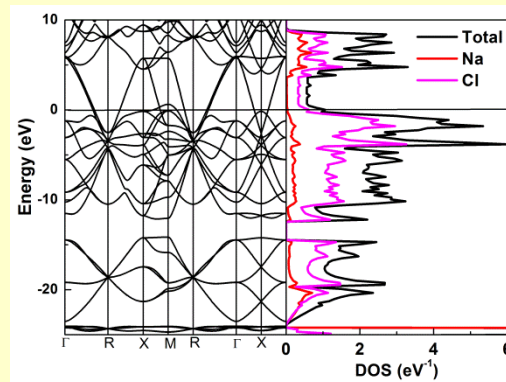
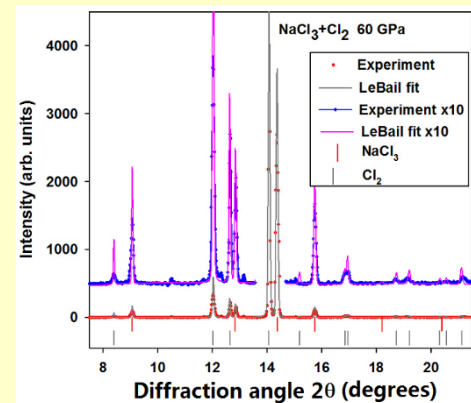
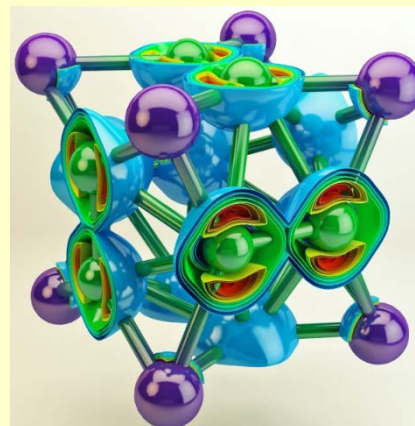
Na_3Cl , Na_2Cl , Na_3Cl_2 , NaCl , NaCl_3 , NaCl_7 are stable under pressure
 [Zhang, Oganov, et al. *Science*, 2013].



Stability fields of sodium chlorides

Chemical anomalies:

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



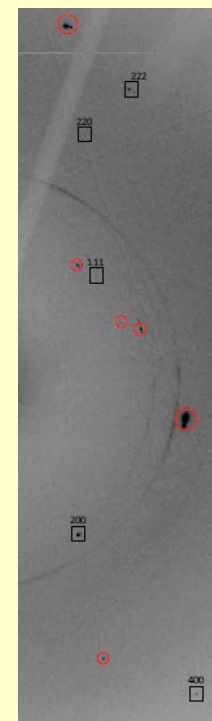
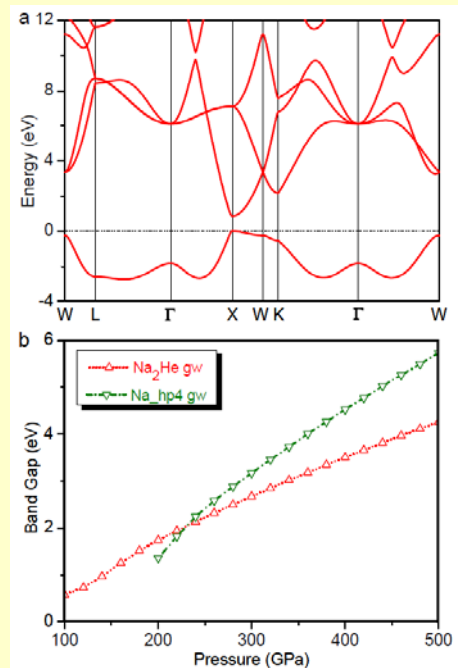
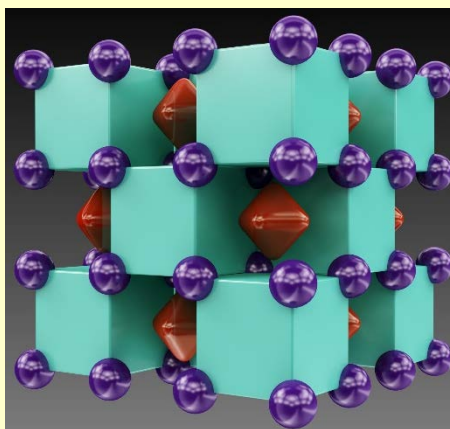
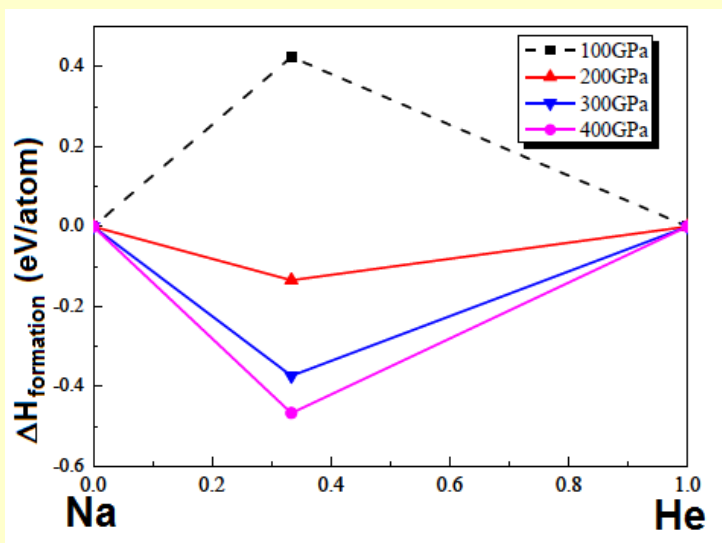
NaCl_3 : atomic and electronic structure, and experimental XRD pattern

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

Helium chemistry? Yes!

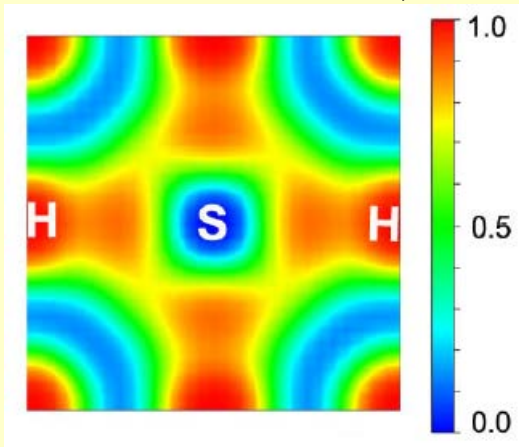
[Dong, Oganov, Goncharov, *Nature Chemistry* 2017]

- 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 NeHe₂ (Loubeyre et al., 1993).



1. Na₂He is stable at >113 GPa, at least up to 1000 GPa.
2. New stable helium compounds: Na₂HeO (Dong & Oganov, 2017); CaF₂He, MgF₂He (Liu, 2018).

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



OPEN

Pressure-induced metallization of dense $(\text{H}_2\text{S})_2\text{H}_2$ with high- T_c superconductivity

SUBJECT AREAS:
THEORY AND
COMPUTATION
CONDENSEDMATTER PHYSICS

Defang Duan^{1,2}, Yunxian Liu¹, Fubo Tian¹, Da Li¹, Xiaoli Huang¹, Zhonglong Zhao¹, Hongyu Yu¹, Bingbing Liu¹, Wenjing Tian² & Tian Cui¹

¹State Key Laboratory of Superhard Materials, College of physics, Jilin University, Changchun, 130012, P. R. China, ²State 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_2 -containing compounds $(\text{H}_2\text{S})_2\text{H}_2$ are elucidated by *ab initio* calculations. The ordered crystal structure with $P1$ symmetry is determined, supported by the good agreement between theoretical and experimental X-ray diffraction data, equation of states, and Raman spectra. The C_{2cm} structure is favorable with partial hydrogen bond symmetrization above 37 GPa. Upon further compression, H_2 molecules disappear and two intriguing metallic structures with $R3m$ and $Im-3m$ 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 $Im-3m$ 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.

Correspondence and requests for materials should be addressed to T.C. (tcui@jl.u.edu.cn)

SCIENTIFIC REPORTS | 4 : 6968 | DOI: 10.1038/srep06968

1

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

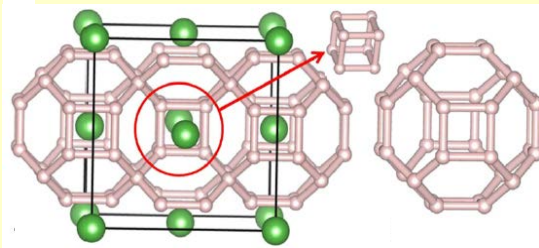
Nature (2015) | doi:10.1038/nature14964

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 system¹: 133 kelvin at ambient pressure² and 164 kelvin at high pressures³. 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 states⁴. 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 hydrides⁷, but only a moderate T_c of 17 kelvin has been observed experimentally⁸. Here we investigate sulfur hydride⁹, where a T_c of 80 kelvin has been predicted¹⁰. 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_2S , formed from H_2S_2 by decomposition under pressure. These findings raise hope for the prospects for achieving room-temperature superconductivity in other hydrogen-based materials.

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

And the record is broken again: LaH_{10} ($T_c = 250\text{-}260\text{ K}$ at 170 GPa)



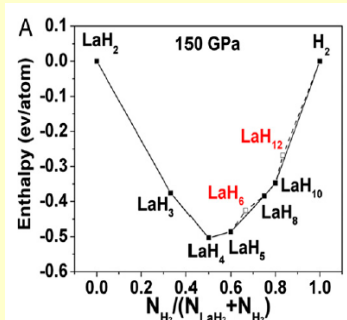
The maximal $T_c \sim 250\text{-}260\text{ K}$

Potential high- T_c superconducting lanthanum and yttrium hydrides at high pressure

Hanyu Liu^a, Ivan I. Naumov^b, Roald Hoffmann^c, N. W. Ashcroft^d, and Russell J. Hemley^{d,e,1}

^aGeophysical Laboratory, Carnegie Institution of Washington, Washington, DC 20015; ^bDepartment of Chemistry and Chemical Biology, Cornell University, Ithaca, NY 14853; ^cLaboratory of Atomic and Solid State Physics, Cornell University, Ithaca, NY 14853; ^dDepartment of Civil and Environmental Engineering, The George Washington University, Washington, DC 20052; and ^eSchool of Applied and Engineering Physics, Cornell University, Ithaca, NY 14853

Contributed by Russell J. Hemley, May 5, 2017 (sent for review March 20, 2017; reviewed by Panchapakesan Ganesh, Jeffrey M. McMahon, and Dimitrios Papaconstantopoulos)



Superconductivity at 215 K in lanthanum hydride at high pressures

A. P. Drozdov, V. S. Minkov, S. P. Besedin, P. P. Kong, M. A. Kuzovnikov, D. A. Knyazev, M. I. Erements

(Submitted on 21 Aug 2018)

Evidence for superconductivity above 260 K in lanthanum superhydride at megabar pressures

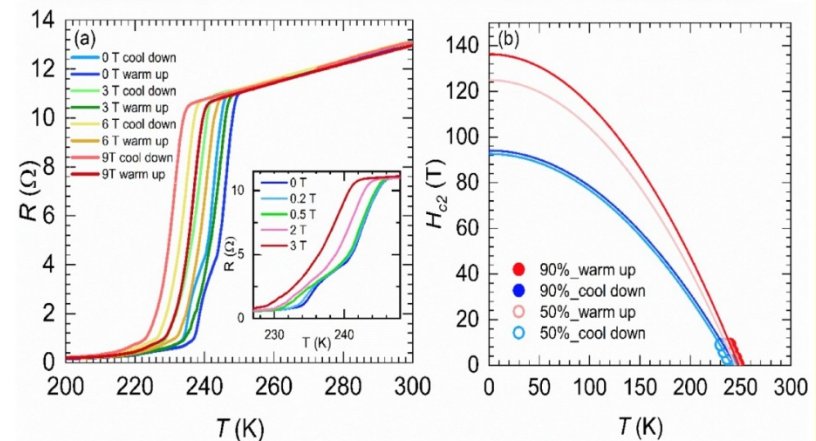
Maddury Somayazulu, Muhtar Ahart, Ajay K Mishra, Zachary M. Geballe, Maria Baldini, Yue Meng, Viktor V. Struzhkin, Russell J. Hemley

(Submitted on 23 Aug 2018 (v1), last revised 29 Aug 2018 (this version, v3))

Superconductivity at 250 K in lanthanum hydride under high pressures

A. P. Drozdov, P. P. Kong, V. S. Minkov, S. P. Besedin, M. A. Kuzovnikov, S. Mozaffari, L. Balicas, F. Balakirev, D. Graf, V. B. Prakapenka, E. Greenberg, D. A. Knyazev, M. Tkacz, M. I. Erements

(Submitted on 4 Dec 2018)



...and record is broken again: mysterious S-C-H compound ($T_c = 288 \text{ K}$ at 267 GPa)

Room-temperature superconductivity in a carbonaceous sulfur hydride

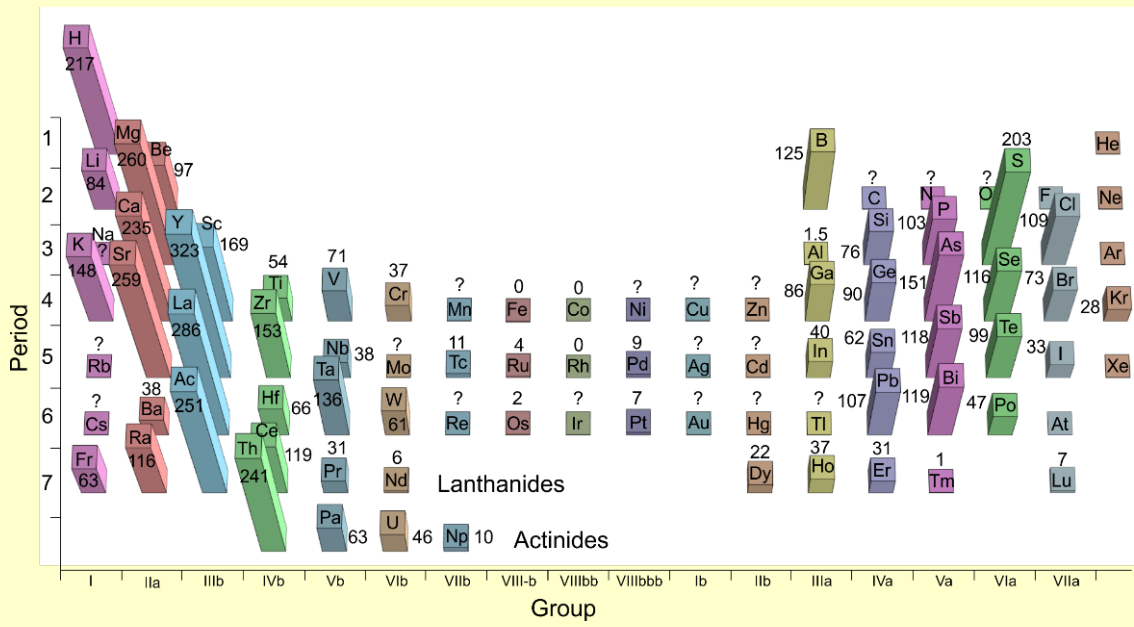
Elliot Snider, Nathan Dasenbrock-Gammon, Raymond McBride, Mathew Debessai, Hiranya Vindana, Kevin Vencatasamy, Keith V. Lawler, Ashkan Salamat & Ranga P. Dias 

Nature **586**, 373–377(2020) | [Cite this article](#)

One of the long-standing challenges in experimental physics is the observation of room-temperature superconductivity^{1,2}. Recently, high-temperature conventional superconductivity in hydrogen-rich materials has been reported in several systems under high pressure^{3,4,5}. An important discovery leading to room-temperature superconductivity is the pressure-driven disproportionation of hydrogen sulfide (H_2S) to H_3S , with a confirmed transition temperature of 203 kelvin at 155 gigapascals^{3,6}. Both H_2S and CH_4 readily mix with hydrogen to form guest–host structures at lower pressures⁷, and are of comparable size at 4 gigapascals. By introducing methane at low pressures into the $\text{H}_2\text{S} + \text{H}_2$ precursor mixture for H_3S , molecular exchange is allowed within a large assemblage of van der Waals solids that are hydrogen-rich with H_2 inclusions; these guest–host structures become the building blocks of superconducting compounds at extreme conditions. Here we report superconductivity in a photochemically transformed carbonaceous sulfur hydride system, starting from elemental precursors, with a maximum superconducting transition temperature of 287.7 ± 1.2 kelvin (about 15 degrees Celsius) achieved at 267 ± 10 gigapascals. The superconducting state is observed over a broad pressure range in the diamond anvil cell, from 140 to 275 gigapascals, with a sharp upturn in transition temperature above 220 gigapascals. Superconductivity is established by the observation of zero resistance, a magnetic susceptibility of up to 190 gigapascals, and reduction of the transition temperature under an external magnetic field of up to 9 tesla, with an upper critical magnetic field of about 62 tesla according to the Ginzburg–Landau model at zero temperature. The light, quantum nature of hydrogen limits the structural and stoichiometric determination of the system by X-ray scattering techniques, but Raman spectroscopy is used to probe the chemical and structural transformations before metallization. The introduction of chemical tuning within our ternary system could enable the preservation of the properties of room-temperature superconductivity at lower pressures.

