

Professor Artem R. Oganov FRSC MAE

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ADDRESS: Skolkovo Institute of Science and Technology, Bolshoy Boulevard 30, bld. 1, 121205 Moscow, Russia. E-mail: a.oganov@skoltech.ru. Telephone: +7-(495)-240-1481.

DATE OF BIRTH: 03.03.1975.

PERSONAL INFORMATION: Married, four children (daughters Jeanne and Adriana, sons Lev and Alexander). Speak five languages (native Russian, fluent English, intermediate French, basic Italian and German).

PROFESSIONAL EXPERIENCE AND EDUCATION:

- 2015-now : Professor, Skolkovo Institute of Science and Technology, Russia.
- 2021-now : Head of Laboratory of Crystal Chemistry, Institute of Geochemistry and Analytical Chemistry, Russian Academy of Sciences, Moscow, Russia.
- 2020-now : Professor, MISIS University, Moscow, Russia.
- 2017 : Founded and directed (until 2020) the International Center for Materials Discovery, Northwestern Polytechnical University (China)
- 2013-2020 : Head of Laboratory and Professor, Moscow Institute of Physics and Technology, Russia
- 2008-2017 : Professor (2010-2017) and Associate Professor (2008-2010), Dept. Geosciences & Institute for Advanced Computational Sciences, Stony Brook University, U.S.A.
- 2007 : Habilitation, Dept. Materials, ETH Zurich, Switzerland - in 2016 accepted as equivalent to Doctor of Physical & Mathematical Sciences (Russian highest degree)
- 2003-2008 : Senior scientist (2003-2007) and Privatdozent (2007-2008), Dept. Materials, ETH Zurich, Switzerland
- 2002-2003 : Research Fellow, University College London, U.K.
- 2002 : PhD in Crystallography, University College London, U.K.
- 1997 : M.Sc. in Crystallography, Moscow State University, *magna summa cum laude*.

PUBLICATIONS: 307 papers (including 5 in *Nature* and 2 in *Science*) and book chapters. Total citation = 19,308 (Web of Science) and 26,228 (Google Scholar). H-index = 67 (Web of Science) and 75 (Google Scholar). Published two books (at Wiley-VCH and Royal Society of Chemistry) as editor.

INVITED LECTURES: >400 seminars and invited talks at conferences. 65 plenary and keynote lectures.

VISITING APPOINTMENTS: Adjunct Professor of Moscow State University since 2006 and Northwestern Polytechnical University (China) since 2012. Since 2005 was an invited professor in Italy (Milan), France (Paris, Lille and Poitiers), China (Guilin, Beijing, Hong Kong, Kaifeng, Urumqi).

MAJOR DISTINCTIONS:

- 2021 : Lifetime Honorary Member of RASA-USA
- 2020 : Fellow of the American Physical Society
- 2020 : Fellow of the Royal Society of Chemistry (FRSC)
- 2019 : Friendship award of Chinese government
- 2017 : George Gamow award
- 2017 : Concord award
- 2017 : Member of Academia Europaea (M.A.E.)
- 2017 : Russian Highly Cited Researcher in Physics (Clarivate Analytics)
- 2017 : Chinese Academy of Sciences Presidential Visiting Fellowship
- 2017 : Paper (*J. Chem. Phys.* 2006) declared citation classic by Google Scholar
- 2016 : Russian Highly Cited Researcher award (Chemistry), by Clarivate Analytics
- 2015 : Japan Society for Promotion of Science Invitation Fellow
- 2015 : Professor of Russian Academy of Sciences
- 2013 : Fellow of the Mineralogical Society of America
- 2013 : Megagrant of Russian government
- 2012 : 1000 talents professor of People's Republic of China
- 2012 : Honorary Professor, Yanshan University, China
- 2007 : Research Excellence Medal of the European Mineralogical Union
- 2006 : University Latsis Prize
- 2004 : European High-Pressure Research Group Award
- 2003 : Young Scientist Award of the European Union of Geosciences
- 2002 : President's Award of the Geological Society of London

IN MEDIA: Ranked among the most successful Russian scientists by Russian Newsweek (2008), Forbes Russia (2011), and Russian Reporter magazine (2014). Ranked among the most influential Russians by GQ (2019).

