CV of Professor Artem R. Oganov (updated 21/01/2019)

ADDRESS: Skolkovo Institute of Science and Technology, 3 Nobel St., 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:

2016 : Doctor of Physical & Mathematical Sciences (Russian highest degree, by equivalence to Habilitation)
2015-now : Professor, Skolkovo Institute of Science and Technology, Russia.
2013-now : 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
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, *summa cum laude.*

PUBLICATIONS: 238 papers (including 5 in *Nature* and 2 in *Science*) and book chapters.
Total citation = 11,564 (Web of Science) and 15,814 (Google Scholar). H-index = 55 (Web of Science) and 62 (Google Scholar). Published two books as editor.

INVITED LECTURES: >300 seminars and invited talks at conferences. 51 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:

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). Biographical and documentary films: "Color of the crystal" (directed by V. Gerchikov, 2012), "Made by Russians" (directed by L. Parfenov, 2015), "Watching the thought fly" (directed by V. Gerchikov, 2017). "House of science: Artem Oganov" (directed by N. Popova, 2018), "Cool story: Return of the professor" (directed by T. Mitkova, 2018).

SELECT PROFESSIONAL SERVICES:

2019-now : Science and Technology Council, Talent & Success Foundation (Russia)
2019-now : Academic Council, Russian Railways Corporation

2017-now : 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.
2009-now : Editorial Board member: *Scientific Reports (Nature Publishing Group)*
2009-now : Editorial Board member of *Journal of Superhard Materials*
2006-2010 : Associate Editor of *American Mineralogist*
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.)

PHD STUDENTS GRADUATED:

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).

List of publications of Artem R. Oganov.

BOOKS:

1. Oganov A.R., Saleh G., Kvashnin A.G. (Editors). *Computational Materials Discovery*. Royal Society of Chemistry. ISBN: 978-1-78262-961-0. (2018).
2. 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:

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.
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 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