Superconductivity is linked with Mendeleev's Table

[Semenok & Oganov, *JPCL*, 2018; *Curr. Opinion Solid St. Mater. Sci.*, 2020]



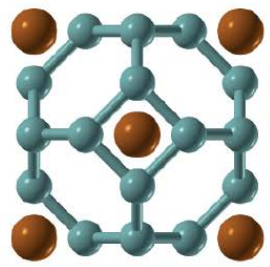
Distribution of Tc for hydrides

LaH₁₀: record Tc (260 K @ 190 GPa)
(Somayazulu et al., 2019).

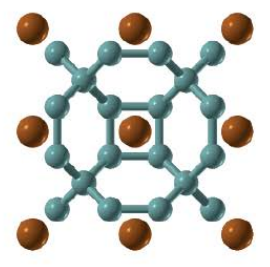
Test of idea: Th and Ac hydrides
have high-Tc superconductivity.

ThH₁₀: Tc=241 K at 100 GPa
(Kvashnin & Oganov, 2018).

Metal atom is VERY important!

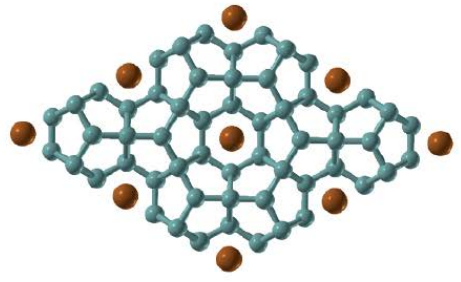


CaH₆
(T_c = 220–235 K)



LaH₁₀ (T_c = 274–286 K)
YH₁₀ (T_c = 305–326 K)

AcH₁₀ (T_c = 226–251 K)
ThH₁₀ (T_c = 220–241 K)



AcH₁₆
(T_c = 221–241 K)

Polyhydride superconductors: surge of interest!

nature
International journal of science

Letter | Published: 22 May 2019

Superconductivity at 250 K in lanthanum hydride under high pressures

A. P. Drozdov, P. P. Kong, V. S. Minkov, S. P. Besedin, M. A. Kuzovnikov, S. Mozaffari, L. Balicas, F. F. Balakirev, D. E. Graf, V. B. Prakapenka, E. Greenberg, D. A. Knyazev, M. Tkacz & M. I. Erements

Nature 569, 528–531 (2019) | Download Citation

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International journal of science

Letter | Published: 17 August 2015

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

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

Nature 525, 73–76 (03 September 2015) | Download Citation

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Article | Open Access | Published: 01 August 2019

Polyhydride CeH₉ with an atomic-like hydrogen clathrate structure

Xin Li, Xiaoli Huang, Defang Duan, Chris J. Pickard, Di Zhou, Hui Xie, Quan Zhuang, Yanping Huang, Qiang Zhou, Bingbing Liu & Tian Cui

Nature Communications 10, Article number: 3461 (2019) | Download Citation

materialstoday
Volume 33, March 2020, Pages 36–44

Research

Superconductivity at 161 K in thorium hydride ThH₁₀: Synthesis and properties

Dmitry V. Semenov, Alexander G. Kvashnin, Anna G. Ivanova, Volodymyr Svitlyk, Vyacheslav Yu. Fomin, Andrey V. Sadakov, Oleg A. Sobolevskiy, Vladimir M. Pudalov, Ivan A. Troyan, Artem R. Oganov

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Superconducting praseodymium superhydrides

Di Zhou^{1,2}, Dmitry V. Semenov^{1,2}, Defang Duan^{1,2}, Hui Xie¹, Wuhao Chen¹, Xiaoli Huang^{1,2}, Xin Li¹, Bingbing Liu¹, Tian Cui¹

Science Advances 28 Feb 2020
Vol. 6, no. 5, eaax6849
DOI: 10.1126/sciadv.aax6849

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High-Pressure Synthesis of Magnetic Neodymium Polyhydrides

Di Zhou, Dmitrii V. Semenov, Hui Xie, Xiaoli Huang*, Defang Duan, Alex Aperis, Peter M. Oppeneer, Michele Galasso, Alexey I. Kartsev, Alexander G. Kvashnin*, Artem R. Oganov*, and Tian Cui*

Cite this: *J. Am. Chem. Soc.* 2020, 142, 6, 2803–2811
Publication Date: January 22, 2020
<https://doi.org/10.1021/jacs.9b10439>
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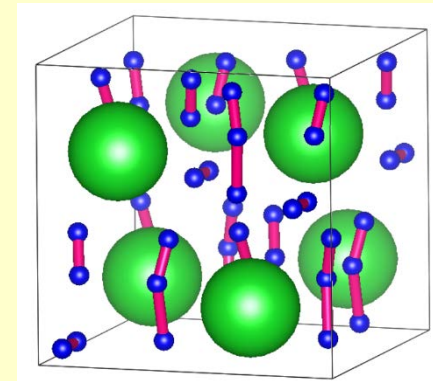
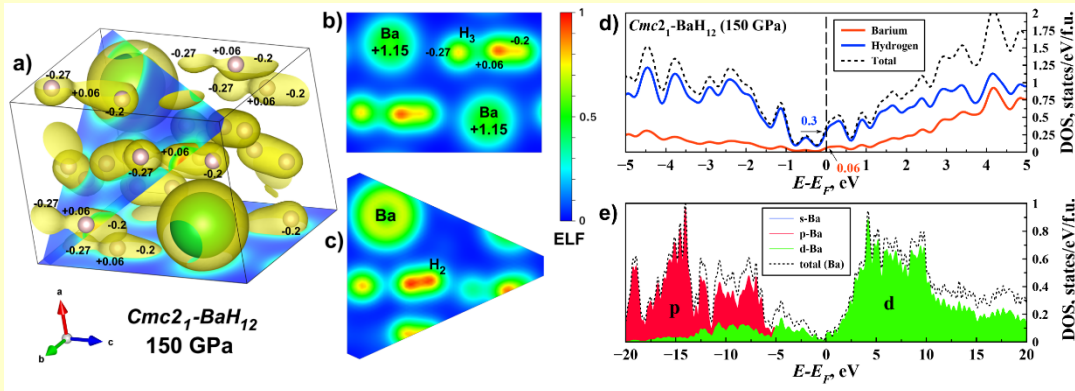
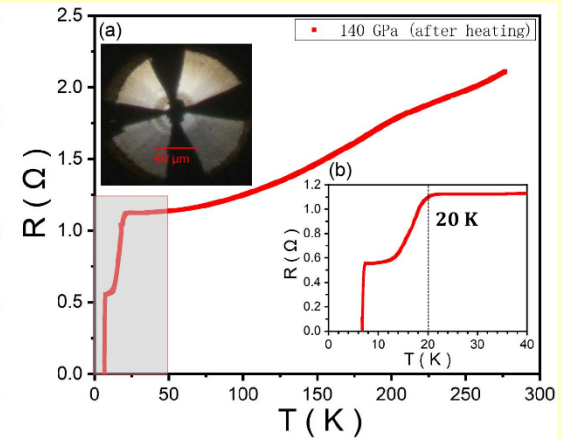
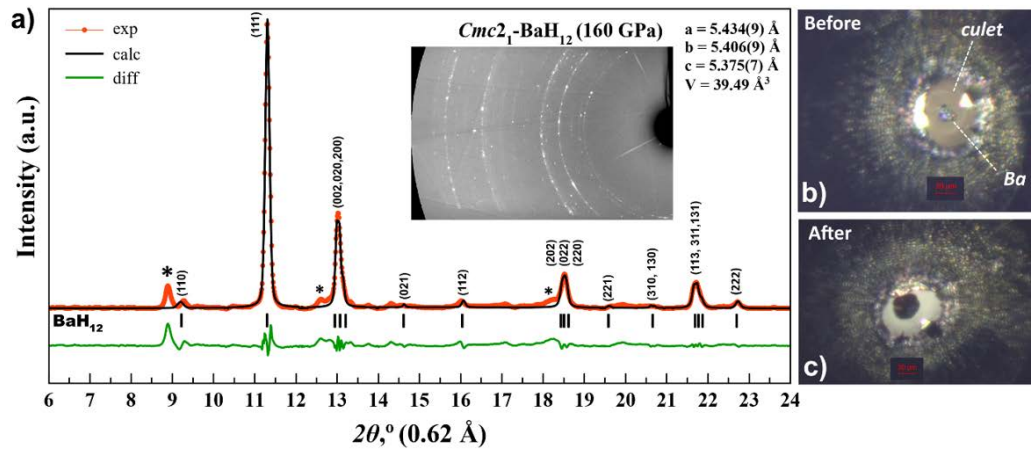
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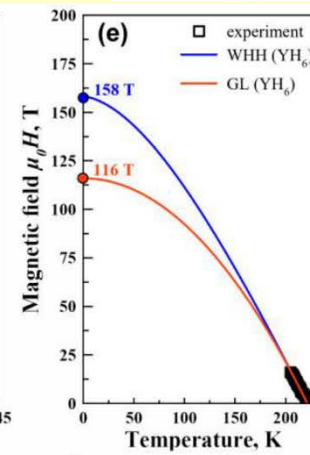
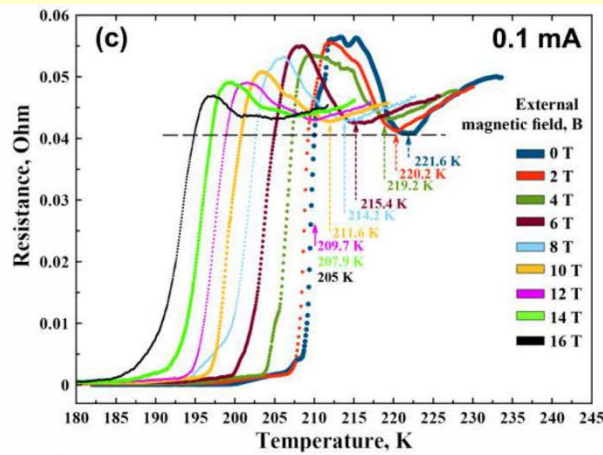
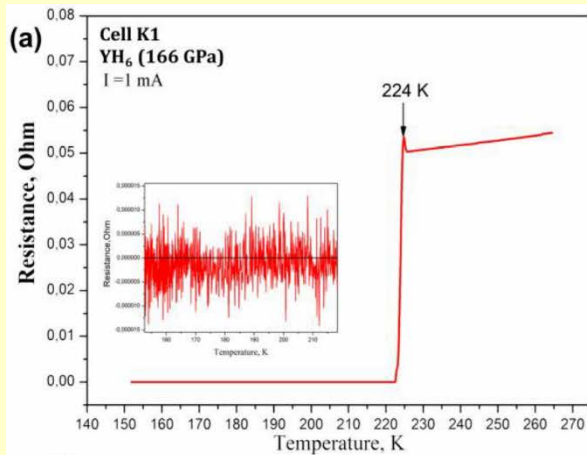
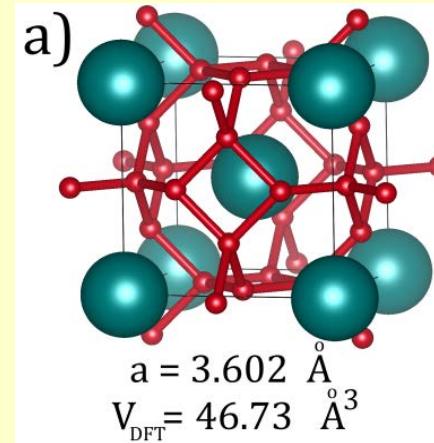
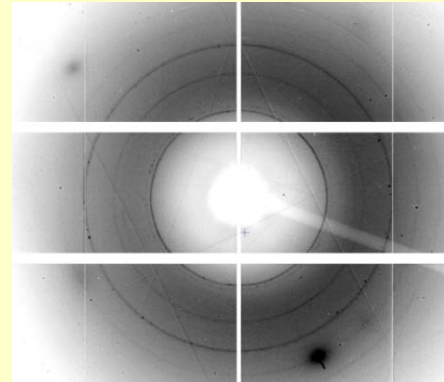
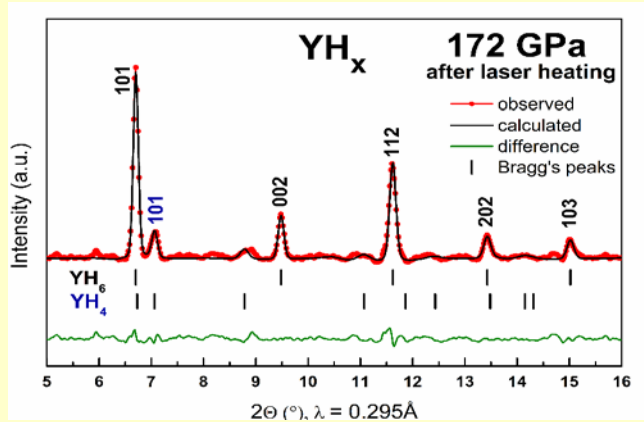
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Pseudocubic BaH₁₂: molecular metal