Participated in films about science and scientists: “Watching the thought fly” (directed by V. Gerchikov, 2017), “New element in the Russian table” (directed by E. Tukhareli, 2019).

Biographical and documentary films about Artem R. Oganov:

“Color of the crystal” (directed by V. Gerchikov, 2012),

“Made by Russians” (directed by L. Parfenov, 2015),

“House of science: Artem Oganov” (directed by N. Popova, 2018),

“Cool story: Return of the professor” (directed by T. Mitkova, 2018).

SELECT PROFESSIONAL SERVICES:

2021-now : Editorial Board (Chemistry section) of Russian Encyclopedia

2021-now : Expert Council of Russian Government on Artificial Intelligence

2021-now : Science and Technology Council, Rusnano Corporation

2021-now : Academic Council, MISIS University, Russia

2021-now : Academic Council for Materials and Nanomaterials, Russian Academy of Sciences

2021-now : Academic Council for Geochemistry Problems, Russian Academy of Sciences

2019-now : Academic Council for Chemical Physics, Russian Academy of Sciences

2019-now : Academic Council, Russian Railways Corporation

2019 : Science and Technology Council, “Talent and Success” Foundation

2017-2020 : Member of Russian Presidential Council for Science and Education

2017-2020 : Consultant, Commission on Crystallography of Materials of IUCr

2017 : Co-chairman of two panels at World Economic Forum (Dalian, June 2017)

2017 : Award Committee, RusnanoPrize

2016-now : Academic Council, Fersman Mineralogical Museum

2016-2019 : Academic Council, Skolkovo Institute of Science and Technology

2011-2017 : Founder and Chairman, Commission on Crystallography of Materials of IUCr

2011-2019 : Organized 16 workshops on crystal structure prediction in France, China, India, Canada, USA, Switzerland, Italy, Russia.

2010-now : Member of program and scientific advisory committees of several international conferences, e.g., the International Union of Crystallography (IUCr) meeting, Montreal, August 2014.

2009-2012 : Member of the University Senate, Stony Brook University.

2006-now : member of editorial boards of *Scientific Reports* (2006-now), *Journal of Superhard Materials* (2009-now), *Geochemistry International* (2021-), Associate Editor of *American Mineralogist* (2006-2010), *Crystals* (2020-), *Geochemistry International* (2021-).

2005-2014 : Organized 6 highly cited special issues: “Computational Crystallography” (*Zeitschrift fuer Kristallographie*, 2005); “Computational Materials Discovery” (*Acta Crystallographica.C*, 2014); Special issues of the *Journal of Superhard Materials*: “Theory of Superhard Materials” (2010), “Boron and Boron-rich Solids” (2011), “Superhard Carbon” (2012), “Novel Superhard Materials” (2014).

2005-now : referee for >60 journals (including *Nature*, *Science*; *Nature Chemistry*, *Nature Materials*; *Nature Geoscience*; *PNAS*, *Phys. Rev. Lett.*, etc.) and for numerous funding agencies around the world.

PROFESSORS TRAINED:

Yanming Ma (was my postdoc in 2006-2008, now Professor at Jilin U., China).

Qiang Zhu (PhD student in 2009-2013, now Assistant Prof. at UNLV, USA).

Maribel Nunez Valdez (2015-2016, now Prof. at Frankfurt U., Germany).

Andriy O. Lyakhov (postdoc in 2007-2011, then Res. Asst. Prof. at Stony Brook U., USA).

Yu Xie (PhD student in 2007-2010, now Professor at Jilin U., China).

Fei Qi (postdoc in 2013-2015, now Assoc. Prof. at Xidian U., China).

Qinggao Wang (postdoc in 2013-2016, now Professor at Henan U., China).

Xiaohu Yu (postdoc in 2013-2015, now Assoc. Prof. at Henan Normal U., China).

Huafeng Dong (postdoc in 2013-2015, now Assoc. Prof., Guangdong U. of Tech., China).

Xiang-Feng Zhou (postdoc in 2012-2015, now Prof. at Yanshan U., China).

Dongxu Li (visiting scientist in 2013-2014, now Assoc. Prof., Huaqiao U., China).

Qianku Hu (visiting scientist in 2013-2014, now Asst. Prof. at Henan Polytechnic U., China).

Xiao Dong (visiting PhD student in 2012-2014, now Assoc. Prof. at Nankai U., China).