218. Lepeshkin S.V., Baturin V.S., Uspenskii Yu.A., Oganov A.R. (2019). Method for simultaneous prediction of atomic structure of nanoclusters in a wide area of compositions. *J. Phys. Chem. Lett.* **10**, 102-106.
217. Dong B.J., Wang Z.H., Hung N.T., Oganov A.R., Yang T., Saito R., Zhang Z.D. (2019). New two-dimensional phase of tin chalcogenides: Candidates for high-performance thermoelectric materials. *Phys. Rev. Materials* **3**, 013405.
216. Oganov A.R. (2018). Crystal structure prediction: reflections on present status and challenges. *Faraday Discussions* **211**, 643-660.
215. Bushlanov P.V., Blatov V.A., Oganov A.R. (2019). Topology-based crystal structure generator. *Comp. Phys. Comm.*, in press.
214. Kvashnin A.G., Semenok D.V., Kruglov I.A., Wrona I.A., Oganov A.R. (2018). High-temperature superconductivity in a Th-H system under pressure conditions. *ACS Appl. Mater. Interf.* **10**, 43809-43816.
213. Yu X.H., Oganov A.R., Zhu Q., Qian G.R. (2018). The stability and unexpected chemistry of oxide clusters. *Phys. Chem. Chem. Phys.* **20**, 30437-30444.
212. Dong H.F., Oganov A.R., Brazhkin V.V., Wang Q.G., Zhang J., Davari Esfahani M.M., Zhou X.-F., Wu F.G., Zhu Q. (2018). Boron oxides under pressure: Prediction of the hardest oxides. *Phys. Rev.* **B98**, 174109.
211. Zhao C.M., Duan Y.F., Gao J., Liu W.J., Dong H.M., Dong H.F., Zhang D.K., Oganov A.R. (2018). Unexpected stable phases of tungsten borides. *Phys. Chem. Chem. Phys.* **20**, 24665-24670.
210. Kruglov I.A., Kvashnin A.G., Goncharov A.F., Oganov A.R., Lobanov S.S., Holtgrewe N., Jiang S.Q., Prakapenka V.B., Greenberg E., Yanilkin A.V. (2018). Uranium polyhydrides at moderate pressures: prediction, synthesis, and expected superconductivity. *Science Advances* **4**, eaat9776.
209. Shorikov A.O., Roizen V.V., Oganov A.R., Anisimov V.I. (2018). Role of temperature and Coulomb correlation in the stabilization of CsCl-type phase in FeS under pressure. *Phys. Rev.* **B98**, 094112.
208. Streltsov S.V., Roizen V.V., Ushakov A.V., Oganov A.R., Khomskii D.I. (2018). Old puzzle of incommensurate crystal structure of calaverite $AuTe_2$ and predicted stability of novel AuTe compound. *Proc. Natl. Acad. Sci. USA* **115**, 9945-9950.
207. Feya O.D., Wang Q.G., Lepeshkin S.V., Baturin V.S., Uspenskii Yu.A., Oganov A.R. (2018). Tetrahedral honeycomb surface reconstructions of quartz, cristobalite and stishovite. *Sci. Rep.* **8**, 11947.
206. Oganov A.R. (2018). 2D materials worth their salt. *Nature Chem.* **10**, 694-695.
205. Yao X., Xie C.W., Dong D., Oganov A.R., Zeng Q.F. (2018). Novel high-pressure calcium carbonates. *Phys. Rev.* **B98**, 014108.
204. Kvashnin A.G., Zakaryan H., Zhao C.M., Duan Y.F., Kvashnina Y.A., Xie C.W., Dong H.F., Oganov A.R. (2018). New tungsten borides, their stability and outstanding mechanical properties. *J. Phys. Chem. Lett.* **9**, 3470-3477.
203. Mazitov A., Oganov A.R., Yanilkin A.V. (2018). Titanium-hydrogen interaction at megabar pressure. *J. Appl. Phys.* **123**, 235901.
202. Frolov T., Setyawan W., Kurtz R., Marian J., Oganov A.R., Rudd R.E., Zhu Q. (2018). Grain boundary phases in bcc metals. *Nanoscale* **10**, 8253-8268.
201. Fan T., Xie C.W., Wang S.Y., Oganov A.R., Cheng L.F. (2018). First-principles study of thermoelectric properties of Mg_2Si-Mg_2Pb semiconductor materials. *RSC Advances* **8**, 17168-17175.
200. Cherednichenko K.A., Kruglov I.A., Oganov A.R., Le Godec Y., Mezouar M., Solozhenko V.L. (2018). Boron monosulfide: equation of state and pressure-induced phase transition. *J. Appl. Phys.* **123**, 135903.
199. Semenok D.V., Kvashnin A.G., Kruglov I.A., Oganov A.R. (2018). Actinium hydrides AcH_{10}, AcH_{12}, AcH_{16} as high-temperature conventional superconductors. *J. Phys. Chem. Lett.* **9**, 1920-1926.
198. He X.L., Dong X., Wu Q.S., Zhao Z.S., Zhu Q., Oganov A.R., Tian Y.J., Yu D.L., Zhou X.F., Wang H.T. (2018). Predicting the ground-state structure of sodium boride. *Phys. Rev.* **B97**, 100102 (Rapid Communications).
197. He X.L., Weng H.J., Zhang Y., Zhao Z.S., Wang Z.H., Xu B., Oganov A.R., Tian Y.J., Zhou X.F., Wang H.T. (2018). Two-dimensional boron on Pb (110) surface. *FlatChem* **7**, 34-41.
196. Hu X.B., Niu H.Y., Ma X.L., Oganov A.R., Fisher C.A.J., Sheng N.C., Liu J.D., Jin T., Sun X.F., Ikuhara Y. (2018). Atomic-scale observation and analysis of chemical ordering in M_3B_2 and M_5B_3 borides. *Acta Materialia* **149**, 274-284.
195. Kvashnin A.G., Kruglov I.A., Semenok D.V., Oganov A.R. (2018). Iron superhydrides FeH_5 and FeH_6: stability, electronic properties and superconductivity. *J. Phys. Chem.* **C122**, 4731-4736.
194. James A., Davari Esfahani M.M., Woerner W.R., Sinclair A., Ehm L., Oganov A.R., Parise J.B. (2018). Theoretical and experimental investigations into novel oxynitride discovery in the GaN-TiO_2 system at high pressure. *Crystals* **8**, 15.
193. Walsh D.W., Butler K.T., Skelton J.M., Xie C.W., Oganov A.R., Walsh A. (2018). Computer-aided design of metal chalcogenide semiconductors: from chemical composition to crystal structure using data-mining and evolutionary global optimisation. *Chem. Science* **9**, 1022-1030.
192. Nunez-Valdez M., Allahyari Z., Oganov A.R. (2018). Efficient technique for computational design of thermoelectric materials. *Comp. Phys. Comm.* **222**, 152-157.