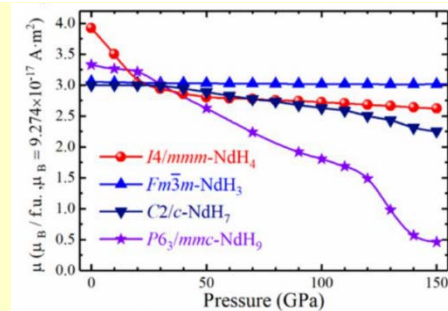
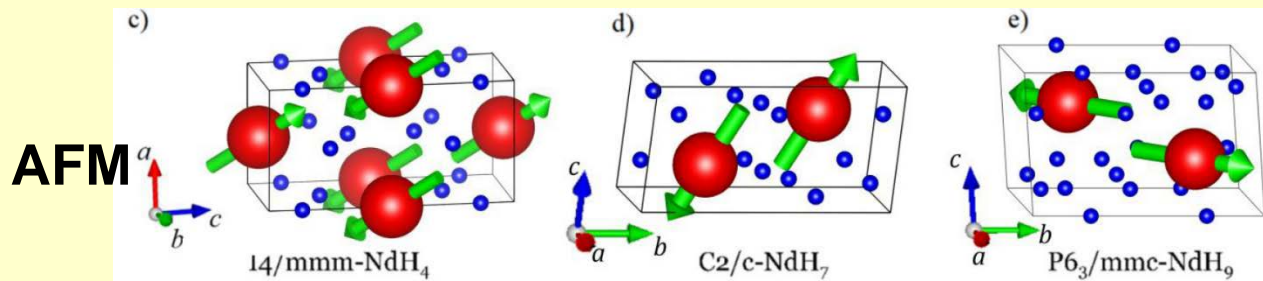
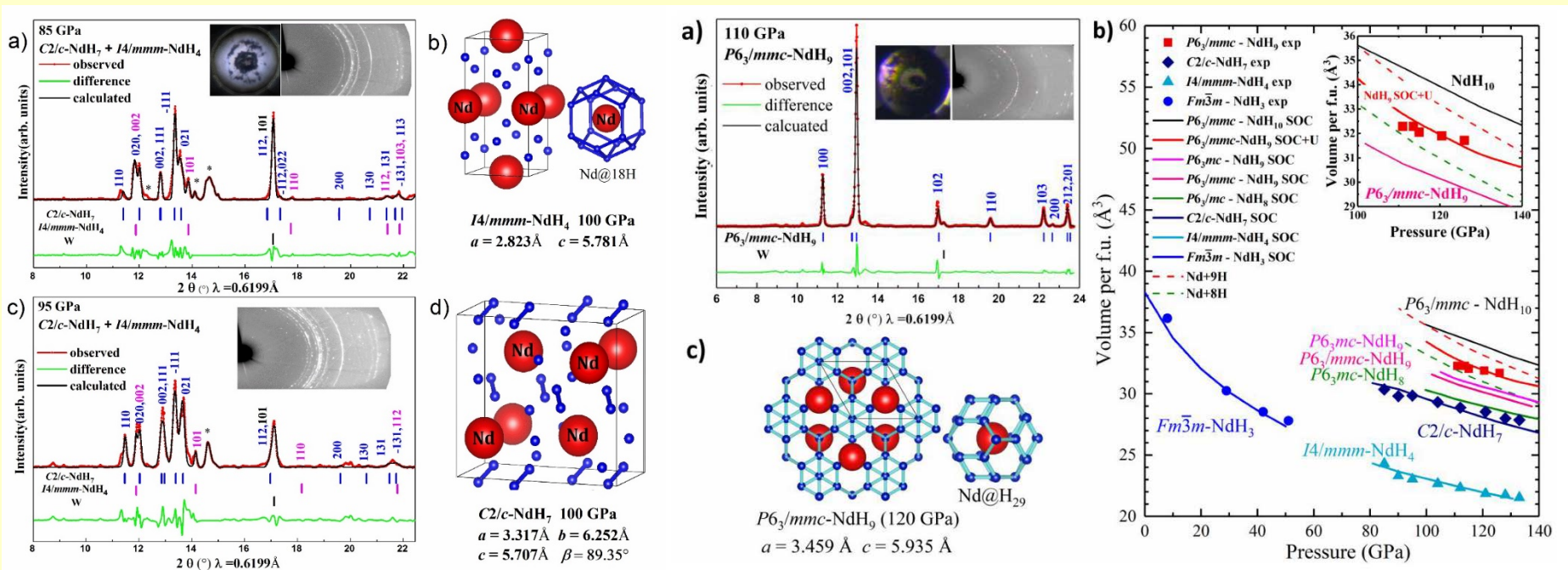


BaH₁₂ (H₂, H₃⁻ groups)

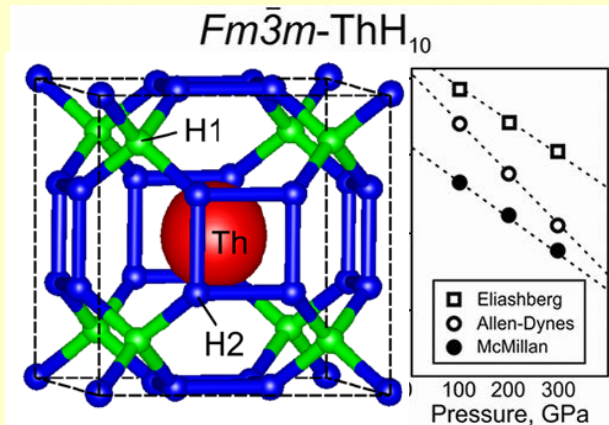
Yttrium hydride YH_6 ($T_C = 224 \text{ K}$, $B_C = 116\text{-}158 \text{ T}$)



Magnetic neodymium hydrides NdH_9 and NdH_7



Thorium hydride ThH_{10} ($T_C = 159\text{-}161\text{ K}$)



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Research Article

High-Temperature Superconductivity in a Th–H System under Pressure Conditions

Alexander G. Kvashnin^{1†}, Dmitrii V. Semenov^{2‡}, Ivan A. Kruglov^{3§}, Izabela A. Wrona⁴, and Artem R. Oganov^{1‡§}

¹ Skolkovo Institute of Science and Technology, Skolkovo Innovation Center, 3 Nobel Street, Moscow 143026, Russia
² Moscow Institute of Physics and Technology, 9 Institutskiy Lane, Dolgoprudny 141700, Russia
³ Dukhov Research Institute of Automatics (VNIIA), Moscow 127055, Russia
⁴ Institute of Physics, Jan Dlugosz University in Czestochowa, Armii Krajowej 13/15 Avenue, 42-200 Czestochowa, Poland
⁵ International Center for Materials Discovery, Northwestern Polytechnical University, Xi'an 710072, China

ACS Appl. Mater. Interfaces, 2018, 10 (50), pp 43809–43816
 DOI: 10.1021/acsami.8b17100
 Publication Date (Web): December 4, 2018
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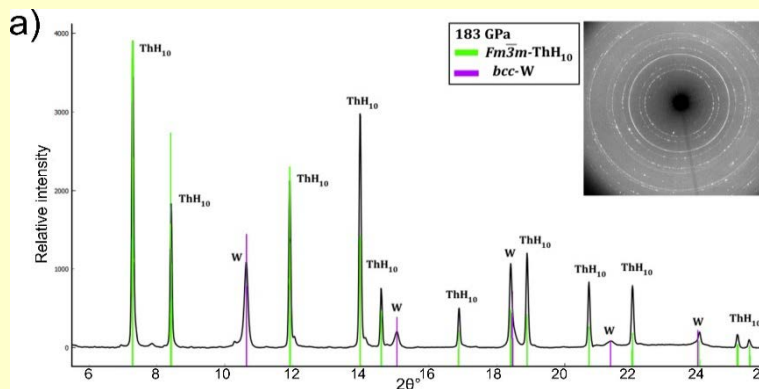
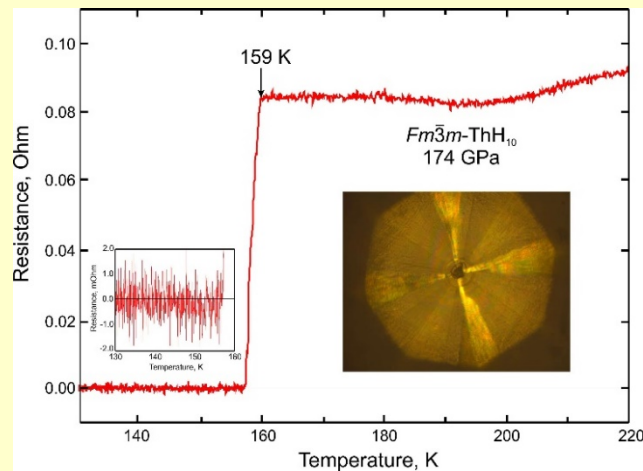
*E-mail: A.Kvashnin@skoltech.ru (A.G.K.), *E-mail: A.Oganov@skoltech.ru (A.R.O.)

Cite this: ACS Appl. Mater. Interfaces 2018, 10, 50, 43809–43816

RIS Citation GO

We predicted ThH_{10} in 2018 -

and just a year later we made it in the diamond anvil cell at 174 GPa!



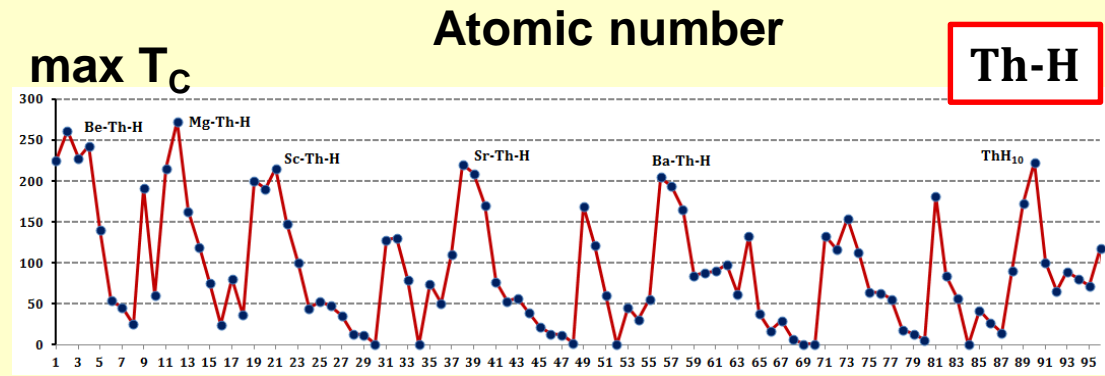
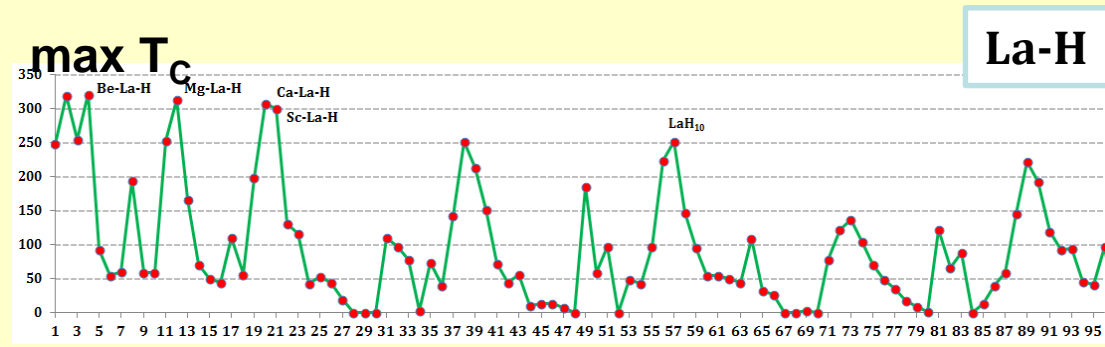
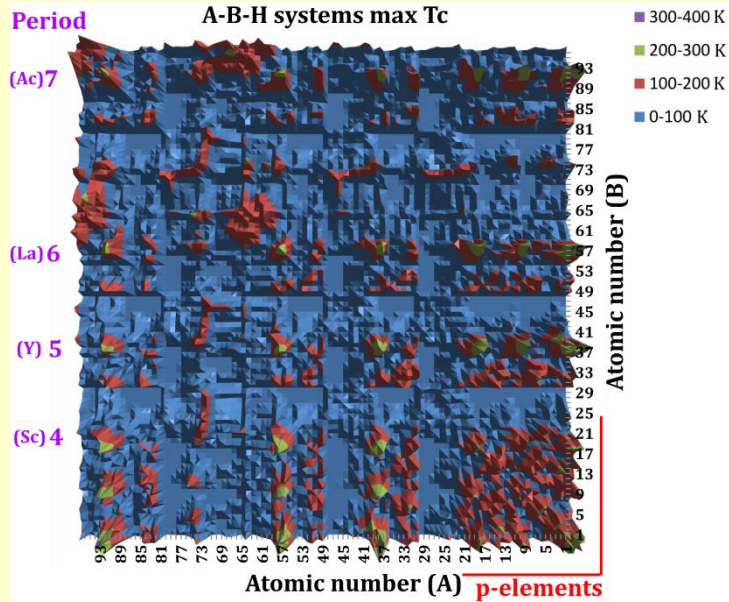
At higher chemical complexity, we may get higher T_c

Element	T_c (K)	Element	T_c (K)	Element	T_c (K)
Al	1.19	Nb	9.2	Tc	7.8
Be	0.026	Np	0.075	Th	1.37
Cd	0.55	Os	0.65	Ti	0.39
Ga	1.09	Pa	1.3	Tl	2.39
Hf	0.13	Pb	7.2	U	0.2
Hg	4.15	Re	1.7	V	5.3
In	3.40	Rh	0.0003	W	0.012
Ir	0.14	Ru	0.5	Zn	0.9
La	4.8	Sn	3.75	Zr	0.55
Mo	0.92	Ta	4.39		

Compound	T_c (K)	Compound	T_c (K)	Compound	T_c (K)
Nb ₃ Sn	18.1	MgB ₂	39	UPt ₃	0.5
Nb ₃ Ge	23.2	PbMo ₆ S ₈	15	UPd ₂ Al ₃	2
Cs ₃ C ₆₀	19	YPd ₂ B ₂ C	23	(TMTSF) ₂ ClO ₄	1.2
Cs ₃ C ₆₀	40	HoNi ₂ B ₂ C	7.5	(ET) ₂ Cu[Ni(CN) ₂]Br	11.5

High- T_c superconductor	T_c (K)	High- T_c superconductor	T_c (K)
La _{1.83} Sr _{0.17} CuO ₄	38	Tl ₂ Ba ₂ Ca ₂ Cu ₃ O _{10+x}	125
YBa ₂ Cu ₃ O _{6+x}	93	HgBa ₂ Ca ₂ Cu ₃ O _{8+x}	135
Bi ₂ Sr ₂ Ca ₂ Cu ₃ O _{10+x}	107	Hg _{0.8} Tl _{0.2} Ba ₂ Ca ₂ Cu ₃ O _{8.33}	134

A glimpse at superconductivity of ternary hydrides



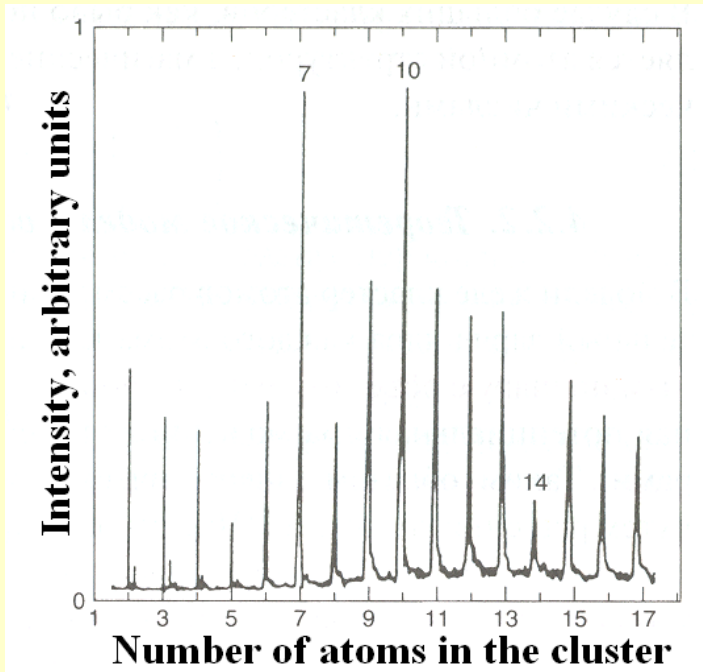
Ternary hydrides may have higher T_c at lower pressure and lower hydrogen content