Qingfeng Zeng (visiting scientist in 2011-2012, now Assoc. Prof., Northwestern Polytechnical U., China).

Chaohao Hu (visiting scientist in 2011-2012, now Professor at Guilin U. of Electronic Technology, China).

Weiwei Zhang (visiting scientist in 2011-2013, now Professor at China Agricultural University).

Feiwu Zhang (PhD student in 2005-2008, now Professor in Inst. Geochemistry, Chinese Acad. Sci.).

Evgeny Tikhonov (postdoc in 2014-2018, now Assistant Prof. at Northwestern Polytechnical U., China).
Haiyang Niu (visiting PhD student in 2014, then postdoc in 2015-2016, now Professor at Northwestern Polytechnical U., China).
Alexander Kvashnin (postdoc in 2015-2021, now Associate Professor at NUST-MISIS, Russia).

PHD STUDENTS GRADUATED:

Zahed Allahyari (2016-2020), Christian Tantardini (2018-2020), Valery Roizen (2015-2019), Congwei Xie (2015-2019), Oleg Feyta (2014-2019), Ivan Kruglov (2014-2018), Jin Zhang (2014-2017), Mahdi Davari (2013-2017), Shengnan Wang (2013-2016), Guangrui Qian (2011-2015), Qiang Zhu (2009-2013), Yu Xie (2007-2010), Feiwu Zhang (2005-2008), Colin W. Glass (2006-2009), Donat Adams (2004-2007), Kai H. Hassdenteufel (2003-2006), Daniel Y. Jung (2004-2008).

DSC THESIS SUPERVISED:

Alexander Kvashnin (2021).

List of publications of Artem R. Oganov.

BOOKS:

1. Kuzmin M.I., Yarmolyuk V.V., Gladkochub D.P., Goryachev N.A., Derevyanko A.P., Didenko A.N., Donskaya T.V., Kravchinsky V.A., Oganov A.R., Pisarevsky S.A. (2021). Geological evolution of the Earth: from space dust to the home of mankind. Academic Publishing House "Geo", Novosibirsk. (in Russian).
2. Oganov A.R., Saleh G., Kvashnin A.G. (Editors). *Computational Materials Discovery*. Royal Society of Chemistry. ISBN: 978-1-78262-961-0. (2018).
3. Oganov A.R. (Editor). *Modern Methods of Crystal Structure Prediction*. Berlin: Wiley-VCH. ISBN: 978-3-527-40939-6. (2010).

REVIEWS AND CHAPTERS IN BOOKS:

21. Oganov A.R., Konson G.R. (2020). The way the people of art and science study the world. In: *Art History in the Context of Other Sciences in Modern World: Parallels and Interactions* (Proceedings of the international academic conference, April 21-26, 2019), pp. 278-291.
20. Kruglov I.A., Dolgirev P.E., Oganov A.R., Mazitov A.B., Pozdnyakov S.N., Mazhnik E.A., Yanilkin A.V. (2019). Machine learning interatomic potentials for global optimization and molecular dynamics simulation. In: *Materials Informatics* (edited by O. Isayev, A. Tropsha, S. Curtarolo), pp. 253-288; Wiley-VCH.
19. Allahyari Z., Oganov A.R. (2018). Multi-objective optimization as a tool for materials design. In: *Handbook of Materials Modeling* (ed. W. Andreoni, S. Yip). Volume 2 Applications: Current and Emerging Materials. Springer Verlag, pp. 2777-2790.
18. Oganov A.R., Kvashnin A.G., Saleh G. (2018). Computational materials discovery: dream or reality? In: *Computational Materials Discovery*. Eds.: Oganov A.R., Kvashnin A.G., Saleh G. Royal Society of Chemistry, pp. 1-14.
17. Oganov A.R., Kruglov I.A., Zhang J., Davari Esfahani M. (2018). Computational materials discovery using evolutionary algorithms. In: *Computational Materials Discovery*. Eds.: Oganov A.R., Kvashnin A.G., Saleh G. Royal Society of Chemistry, pp. 15-65.
16. Dong X., Oganov A.R. (2017). Electrified and their high-pressure chemistry. In: *Correlations in Condensed Matter Under Extreme Conditions*, ed. G.N.N. Angilella & A. La Magna, Springer Verlag. pp. 69-84.
15. Yu X.H., Oganov A.R., Wang Z.H., Saleh G., Baturin V.S., Sharma V., Zhu Q., Wang Q.G., Zhou X.F., Popov I.A., Boldyrev A.I. (2017). Predicting the structure and chemistry of low-dimensional materials. *Handbook of Solid State Chemistry*, v.5, eds. R. Dronskowski, S. Kikkawa, A. Stein. Pp. 527-570.
14. Oganov A.R., Lyakhov A.O., Zhu Q. (2014). Theory of superhard materials. In: *Comprehensive Hard Materials Review*, Elsevier, v.3, 59-79.
13. Oganov A.R. (2011). Discovery of γ -B28, a Novel Boron Allotrope with Partially Ionic Bonding. In: *Boron and boron compounds – from fundamentals to applications*. Materials Research Society, ISBN 978-1-61839-514-6, Chapter 1, pp. 1-15.
12. Oganov A.R. (2011). Boron under pressure: phase diagram and novel high-pressure phase. In: "*Boron rich solids*", Chapter 14 (pp. 207-215). Eds. N. Orlovskaya and M. Lugovy, Springer Verlag, Berlin.
11. Oganov A.R., Schön J.C., Jansen M., Woodley S.M., Tipton W.W., Hennig R.G. (2010). First blind test of inorganic crystal structure prediction. In: *Modern Methods of Crystal Structure Prediction* (ed. A.R. Oganov), pp. 223-231. Berlin: Wiley-VCH.
10. Lyakhov A.O., Oganov A.R., Valle M. (2010). Crystal structure prediction using evolutionary approach. In: *Modern methods of crystal structure prediction* (ed. A.R. Oganov), pp. 147-180. Berlin: Wiley-VCH.
9. Oganov A.R. (2010). Crystal structure prediction, a formidable problem. In: *Modern Methods of Crystal Structure Prediction* (ed. A.R. Oganov), pp. xi-xxi. Berlin: Wiley-VCH.
8. Oganov A.R., Ma Y., Lyakhov A.O., Valle M., Gatti C. (2010). Evolutionary crystal structure prediction and novel high-pressure phases. "High-pressure crystallography" (eds. E. Boldyreva, P. Dera), pp. 293-325. Springer Verlag.
7. Oganov A.R., Ma Y., Glass C.W., Valle M. (2007). Evolutionary crystal structure prediction: overview of the USPEX method and some of its applications. *Psi-k Newsletter*, number 84, Highlight of the Month, 142-171 (invited review).
6. Oganov A.R. (2007). Thermodynamics, phase transitions, equations of state and elasticity of minerals at high pressures and temperatures. *Treatise on Geophysics*, vol. 2 (Mineral Physics, edited by G.D. Price), 121-152.
5. Jung D.Y., Oganov A.R. (2005). Basics of first-principles simulation of matter under extreme conditions. *EMU Notes in Mineralogy* v.7 ("High-Pressure Behaviour of Minerals", edited by R. Miletich), 117-138.
4. Adams D.J., Oganov A.R. (2005). Theory of minerals at extreme conditions: predictability of structures and properties. *EMU Notes in Mineralogy* v.7 ("High-Pressure Behaviour of Minerals", edited by R. Miletich), 441-457.
3. Oganov A.R. (2004). Phase diagrams of minerals from first principles. *Proceedings of the CECAM Workshop «First-Principles Simulations: Perspectives and Challenges in Mineral Sciences»* (Berichte aus Arbeitskreisen der DGK, Nr. 14, German Crystallographic Society), pp. 53-62.

2. Oganov A.R. (2003). Theory of Minerals at High and Ultrahigh Pressures: Structure, Properties, Dynamics, and Phase Transitions. In: *High-Pressure Crystallography*, NATO Science Series: II: Mathematics, Physics and Chemistry, vol. 140, p.199-215 (edited by A.Katrusiak, P.F.McMillan). Kluwer Academic Publishers, Dordrecht.
1. Oganov A.R., Brodholt J.P., Price G.D. (2002). Ab initio theory of thermoelasticity and phase transitions in minerals. *EMU Notes in Mineralogy* v.4 ('Energy Modelling in Minerals', edited by C.M. Gramaccioli), pp.83-170.

