

## Professor Artem R. Oganov FRSC MAE

(CV updated 15/01/2023)

**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). Speaks 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 (from 2021 – Head of Department of Semiconductors and Dielectrics).

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:** 319 papers (including 5 in *Nature* and 2 in *Science*) and book chapters.

Web of Science: total citation = 22,221, h-index = 71.

Google Scholar: total citation = 30,007, h-index = 83.

Author and coauthor of three scientific books and one best-selling popular science book.

**INVITED LECTURES:** >470 seminars and invited talks at conferences. 71 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:

2022 : Highly Cited Researcher by Clarivate Analytics

2021 : Lifetime Honorary Member of RASA-USA

2020 : Fellow of the American Physical Society

2020 : Fellow of the Royal Society of Chemistry (FRSC)

2019- : ranked in top 2% most cited scientists (Elsevier)

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:

- 2022- : Science council, Moscow Institute of Physics and Technology  
 2022- : Expert Council, New Technological Initiative  
 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).  
Chao hao 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 Assistant Professor at Skoltech).

**PHD STUDENTS GRADUATED:**

Dmitrii Semenok (2018-2022), Tao Fan (2018-2022), Zahed Allahyari (2016-2020), Christian Tantardini (2018-2020), Valery Roizen (2015-2019), Congwei Xie (2015-2019), Oleg Feya (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:

4. Oganov A.R. *Chemistry*. AST Publishing House. Moscow. (popular science book, in Russian). ISBN 978-5-17-145181-3. (2022).
3. 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. *Geological evolution of the Earth: from space dust to the home of mankind*. Academic Publishing House "Geo", Novosibirsk. (in Russian). ISSN 2686-9993. (2021).
2. Oganov A.R., Saleh G., Kvashnin A.G. (Editors). *Computational Materials Discovery*. Royal Society of Chemistry. ISBN: 978-1-78262-961-0. (2018).
1. 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). Electrides 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  $\gamma$ -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

298. Galasso M., Oganov A.R. (2023). Automag: An automatic workflow software for calculating the ground magnetic state of a given structure and estimating its critical temperature. *Comp. Phys. Comm.* **283**, 108571.
297. Xie C.W., Tudi A., Oganov A.R. (2022). PNO: a promising deep-UV nonlinear optical material with the largest second harmonic generation effect. *Chem. Commun.* **58**, 12491-12494.
296. Marchenko E.A., Oganov A.R., Mazhnik E.A., Eremin N.N. (2022). Stable compounds in the CaO-Al<sub>2</sub>O<sub>3</sub> system at high pressures. *Phys. Chem. Miner.* **49**, art. 44.
295. Troyan I.A., Semenok D.V., Ivanova A.G., Kvashnin A.G., Zhou D., Sadakov A.V., Sobolevsky O.A., Pudalov V.M., Lyubutin I.S., Oganov A.R. (2022). High-temperature superconductivity in hydrides. *Physics-Uspekhi* **192**, 799–813.
294. Rahmanian Koshkaki S., Allahyari Z., Oganov A.R., Solozhenko V.L., Polovov I., Belozherov A., Katanin A., Anisimov V.I., Tikhonov E., Qian G.R., Maksimtshev K., Mukhamadeev A., Chukin A., Korolev A., Mushnikov N., Li H. (2022). Computational prediction of new magnetic materials. *J. Chem. Phys.* **157**, 124704.
293. Rybin N., Chepkasov I., Novoselov D.Y., Anisimov V.I., Oganov A.R. (2022). Prediction of stable silver fluorides. *J. Phys. Chem.* **C126**, 15057–15063.
292. Momenzadeh-Abardeh Z., Salimi A., Oganov A.R. (2022). Crystal structure prediction of N-halide phthalimide compounds: halogen bonding synthons as a touchstone. *CrystEngComm* **24**, 6066-6075.
291. Semenok D.V., Troyan I.A., Sadakov A.V., Zhou D., Galasso M., Kvashnin A.G., Kruglov I.A., Bykov A.A., Terent'ev K.Y., Cherepanin A.V., Sobolevskiy O.A., Pervakov K.S., Seregin A.Yu., Helm T., Förster T., Grochowiak A.D., Tozer S.W., Nakamoto Y., Shimizu K., Pudalov V.M., Lyubutin I.S., Oganov A.R. (2022). Effect of magnetic impurities on superconductivity in LaH<sub>10</sub>. *Adv. Mater.* **34**, 2204038.
290. Lepeshkin S.V., Naumova A.S., Baturin V.S., Oganov A.R. (2022). "Magic" molecules and a new look at chemical diversity of hydrocarbons. *J. Phys. Chem. Lett.* **13**, 7600-7606.
289. Semenok D.V., Chen W., Huang X., Zhou D., Kruglov I.A., Mazitov A.B., Galasso M., Tantardini C., Gonze X., Kvashnin A.G., Oganov A.R., Cui T. (2022). Sr-Doped Molecular Hydrogen: Synthesis and Properties of SrH<sub>22</sub>. *Adv. Mater.* 2200924.
288. Novoselov D.Y., Mazannikova M.A., Korotin D.M., Shorikov A.O., Korotin M.A., Anisimov V.I., Oganov A.R. (2022). Localization mechanism of interstitial electronic states in electride mayenite. *J. Phys. Chem. Lett.* **13**, 7155-7160.
287. 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*, **14**, 794–800.
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.* **119**, e2117416119.
285. 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.* **34**, 183002.
284. 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.
283. Dyachenko A.A., Lukoyanov A.V., Anisimov V.I., Oganov A.R. (2022). Electride properties of ternary silicide and germanide of La and Ce. *Phys. Rev.* **B105**, 085146.
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 Al<sub>2</sub>SiO<sub>5</sub> 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<sub>c</sub> 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 Ca<sub>2</sub>N. *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/Al<sub>2</sub>O<sub>3</sub> 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 Cu<sub>2</sub>F<sub>5</sub>. *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-Yb<sub>5</sub>Sb<sub>3</sub>. *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., Gavriluk 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 YH<sub>6</sub>. *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.
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