Atomic number

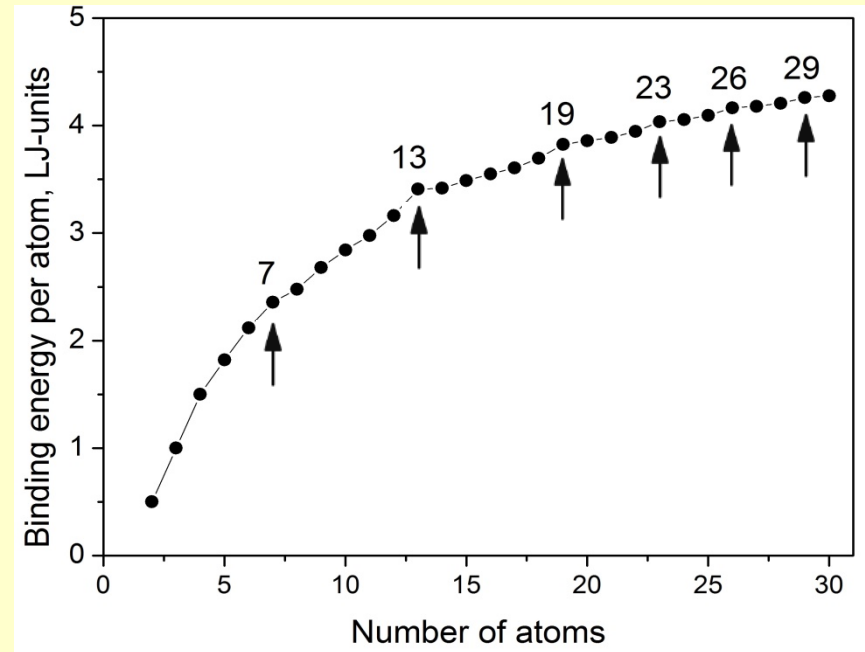
Predicting Stable Nanoclusters

- Only conditional stability. Magic clusters. Similar to atomic nuclei.**
- Unusual stable compositions are typical.**
- Explanation of carcinogenicity of oxide dust?**

Stability of nanoparticles: conditional

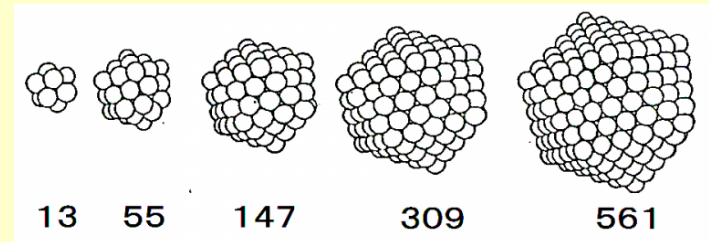


Mass spectrum of Pb_n clusters
(Poole & Owens, 2003)



Lennard-Jones clusters

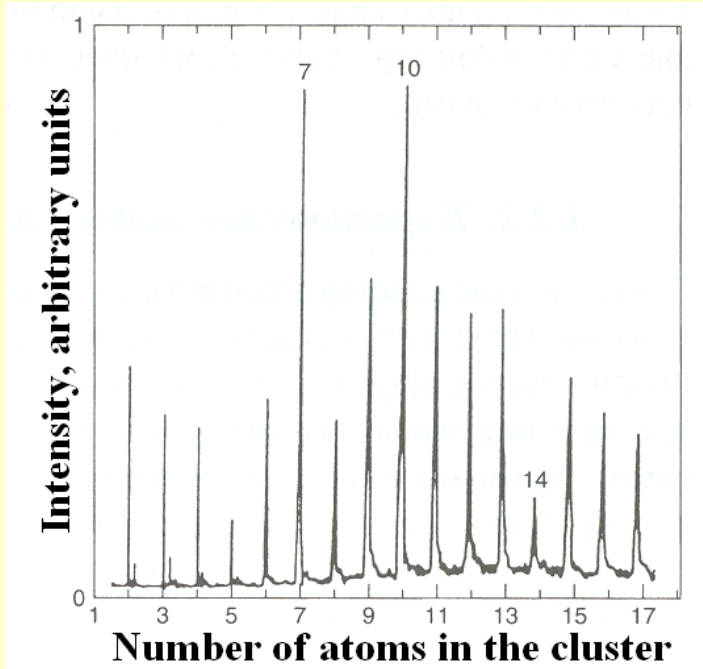
↑ – “magic” clusters



Stability grows with cluster size. We define stability relative to neighboring compositions. Especially stable clusters have filled electronic and/or structural shells.

Stability of clusters

Real system: Pb clusters

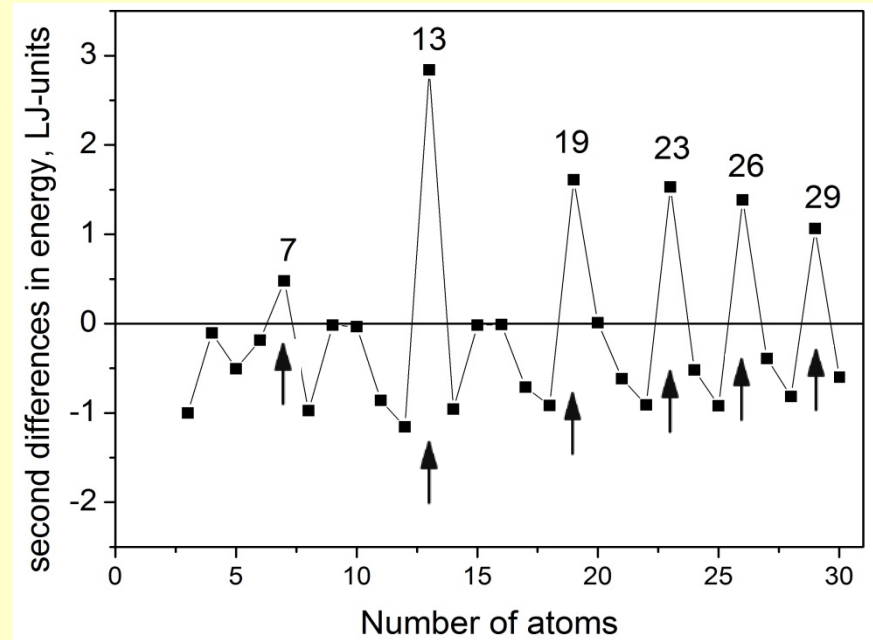


Mass-spectrum of Pb_n clusters
(from Poole & Owens, 2003)

Criterion of local stability (**magic clusters**):

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

Model system: Lennard-Jones clusters



↑ – magic clusters.

For binary clusters (A_mB_n):

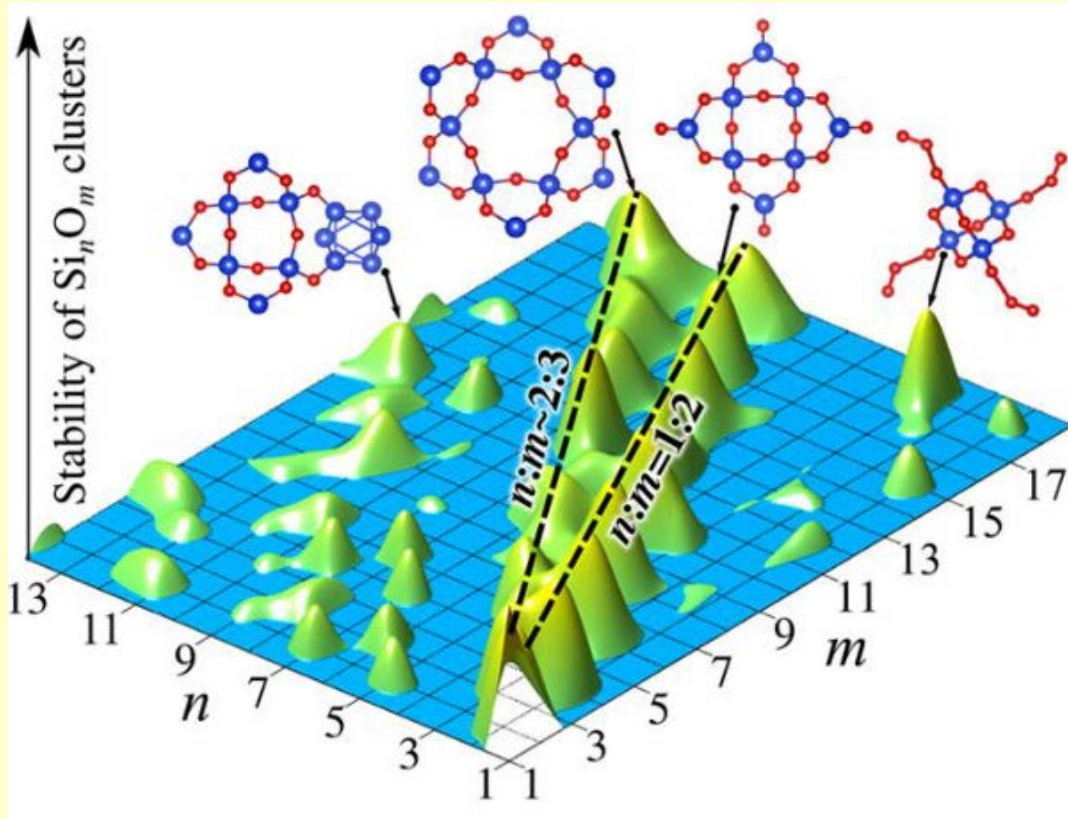
$$\Delta_x^2 E = E(m, n+1) + E(m, n-1) - 2E(m, n) > 0$$

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

Map of stability of Si-O clusters

[Lepeshkin & Oganov, *J. Phys. Chem. Lett.* 2019]

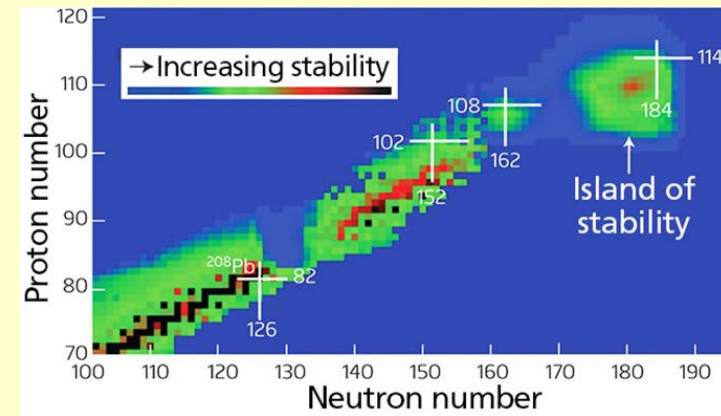
Si-O



Ridges of stability: SiO₂, Si₂O₃
 Islands of stability: e.g., Si₄O₁₈

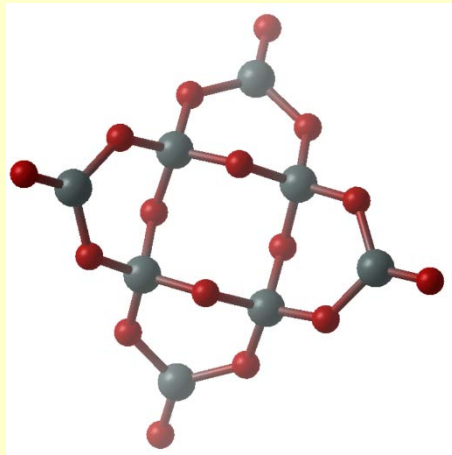
«Magic» nuclei: with filled proton or neutron shells (2, 8, 20, 28, 50, 82, 126 p or n)
 (1s²/2p⁶/3d¹⁰2s²/4f⁸/4f⁶3p⁶5g¹⁰/5g⁸4d¹⁰3s²6h¹²)

Magic numbers of electrons = 2, 10, 18, 36, 54, 86, 118)

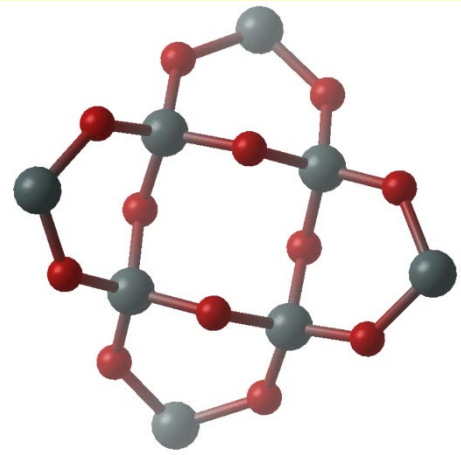


Analogy with
 magic atomic nuclei

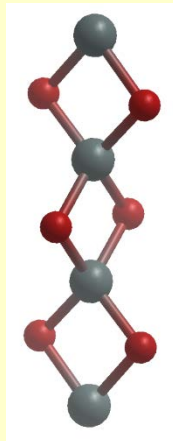
Si-O



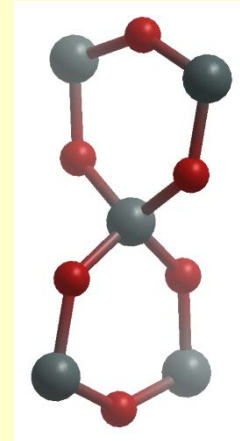
Si₈O₁₆



Si₈O₁₂

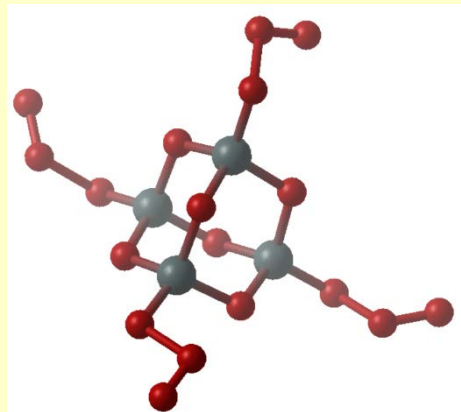


Si₄O₆

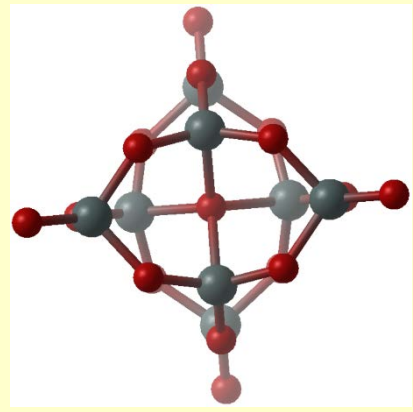


Si₅O₆

Magic clusters. Non-magnetic

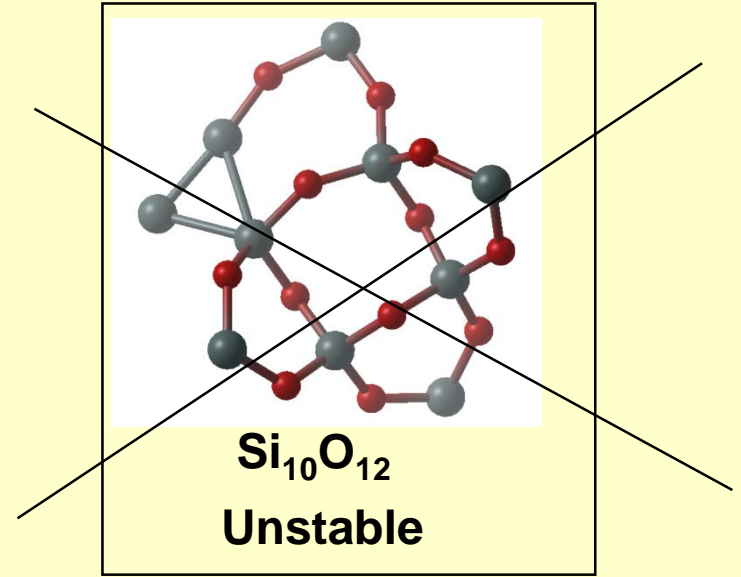


Si₄O₁₈



Si₈O₁₇

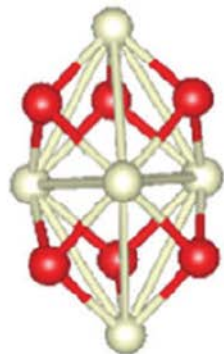
Magic magnetic(!) clusters. Excess of O



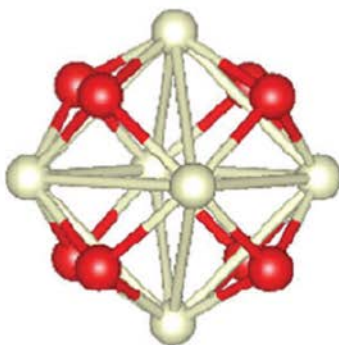
**Si₁₀O₁₂
Unstable**

Unusual compositions of transition metal oxide clusters

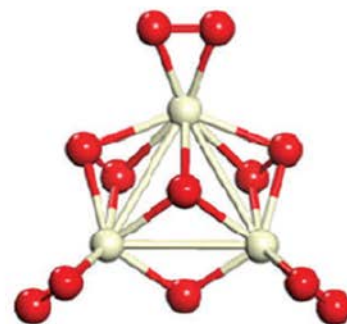
[Yu & Oganov, *Phys. Chem. Chem. Phys.*, 2018]