PAPERS IN REFEREED JOURNALS

286. Dong X., Oganov A.R., Cui H., Zhou X.-F., Wang H.-T. (2022). Electronegativity and chemical hardness of the elements under pressure. *Proc. Natl. Acad. Sci.*, in press.
285. Wang Y., Bykov M., Chepkasov I., Samtsevitch A., Bykova E., Zhang X., Jiang S.-q., Greenberg E., Chariton S., Prakapenka V.B., Oganov A.R., Goncharov A.F. (2022). Stabilization of hexazine rings in potassium polynitride at high pressure. *Nature Chemistry*, in press.
284. Boeri L., Hennig R.G., Hirschfeld P.J., Profeta G., Sanna A., Zurek E., Pickett W.E., Amsler M., Dias R., Eremets M., Heil C., Hemley R.J., Liu H., Ma Y., Pierleoni C., Kolmogorov A., Rybin N., Novoselov D., Anisimov V.I., Oganov A.R., Pickard C.J., Bi T., Arita R., Errea I., Pellegrini C., Requist R., Gross E.K.U., Margine E.R., Xie S.R., Quan Y., Hire A., Fanfarillo L. Stewart G.R., Hamlin J.J., Stanev V., Gonnelli R.S., Piatti E., Romanin D., Daghero D., Valenti R. (2022). The 2021 room-temperature superconductivity roadmap. *J. Phys.: Cond. Matt.*, in press.
283. Li H.F., Oganov A.R., Cui H., Zhou X.-F., Dong X., Wang H.-T. (2022). Ultrahigh-pressure magnesium hydrosilicates as reservoirs of water in early Earth. *Phys. Rev. Lett.* **128**, 035703.
282. Li X., Niu H., Oganov A.R. (2021). COPEX: co-evolutionary crystal structure prediction algorithm for complex systems. *npj Comp. Mater.* **7**, 199.
281. Popov Z.I., Tikhomirova K.A., Demin V.A., Chowdhury S., Oganov A.R., Kvashnin A.G., Kvashnin D.G. (2021). Novel two-dimensional boron oxynitride predicted using USPEX evolutionary algorithm. *Phys. Chem. Chem. Phys.* **23**, 26178-26184.
280. Stavrou E., Maryewski A.A., Lobanov S.S., Oganov A.R., Konopkova Z., Prakapenka V.B., Goncharov A.F. (2021). Ethane and methane at high pressures: structure and stability. *J. Chem. Phys.* **155**, 184503.
279. Zhang J., Li X., Dong X., Dong H., Oganov A.R., McMahon J.M. (2021). Theoretical study of the crystal structure, stability and properties of phases in the V-N system. *Phys. Rev.* **B104**, 134111.
278. Semenok D.V., Troyan I.A., Ivanova A.G., Kvashnin A.G., Kruglov I.A., Hanfland M., Sadakov A.V., Sobolevskiy O.A., Pervakov K.S., Lyubutin I.S., Glazyrin K.V., Giordano N., Karimov D.N., Vasiliev A.L., Akashi R., Pudalov V.M., Oganov A.R. (2021). Superconductivity at 253 K in lanthanum–yttrium ternary hydrides. *Materials Today* **48**, 18-28.
277. Mazitov A.B., Oganov A.R. (2021). Grain boundaries in minerals: atomic structure, phase transitions, and effect on strength of polycrystals. *Zapiski RMO (Proc. Russ. Mineral. Soc.)* **150**, 92-102.
276. Samtsevich A.I., Oganov A.R. (2021). Mechanisms of phase transitions in Al₂SiO₅ phases. *Zapiski RMO (Proc. Russ. Mineral. Soc.)* **150**, 79-91.
275. Fan T., Oganov A.R. (2021). Discovery of high performance thermoelectric chalcogenides through first-principles high-throughput screening. *J. Mater. Chem.* **C9**, 13226-13235.
274. Chen W., Semenok D.V., Huang X., Shu H., Li X., Duan D., Cui T., Oganov A.R. (2021). High-Temperature Superconducting Phases in Cerium Superhydride with a T_c up to 115 K below a Pressure of 1 Megabar. *Phys. Rev. Lett.* **127**, 117001.
273. Novoselov D.Y., Korotin D.M., Shorikov A.O., Anisimov V.I., Oganov A.R. (2021). Interacting electrons in two-dimensional electride Ca₂N. *J. Phys. Chem.* **C125**, 15724-15729.
272. Sandu M.P., Kovtunov M.A., Baturin V.S., Kurzina I., Oganov A.R. (2021). Influence of Pd:Bi ratio on Pd-Bi/A₁₂O₃ catalysts: structure, surface and activity in glucose oxidation. *Phys. Chem. Chem. Phys.* **23**, 14889-14897.
271. Rybin N., Novoselov D.Y., Korotin D.M., Anisimov V.I., Oganov A.R. (2021). Novel copper fluoride analogs of cuprates. *Phys. Chem. Chem. Phys.* **23**, 15989-15993.
270. Yue C., Weng X.-J., Gao G., Oganov A.R., Dong X., Shao X., Wang X., Sun J., Xu B., Wang H.-T., Zhou X.-F., Tian Y. (2021). Formation of copper boride on Cu(111). *Fundamental Research* **1**, 482-487.
269. Korotin D.M., Novoselov D.Y., Anisimov V.I., Oganov A.R. (2021). Mixed spin S=1 and S=1/2 layered lattice in Cu₂F₅. *Phys. Rev.* **B104**, 064410.
268. Tantardini C., Oganov A.R. (2021). Thermochemical electronegativities of the elements. *Nature Communications* **12**, 2087.
267. Kun L., Wang J., Oganov A.R. (2021). High-pressure phase diagram of the Ti-O system. *J. Phys. Chem. Lett.* **12**, 5486-5493.
266. Novoselov D.Y., Anisimov V.I., Oganov A.R. (2021). Strong electronic correlations in interstitial magnetic centers of zero-dimensional electride β-Yb₅Sb₃. *Phys. Rev.* **B103**, 235126.