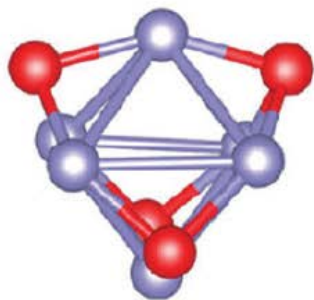
Ce_5O_6 (D_{3h} , 5A_1)



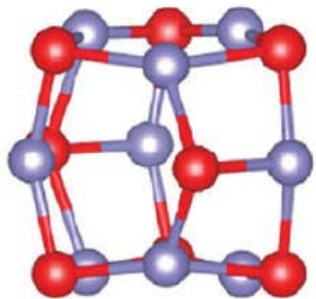
Ce_6O_8 (O_h , $^7A_{1g}$)



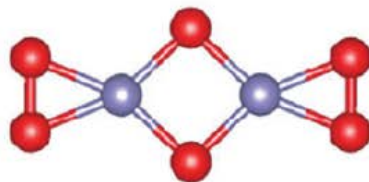
Ce_3O_{12} (C_s , $^3A'$)



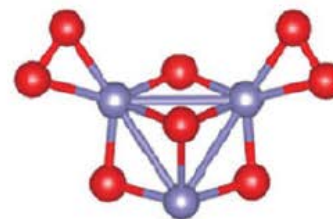
Fe_6O_4 (T_d , 1A_1)



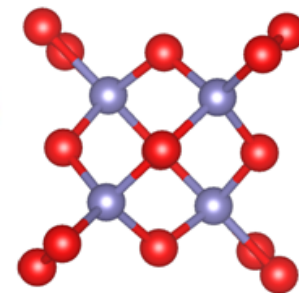
Fe_9O_8 (C_s , $^5A'$)



Fe_2O_8 (C_{2v} , 1A_2)



Fe_3O_8 (C_s , $^3A'$)



Fe_4O_{14} (D_{2d} , 1A)

Do crystals grow from such particles?

Predicting Optimal Materials

- Superior thermoelectrics: possible!**
- New superhard materials: WB_5 etc.**

- Pareto optimization of properties & stability.**
- Mendelevian search for exploring chemical space.**

Towards materials design: example of thermoelectrics

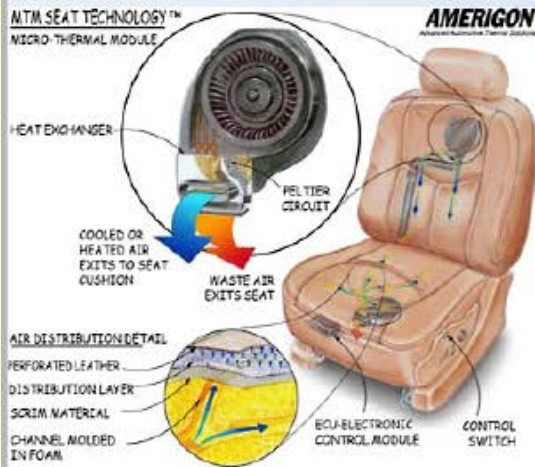
Applications

Water/Beer/Wine Cooler



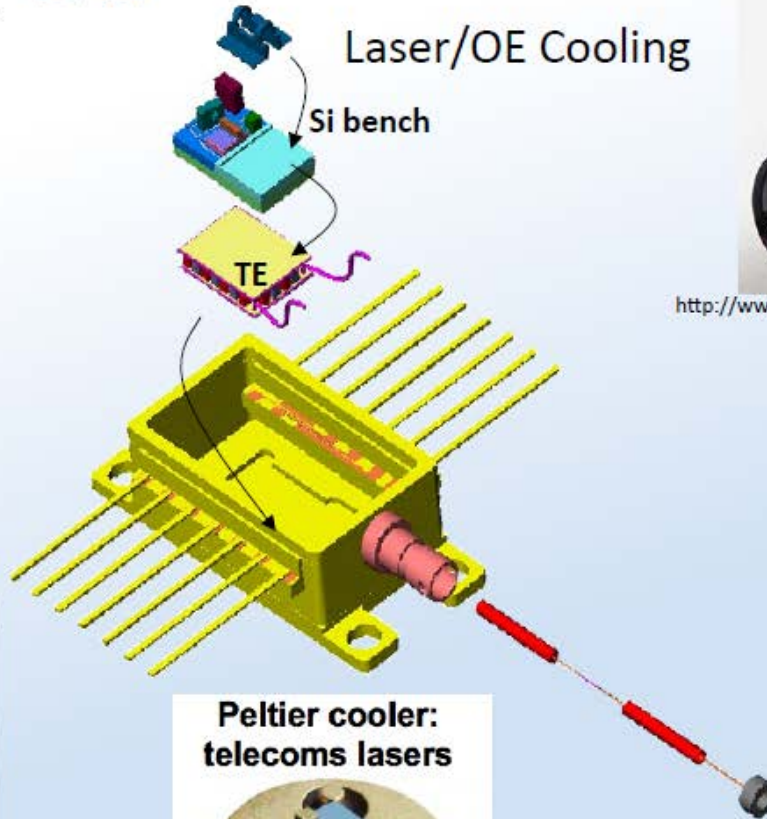
www.kingsbottle.com

Cooled Car Seat



http://wardsauto.com/ar/cooled_seats_mpg

Laser/OE Cooling



Peltier cooler: telecom lasers



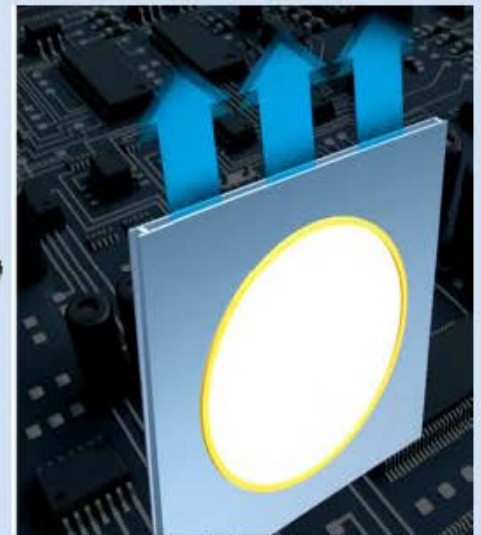
Copyright Micropelt

Cryogenic IR Night Vision



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

Electronic Cooling

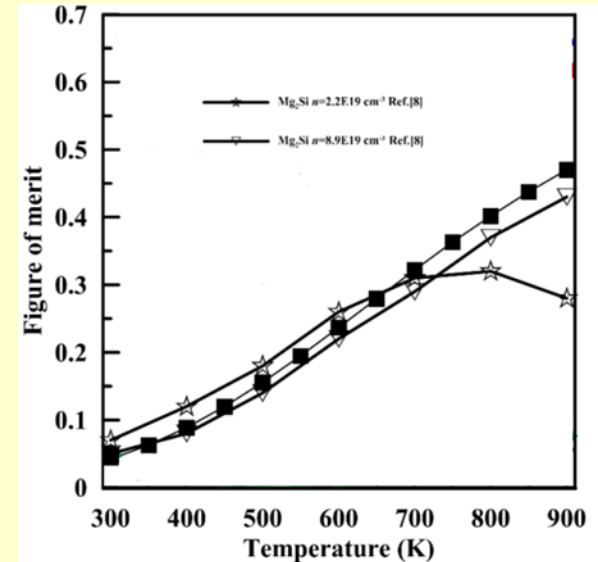
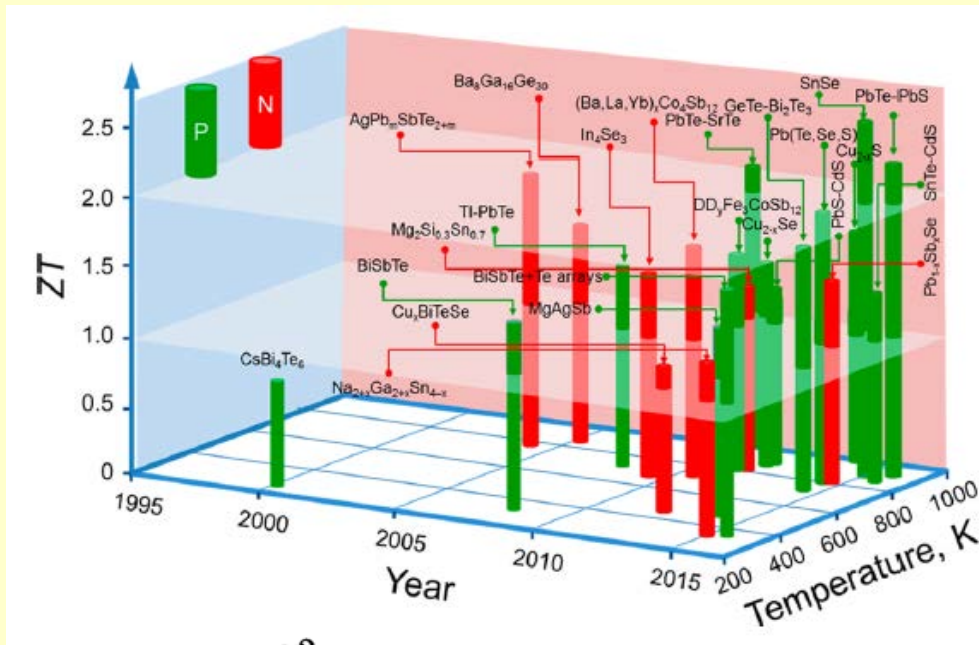


<http://www.gizmag.com/ge-dual-piezo-cooling-jet/25447/>

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)]

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

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

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

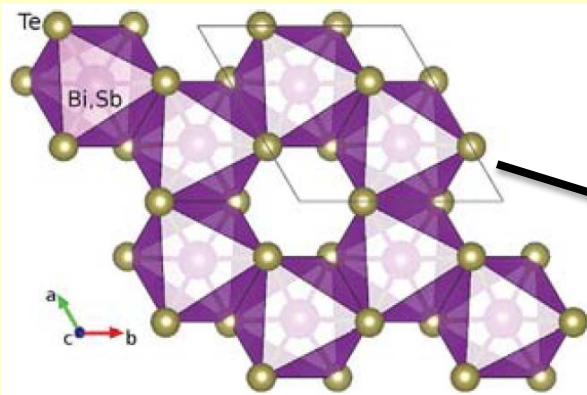
- efficiency

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

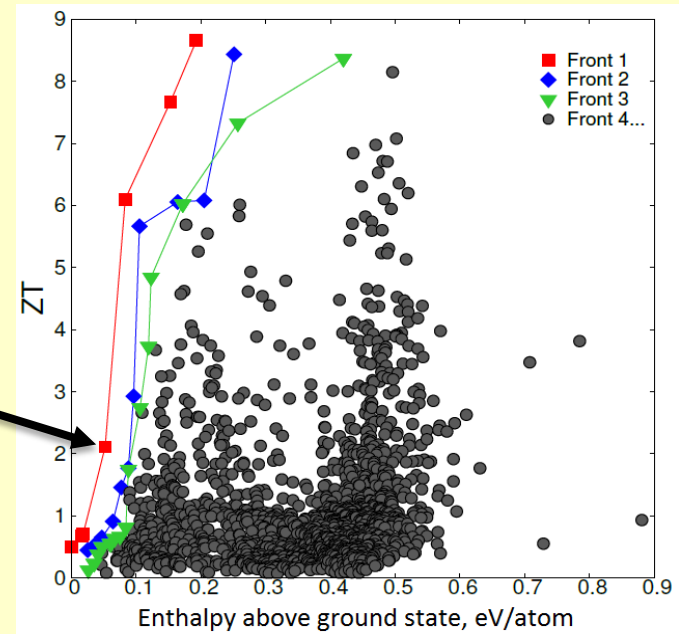
Computer Physics Communications 222 (2018) 152–157

Efficient technique for computational design of thermoelectric materials

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

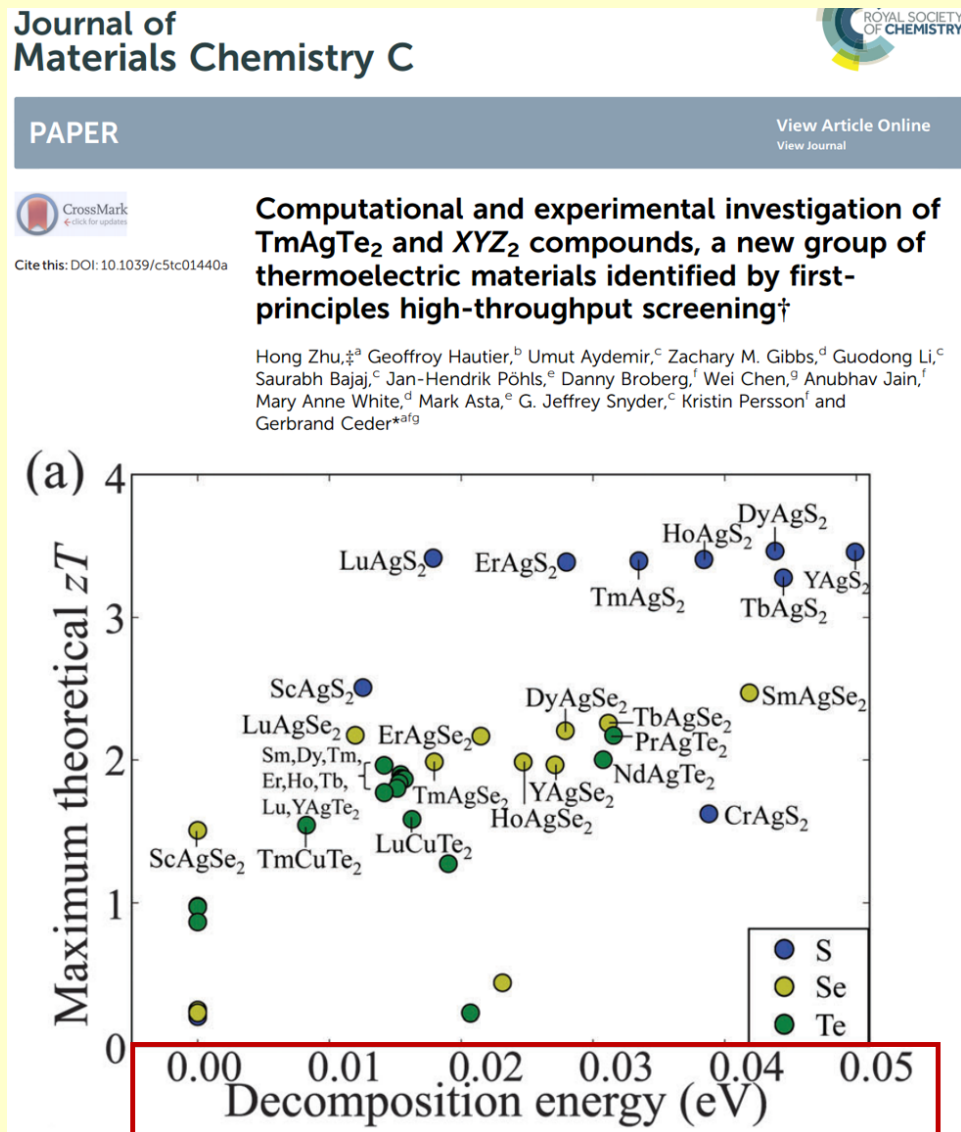


Predicted $P6_3cm$ structure of Bi_2Te_3

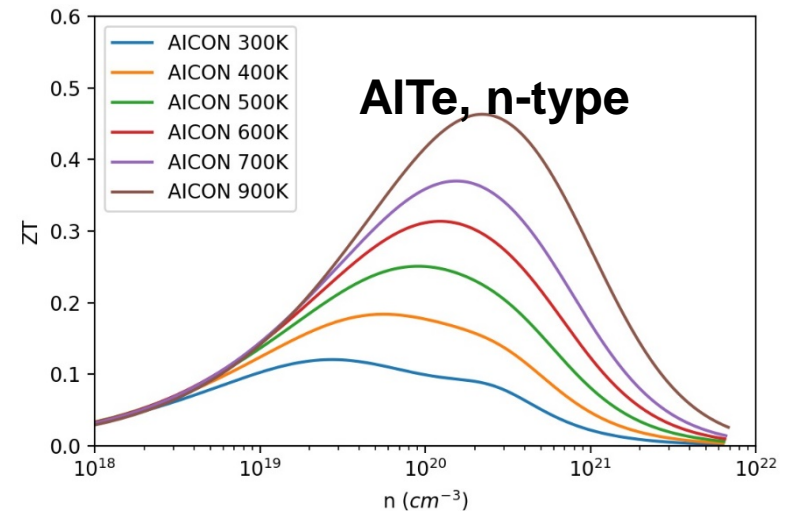
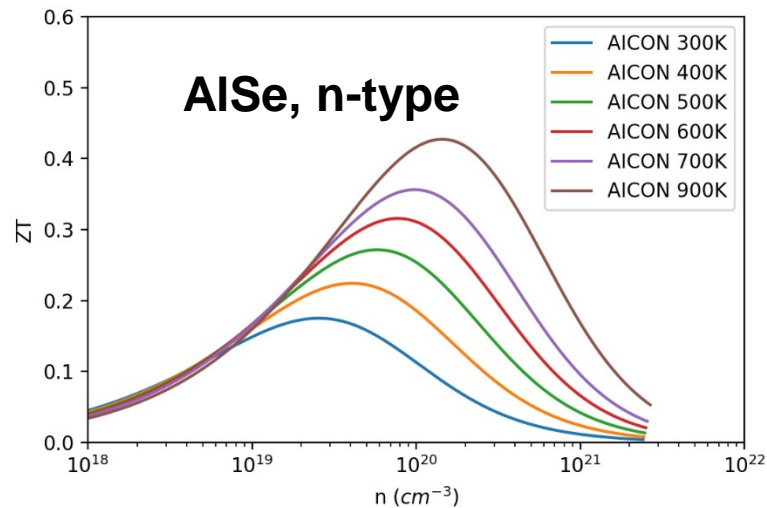
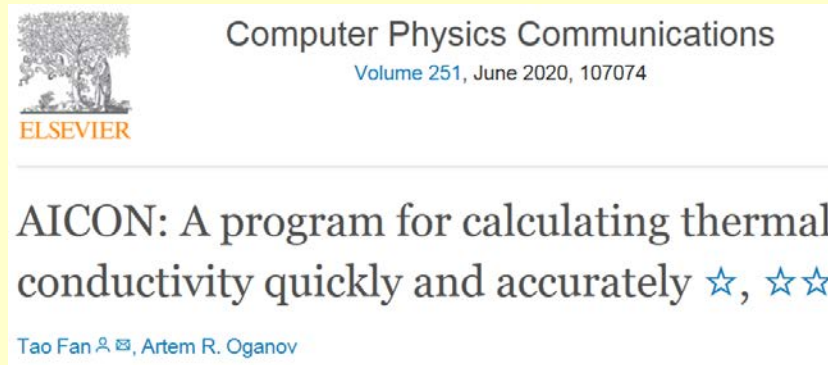


Pareto optimization of ZT and stability in the Bi-Te system

Similar conclusions from data mining



Fast and reliable calculations of thermoelectric properties are enabled by AICON program (Fan & Oganov, 2020; Fan & Oganov, submitted).

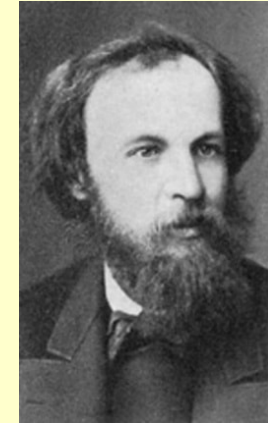
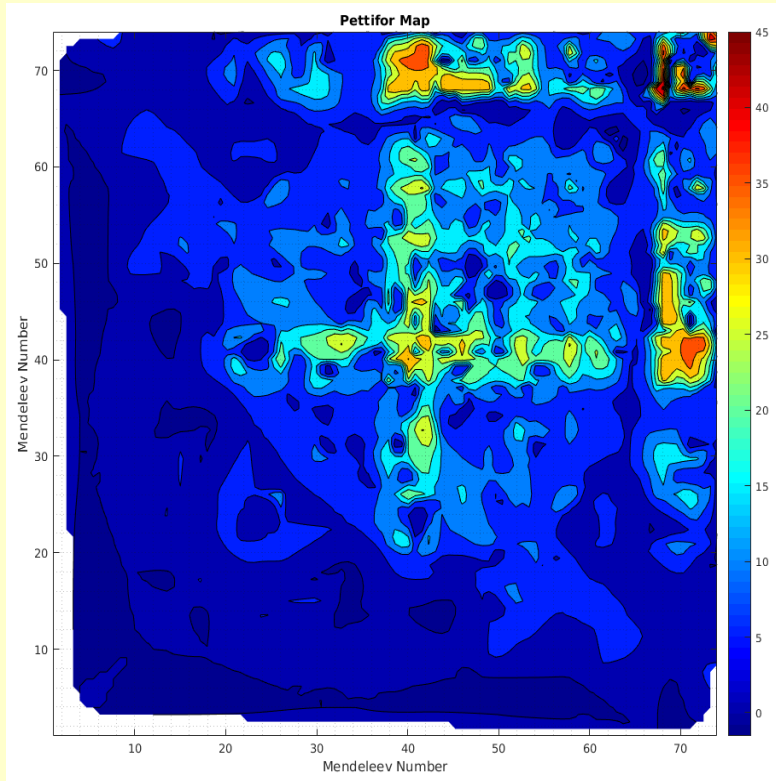


We can simultaneously optimize composition, structure, stability and other properties for a given chemical system.

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

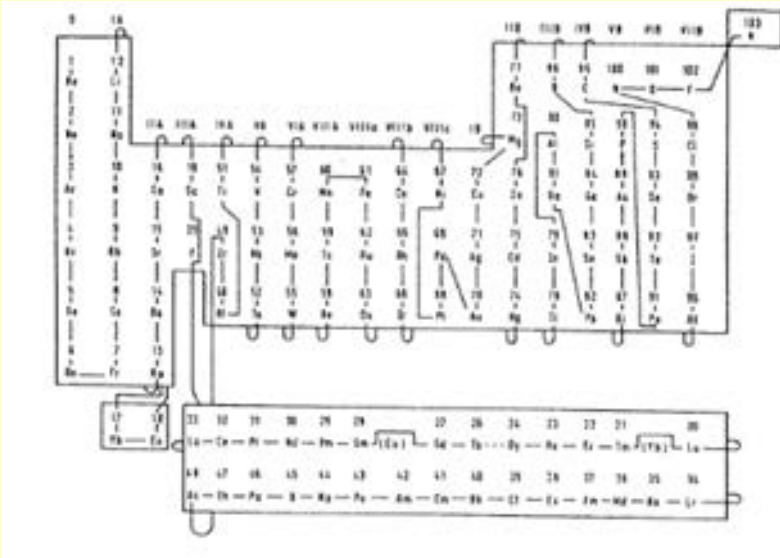
Mendelevian Search – breakthrough method for discovering best materials among all possible compounds

[Allahyari & Oganov, *NPJ Comp. Mat.*, 2020]



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

Mendeleev number (Pettifor, 1984). Prediction of stability, structure, and properties of materials



Mendeleev numbers of the elements

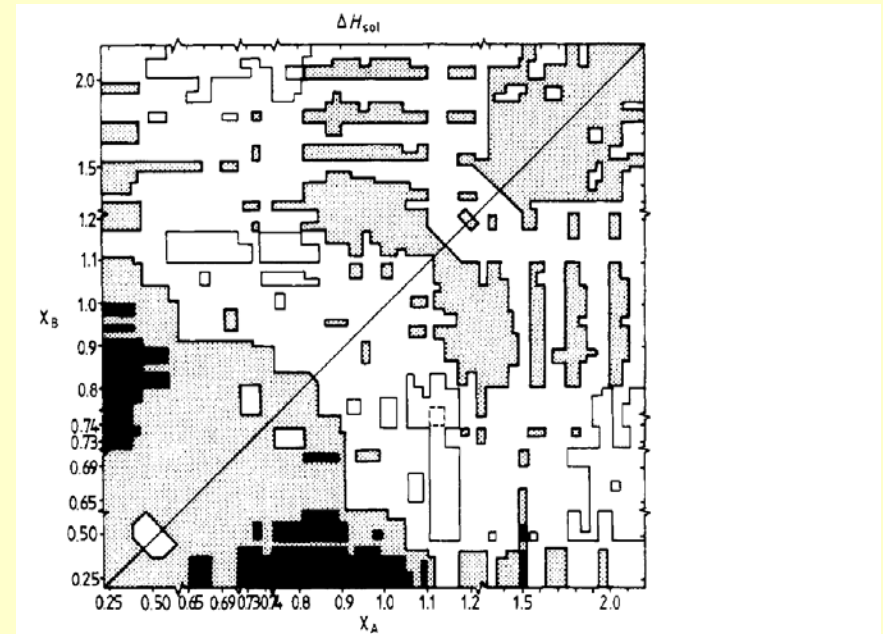


Figure 5. The heat of solution of B in liquid metal A according to the semi-empirical model of Miedema *et al* (1977). The full-solid lines and the diagonal correspond to the contour $\Delta H_{sol} = 0$. The dotted and full shaded regions correspond to $0 < \Delta H_{sol} < 200$ and $\Delta H_{sol} > 200 \text{ kJ mol}^{-1}$ respectively. The light full and broken lines correspond to the contours $\Delta H_{sol} = -200$ and $\Delta H_{sol} = -400 \text{ kJ mol}^{-1}$ respectively.

Enthalpies of formation of compounds

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

[Pettifor, 1984; Allahyari & Oganov, *NPJ Comp. Mat.*, 2020; *J. Phys. Chem. C*, in press]

Mendeleev Number	Atom	Mendeleev Number	Atom	Mendeleev Number	Atom
1	Fr	32	Tl	62	Po
2	Ce	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				

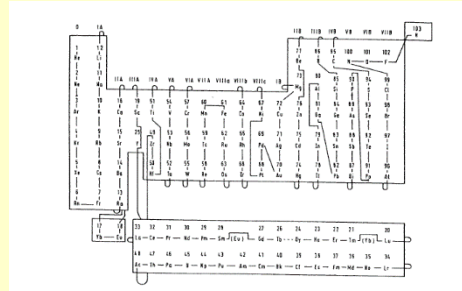
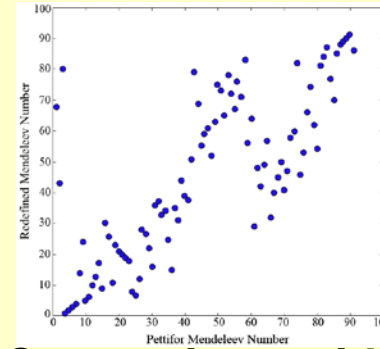
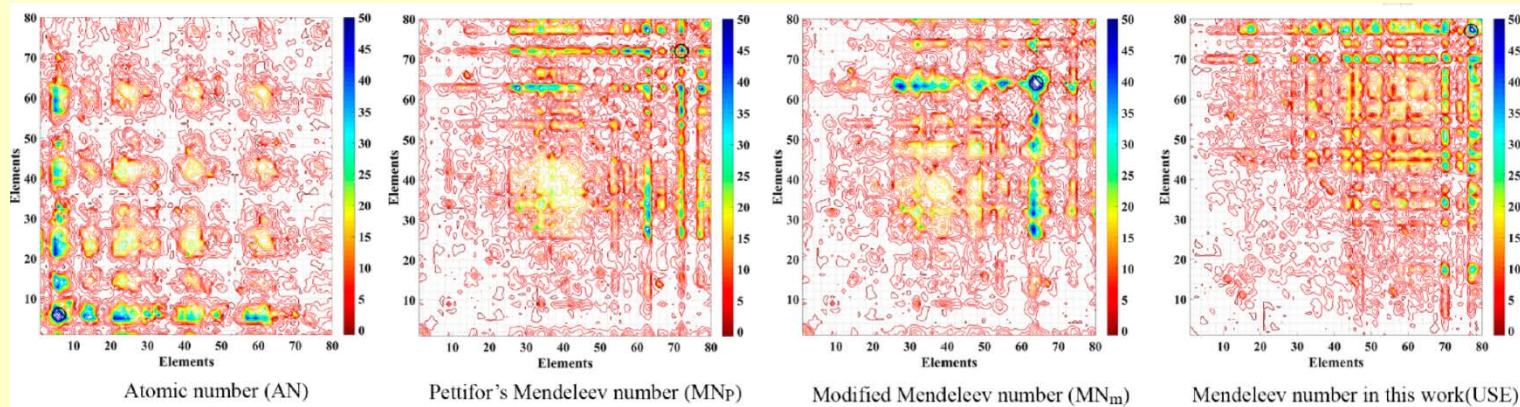


Fig. 1.8 The string running through this modified periodic table puts all the elements in sequential order, given by the relative ordering number *n*. From Pettifor (1988).

Pettifor's construction



Comparison with Pettifor's numbers

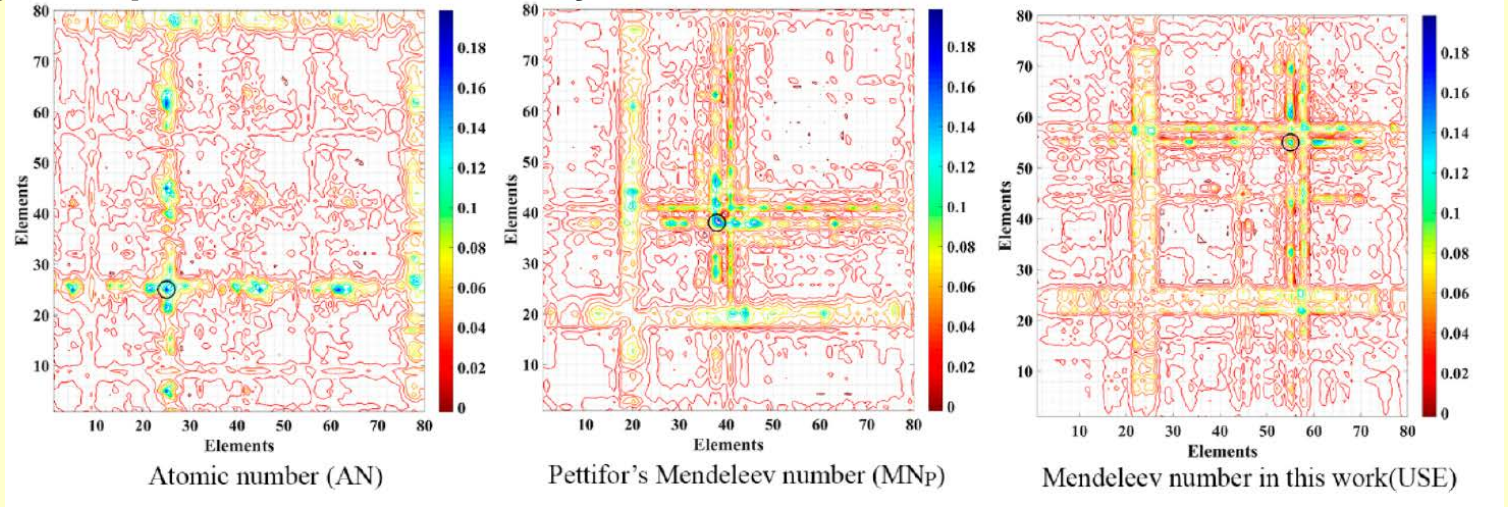


Grouping of hardness by (a) sequential number, empirical (Pettifor's and Glawe's) and our non-empirical Mendeleev numbers.