265. Naumova A.S., Lepeshkin S.V., Bushlanov P.V., Oganov A.R. (2021). Unusual chemistry of the C-H-N-O system under pressure and implications for giant planets. *J. Phys. Chem.* **A125**, 3936-3942.
264. Fan T., Oganov A.R. (2021). AICON2: A program for calculating transport properties quickly and accurately. *Computer Phys. Comm.* **266**, 108027.
263. Li K., Wang J., Blatov V.A., Gong Y., Umezawa N., Tada T., Hosono H., Oganov A.R. (2021). Crystal and electronic structure engineering of tin monoxide by external pressure. *J. Adv. Ceramics* **10**, 565–577.
262. Li H., Min J., Yang Z., Wang Z., Pan S., Oganov A.R. (2021). Prediction of Novel van der Waals Boron Oxides with Superior Deep-Ultraviolet Nonlinear Optical Performance. *Angew. Chem. Int. Ed.* **60**, 10791-10797.
261. Troyan I.A., Semenok D.V., Kvashnin A.G., Sadakov A.V., Sobolevskiy O.A., Pudalov V.M., Ivanova A.G., Prakapenka V.B., Greenberg E., Gavriilyuk A.G., Lyubutin I.S., Struzhkin V.V., Bergara A., Errea I., Bianco R., Calandra M., Mauri F., Monacelli L., Akashi R., Oganov A.R. (2021). Anomalous high-temperature superconductivity in YH₆. *Adv. Mater.*, 2006832.
260. Knyazev A., Savushkin I., Mirsaidov U., Lukoyanov A., Oganov A. (2021). Synthesis and structure of triple thorium phosphates with monazite structure. *J. Radioanalyt. Nucl. Chem.* **327**, 1105–1112.
259. Hou J., Weng X.J., Oganov A.R., Shao X., Gao G., Dong X., Wang H.T., Zhou X.F., Tian Y. (2021). Helium-Induced Nitrogen Salt at High Pressure. *Phys. Rev.* **B103**, L060102.
258. Chen W., Semenok D.V., Kvashnin A.G., Huang X., Kruglov I.A., Galasso M., Song H., Duan D., Goncharov A.F., Prakapenka V.B., Oganov A.R., Cui T. (2021). Synthesis of Molecular Metallic Barium Superhydride: Pseudocubic BaH₁₂. *Nature Comm.* **12**, 273.
257. Semenok D.V., Zhou D., Kvashnin A.G., Huang X., Galasso M., Kruglov I.A., Ivanova A.G., Gavriilyuk A.G., Chen W., Tkachenko N.V., Boldyrev A.I., Troyan I., Oganov A.R., Cui T. (2021). Novel Strongly Correlated Europium Superhydrides. *J. Phys. Chem. Lett.* **12**, 32-40.
256. Wang Y., Glazyrin K., Roizen V., Oganov A.R., Chernyshov I., Zhang X., Greenberg E., Prakapenka V.B., Yang X., Jiang S-q., Goncharov A.F. (2020). Novel Hydrogen Clathrate Hydrate. *Phys. Rev. Lett.* **125**, 255702.
255. Allahyari Z., Oganov A.R. (2020). Nonempirical definition of Mendeleev numbers: organizing the chemical space. *J. Phys. Chem.* **C124**, 23867-23878.
254. Chen W.H., Semenok D.V., Troyan I.A., Ivanova A.G., Huang X.L., Oganov A.R., Cui T. (2020). Superconductivity and equation of state of lanthanum at megabar pressures. *Phys. Rev.* **B102**, 134510.