Non-empirical Mendeleev numbers work best

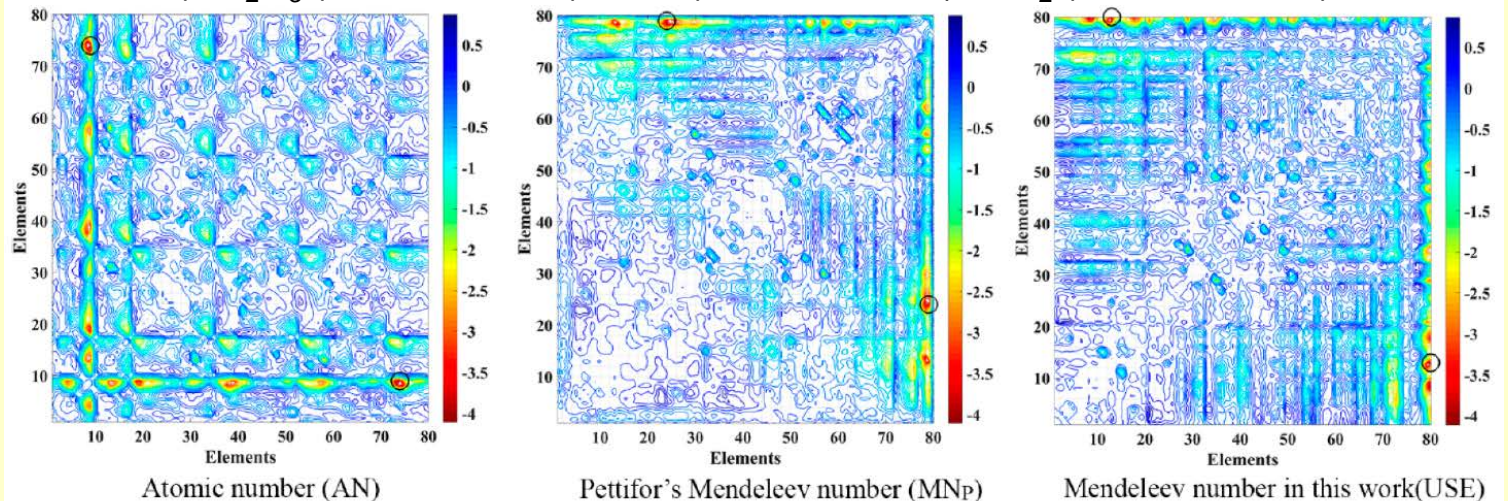
[Allahyari & Oganov, *J.Phys.Chem. C.*, in press]

Highly ferromagnetic phases are formed by Fe and Co, some lanthanoids and actinoids



Most exothermic compounds are formed by very different elements:

ThF₄ (-4.11 eV/atom), AcF₃ (-4.09 eV/atom), CaF₂ (-3.92 eV/atom), ZrF₄ (-3.62 eV/atom), Th₄O₇ (-3.61 eV/atom), Y₂O₃ (-3.48 eV/atom), Al₂O₃ (-2.95 eV/atom), CaO (-2.95 eV/atom), SiO₂ (-2.79 eV/atom).

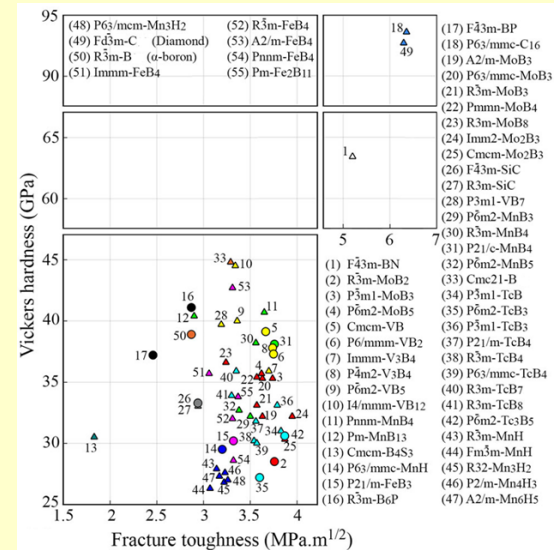
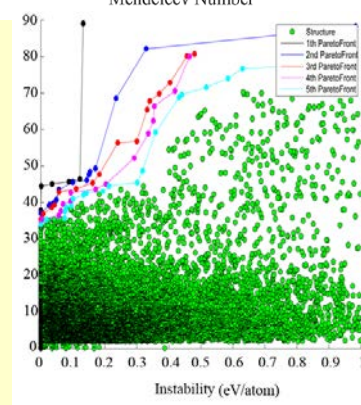
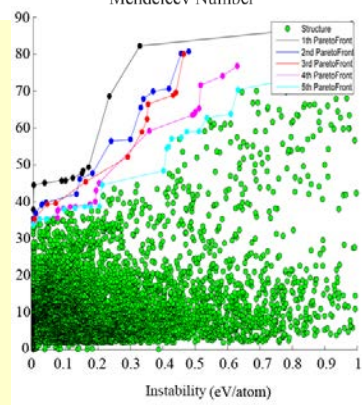
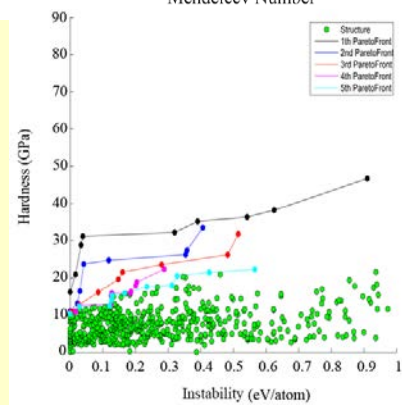
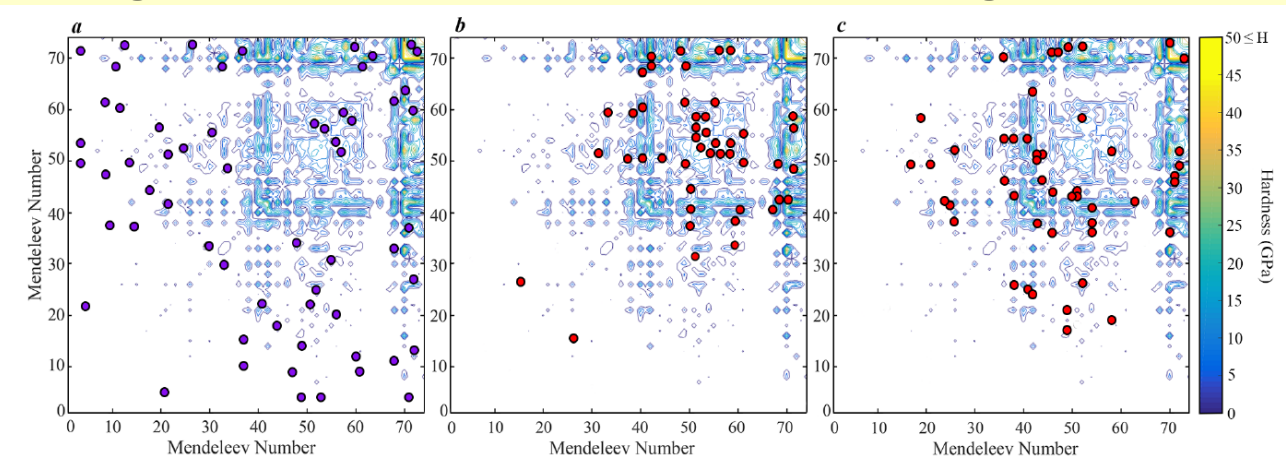


Mendelevian search for the hardest possible material: diamond and lonsdaleite are found!

1st generation

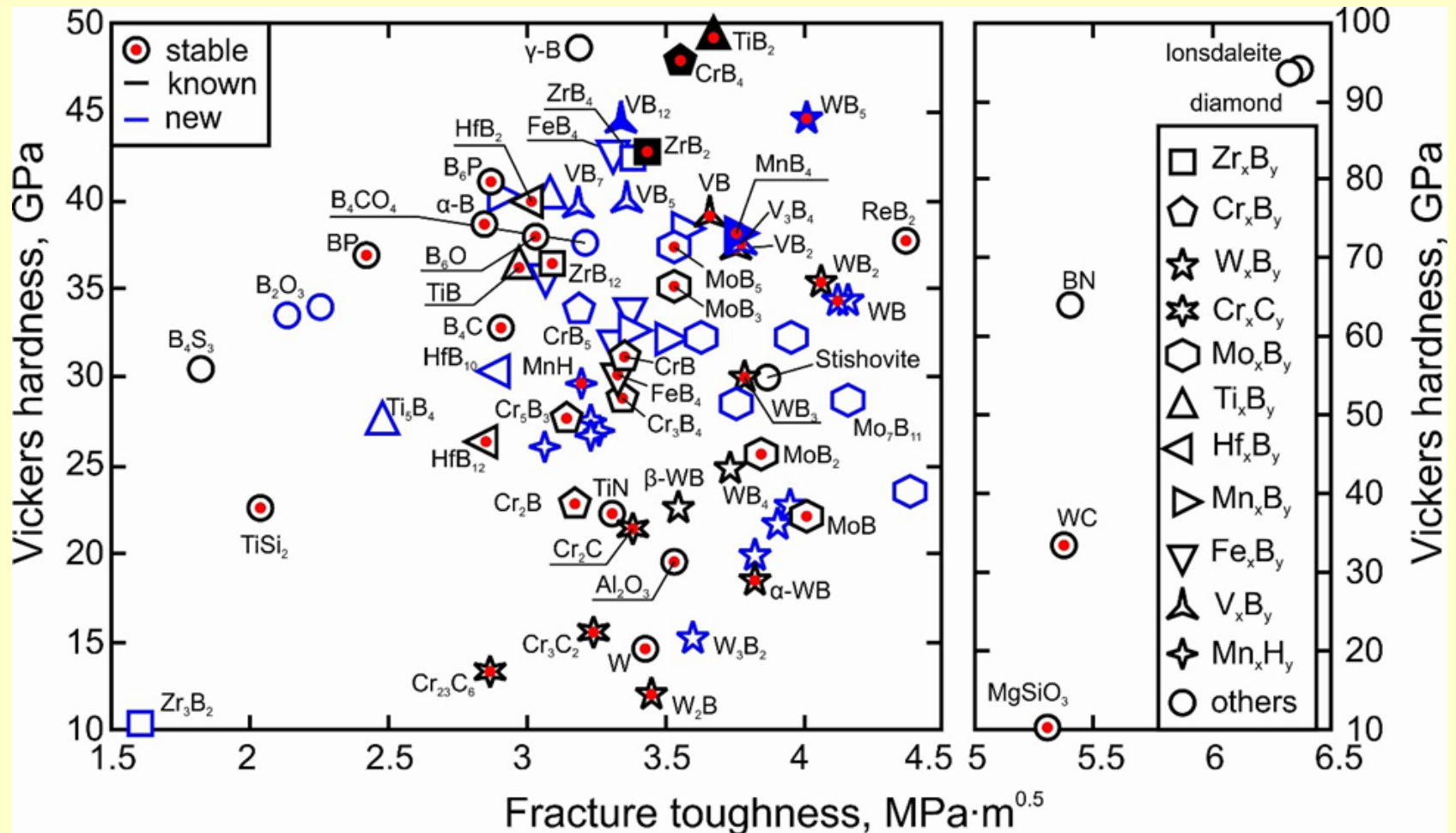
5th generation

10th generation



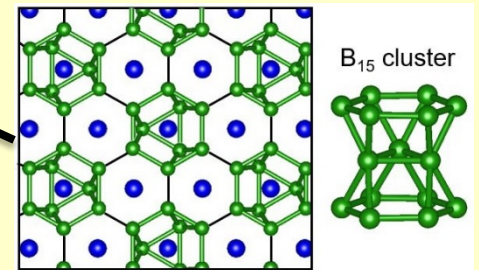
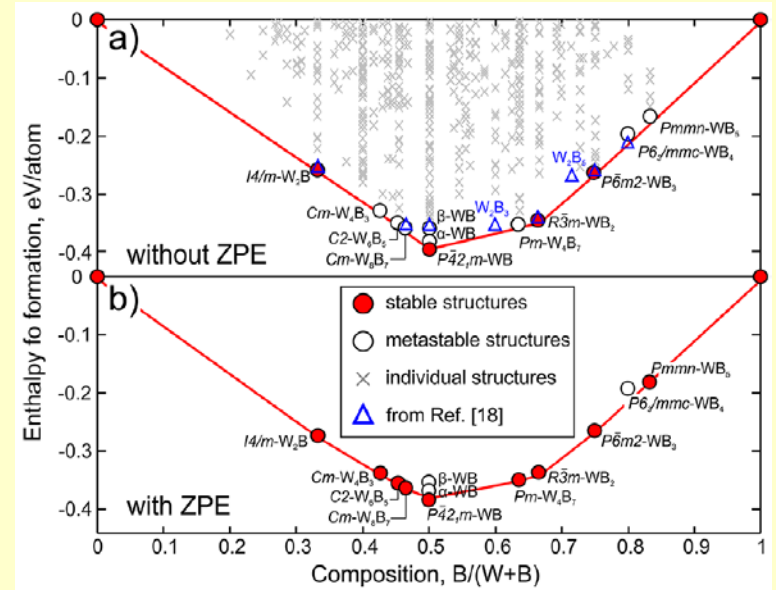
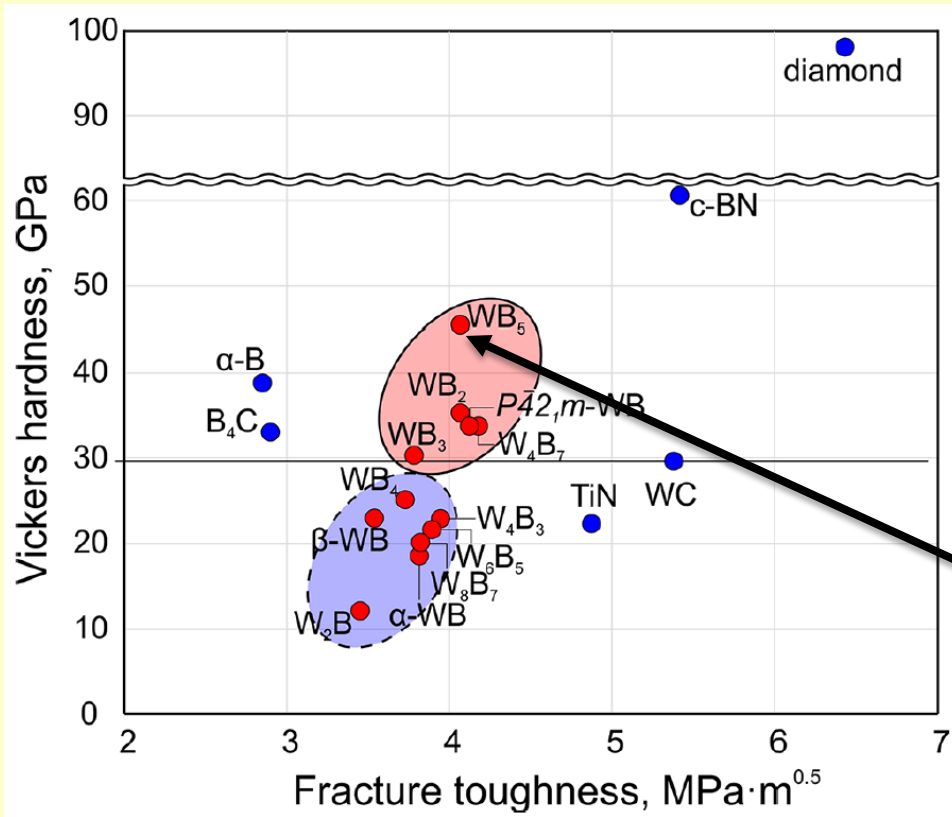
“Treasure” map of superhard materials

[Kvashnin, Allahyari, Oganov, *J. Appl. Phys.*, 2019]



WB_{5-x}: remarkable material

[Kvashnin & Oganov, *J. Phys. Chem. Lett.*, 2018; *Adv. Science*, 2020]



New material WB₅



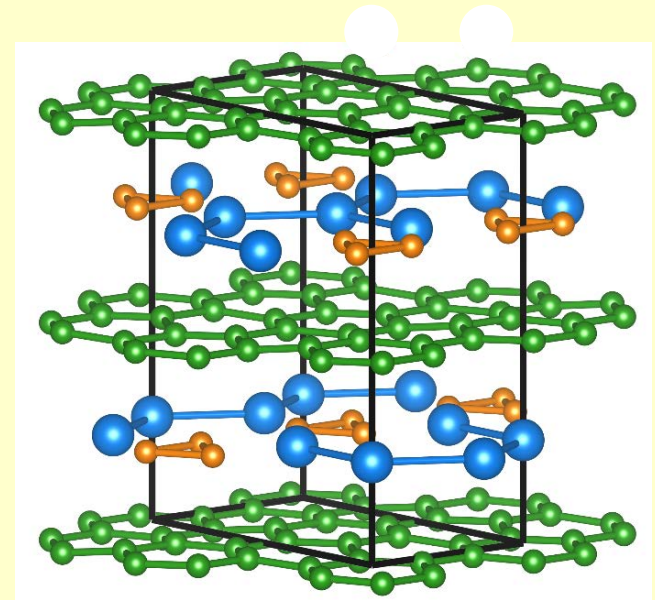
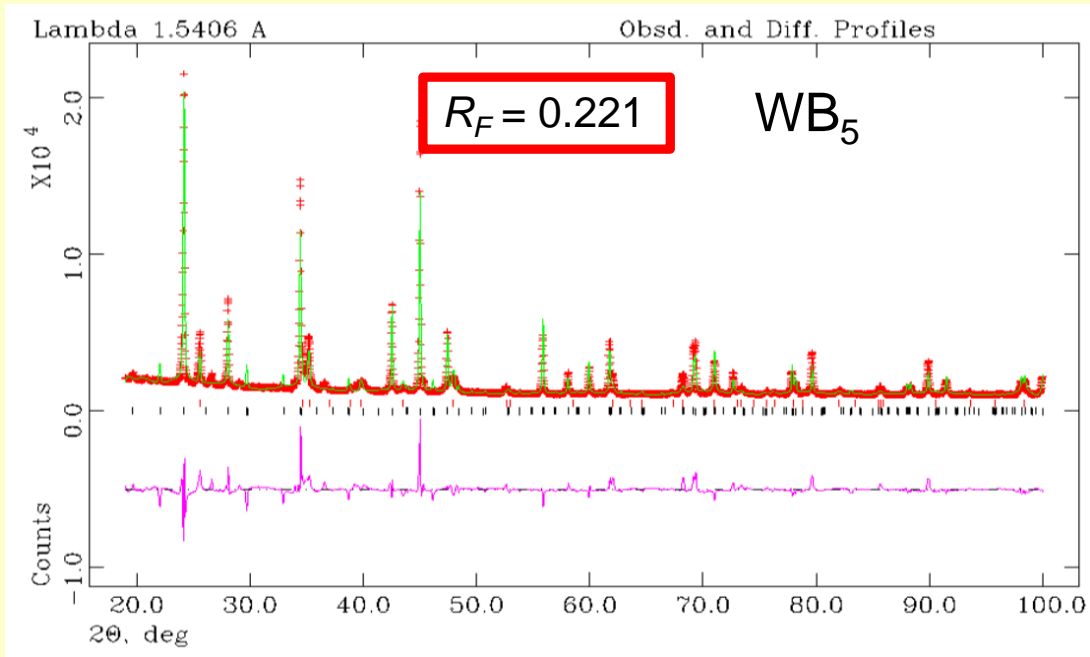
Tungsten carbide WC - standard



Synthesized by
V. Filonenko

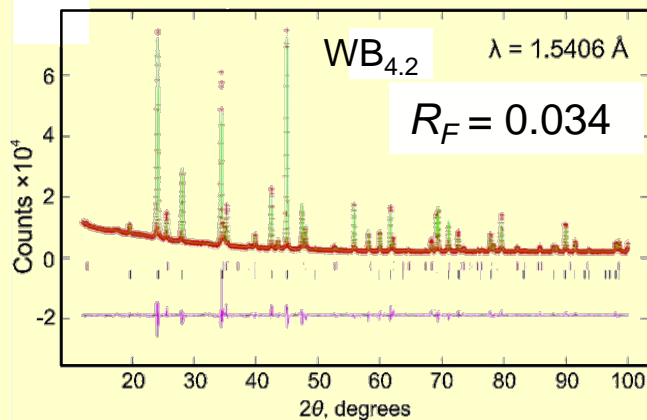
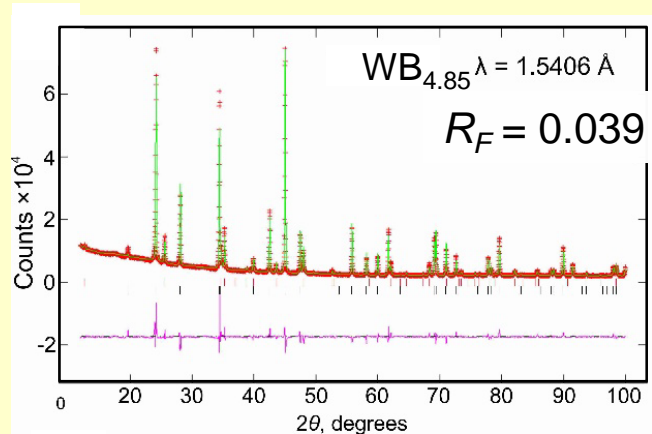
Crystal structure of WB_{5-x}

[Kvashnin & Oganov, *Adv. Science*, 2020]

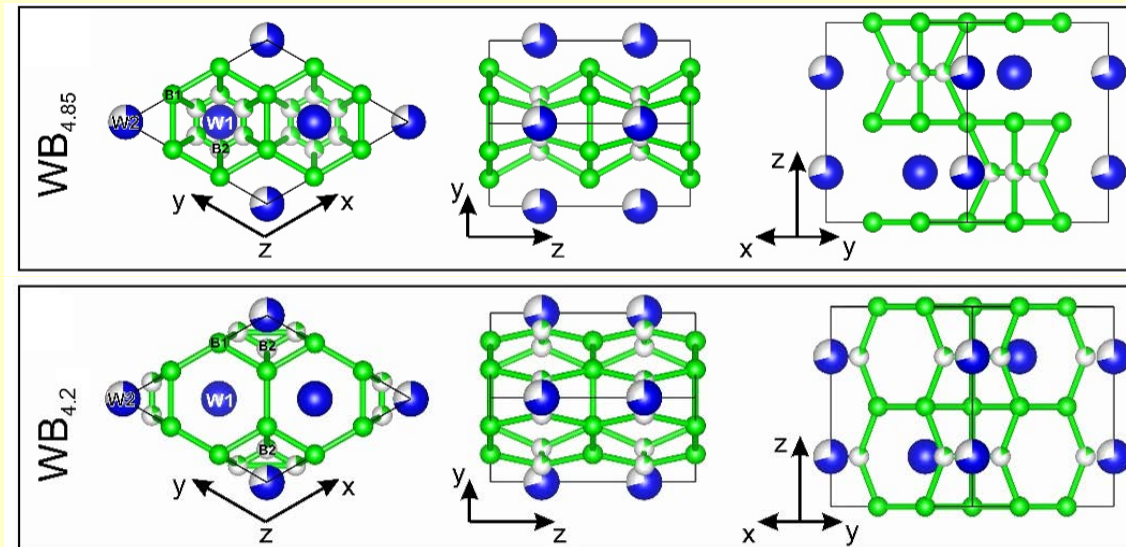


Experiments showed that the actual material has higher symmetry and a non-stoichiometric disordered structure

Crystal structure of WB_{5-x} (Kvashnin & Oganov, *Adv. Science*, 2020)



Synthesized material has composition WB_{5-x}
Two models match XRD



Crystal structure is disordered, actual composition is $WB_{4.2}$
(cf. $MoB_{4.7}$ – Rybkovskiy & Oganov, 2020).

Average structure consistent with the model of Lech et al. (2015) for “ WB_4 ”.

Bonus: very recent story of a material harder than diamond

- Fujii (PRL, 2020) claimed “pentadiamond” to have unique elastic moduli.
- Both machine learning and DFT calculations prove this wrong (Brazhkin & Oganov, arxiv.org).

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MATERIALS

Pentadiamond outshines the original

A theoretical material made of carbon pentagons is lighter and stiffer than a standard diamond

by Sam Lomonick
JULY 6, 2020 | APPEARED IN VOLUME 98, ISSUE 28

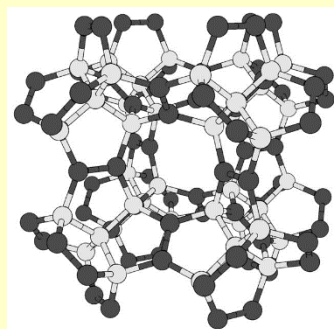






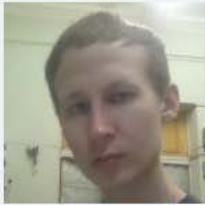







Table 1. Calculated elastic properties of pentadiamond in comparison with Y. Fujii et al. [1].

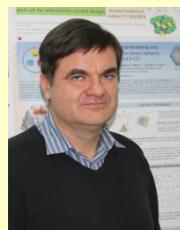
Property	Y. <u>Fujii</u> et al. [1]	This work (Quantum ESPRESSO)	This work (VASP)	This work (machine learning)
a, Å	9.195	9.184	9.191	9.195
E-E(diam), meV/atom	275	263	267	-
C ₁₁ , GPa	1715.3	539	537	409
C ₁₂ , GPa	-283.5	105	106	118
C ₄₄ , GPa	1187.5	141	143	200
B, GPa	381	250	249	215
G, GPa	1113	172	169	176
Y, GPa	1691	420	413	415
σ	-0.241	0.22	0.22	0.18
H _v , GPa	210	20	20	26

Our team. Where great minds do NOT think alike

<p>Artem R. Oganov</p>  <p>Professor Head of Laboratory</p> <p>More</p>	<p>Zahed Allahyari</p>  <p>PhD student</p> <p>Chief developer of USPEX code</p>	<p>Pavel Bushlanov</p>  <p>Postdoc</p>	<p>Efim Mazhnik</p>  <p>PhD student</p>	<p>Tao Fan</p>  <p>PhD student</p>	<p>Michele Galasso</p>  <p>PhD student</p> <p>CV</p>
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A. Goncharov

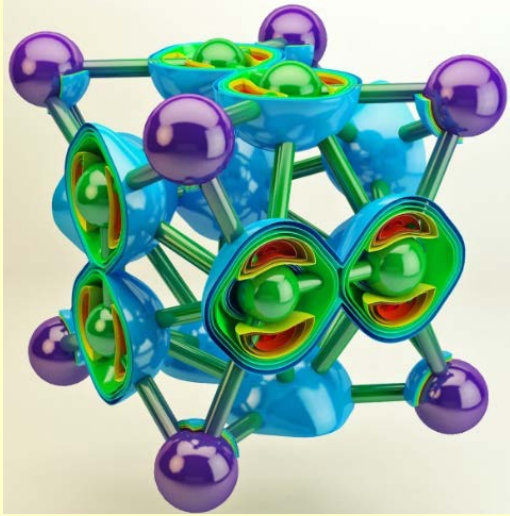


V. Blatov

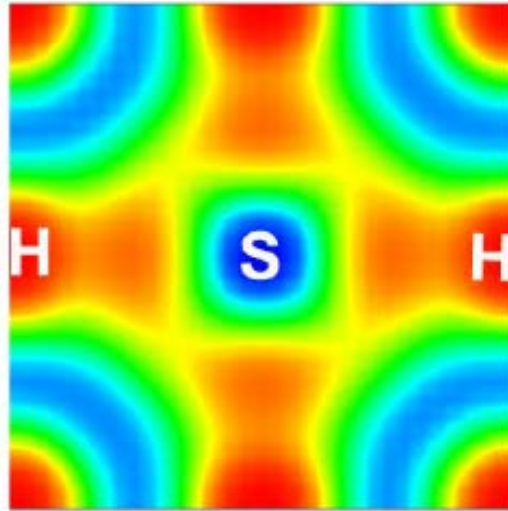


I. Trojan

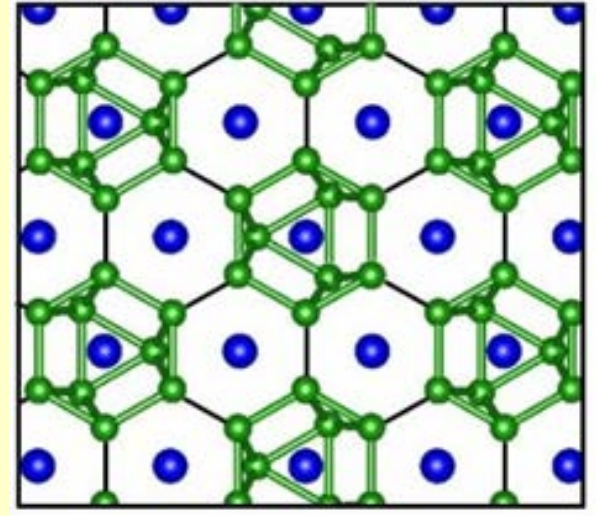
Advanced algorithms predict new supermaterials and help us understand nature



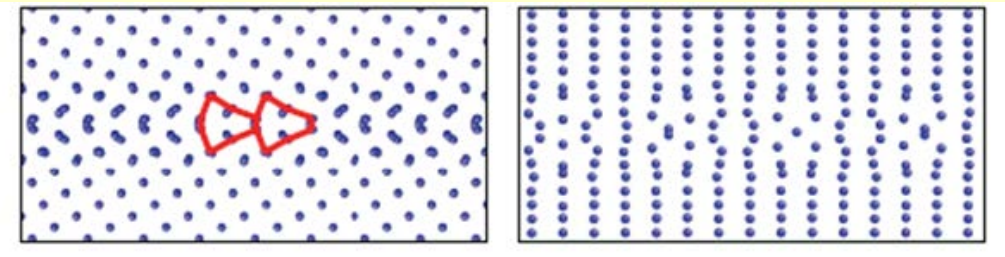
Unusual chemistry at extreme conditions



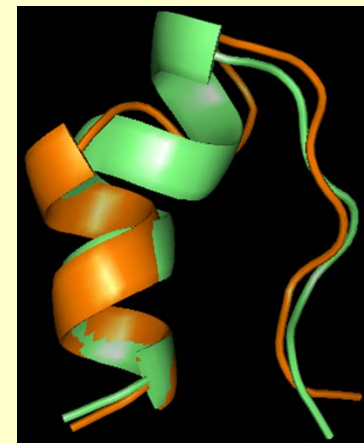
New record of high-Tc superconductivity



New superhard materials



Prediction of grain boundary structures



Protein structure prediction