253. Zhu S.C., Yan X.Z., Oganov A.R., Zhu Q. (2020). A revisited mechanism of the graphite-to-diamond transition at high temperature. *Matter* **3**, 864-878.
252. Ostanin I.A., Oganov A.R., Magnanimo V. (2020). Collapse modes in simple cubic and body-centered cubic arrangements of elastic beads. *Phys. Rev.* **E102**, 032901.
251. Broadway D.A., Scholten S.C., Tan C., Dontschuk N., Lillie S.E., Johnson B.C., Zheng G., Wang Z., Oganov A.R., Tian S., Li C., Lei H., Wang L., Hollenberg L.C.L., Tettienne J.-P. (2020). Imaging domain reversal in an ultrathin van der Waals ferromagnet. *Adv. Mater.*, 2003314.
250. Kvashnin A.G., Tantardini C., Zakaryan H.A., Kvashnina Yu.A., Oganov A.R. (2020). Computational search for new W-Mo-B compounds. *Chem. Mater.* **32**, 7028-7035.
249. Miao N., Wang J., Gong Y., Wu J., Niu H., Wang S., Li K., Oganov A.R., Tada T., Hosono H. (2020). Computational prediction of boron-based MAX phases and MXene derivatives. *Chem. Mater.* **32**, 6947-6957.
248. Novoselov D., Korotin D., Shorikov A.O., Oganov A.R., Anisimov V.I. (2020). Weak Coulomb correlations stabilize the electrified high-pressure phase of elemental calcium. *J. Phys.: Cond. Matt.* **44**, 445501.
247. Mazhnik E., Oganov A.R. (2020). Application of machine learning methods for predicting new superhard materials. *J. Appl. Phys.* **128**, 075102.
246. Pakhnova M.S., Kruglov I., Yanilkin A., Oganov A.R. (2020). Search for stable cocrystals of energetic materials using the evolutionary algorithm USPEX. *Phys. Chem. Chem. Phys.* **22**, 16822-16830.
245. Kvashnin A.G., Rybkovskiy D.V., Filonenko V.P., Bugakov V.I., Zibrov I.P., Brazhkin V.V., Oganov A.R., Osipov A.A., Zakirov A.Ya. (2020). WB_{5-x}: synthesis, properties, and crystal structure – new insights into the long-debated compound. *Adv. Science* **7**, 2000775.
244. Cherednichenko K.A., Mukhanov V.A., Wang Z., Oganov A.R., Kalinko A., Dovgaliuk I., Solozhenko V.L. (2020). Discovery of new boron-rich chalcogenides: orthorhombic B₆X (X=S, Se). *Sci. Rep.* **10**, 9277.
243. Tikhomirova K.A., Tantardini C., Sukhanova E.V., Popov Z.I., Evlashin S.A., Tarkhov M.A., Zhdanov V.L., Dudin A.A., Oganov A.R., Kvashnin D.G., Kvashnin A.G. (2020). Exotic two-dimensional structure: the first case of hexagonal NaCl. *J. Phys. Chem. Lett.* **11**, 3821-3827.
242. Shorikov A., Skorniyakov S.L., Anisimov V.I., Oganov A.R. (2020). Electronic correlations in uranium hydride UH₅ under pressure. *J. Phys.: Cond. Matt.* **32**, 385602.
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