191. Kruglov I., Akashi R., Yoshikawa S., Oganov A.R., Davari M. (2017). Refined phase diagram of the H-S system with high-Tc superconductivity. *Phys. Rev.* **B96**, 220101 (Rapid Comm.).
190. Khrapov N., Roizen V., Posypkin M., Samtsevich A., Oganov A.R. (2017). Volunteer computing for computational materials design. *Lobachevskii J. Mathem.* **38**, 926-930.
189. Kruglov I., Sergeev O., Yanilkin A., Oganov A.R. (2017). Energy-free machine learning force field for aluminum. *Sci. Rep.* **7**, 8512.
188. Lobanov S.S., Dong X., Martirosyan N.S., Samtsevich A.I., Stevanovic V., Gavryushkin P.V., Litasov K.D., Greenberg E., Prakapenka V.B., Oganov A.R., Goncharov A.F. (2017). Raman spectroscopy and X-ray diffraction of *sp3*-CaCO3 at lower mantle pressures. *Phys. Rev.* **B96**, 104101.
187. Zakaryan H.A., Kvashnin A.G., Oganov A.R. (2017). Stable reconstruction of the (110) surface and its role in pseudocapacitance of rutile-like RuO2. *Sci. Rep.* **7**, 10357.
186. Gou H.Y., Zhu L., Huang H.T., Biswas A., Keefer D.W., Chaloux B.L., Prescher C., Yang L.X., Kim D.Y., Ward M.D., Lerach J., Wang S.N., Oganov A.R., Epshteyn A., Badding J.V., Strobel T.A. (2017). From Linear Molecular Chains to Extended Polycyclic Networks: Polymerization of Dicyanoacetylene. *Chem. Mater.* **29**, 6706-6718.
185. Yu S.Y., Huang B., Zeng Q.F., Oganov A.R., Zhang L.T., Frapper G. (2017). Emergence of novel polynitrogen molecule-like species, covalent chains and layers in magnesium-nitrogen MgxNy phases under high pressure. *Phys. Chem. Chem. Phys.* **C121**, 11037−11046.
184. Shtukenberg A.G., Zhu Q., Carter D.J., Vogt L., Hoja J., Schneider E., Song H.X., Pokroy B., Polishchuk I., Tkatchenko A., Oganov A.R., Rohl A.L., Tuckerman M.E., Kahr B. (2017). Powder diffraction and crystal structure prediction identify four new coumarin polymorphs. *Chemical Science* **8**, 4926-4940.
183. Li B.X., Qian G.R., Oganov A.R., Boulfelfel S.E., Faller R. (2017). Mechanism of the fcc-hcp phase transformation in solid Ar. *J. Chem. Phys.* **146**, 214502.
182. Bazhanova Z.G., Roizen V.V., Oganov A.R. (2017). High-pressure behavior of the Fe-S system and composition of the Earth's inner core. *Physics-Uspekhi* **60**, 1025-1032.
181. Esfahani Davari M.M., Zhu Q., Dong H.F., Oganov A.R., Wang S.N., Rakitin M.S., Zhou X.F. (2017). Novel magnesium borides and their superconductivity. *Phys. Chem. Chem. Phys.* **19**, 14486-14494.
180. Zeng Q.F., Yu S.Y., Li D., Oganov A.R., Frapper G. (2017). Emergence of novel hydrogen chlorides under high pressure. *Phys. Chem. Chem. Phys.* **19**, 8236-8242.
179. Esfahani Davari M.M., Niu H.Y., Zhang J., Oganov A.R. (2017). Decomposition of solid germane under high pressure and unexpected chemistry of germanium hydrides with superconductivity. *Phys. Rev.* **B95**, 134506.
178. Zhang J., Oganov A.R., Li X.F., Dong H.F., Davari Esfahani M.M. (2017). First-principles investigation of Zr-O compounds, their crystal structures and mechanical properties. *J. Appl. Phys.* **121**, 155104.
177. Wang D.H., Zhou H.Y., Hu C.H., Zhong Y., Oganov A.R., Rao G.H. (2017). Prediction of thermodynamically stable Li-B compounds at ambient pressure. *Phys. Chem. Chem. Phys.* **19**, 8471-8477.
176. Yu S.Y., Zeng Q.F., Niu H.Y., Huang B., Oganov A.R., Frapper G., Zhang L.T. (2017). First-principles study of Zr-N crystalline phases: phase stability, electronic and mechanical properties. *RSC Advances* **7**, 4697-4703.
175. Kvashnin A.G., Oganov A.R., Allahyari Z. (2017). Computational search for novel hard chromium-based materials. *J. Phys. Chem. Lett.* **8**, 755-764.
174. Zhang J., Oganov A.R., Li X.F., Niu H.Y. (2017). Novel pressure-stabilized hafnium nitrides, and their properties. *Phys. Rev.* **B95**, 020103(R) (Rapid Communications).
173. Dong X., Oganov A.R., Goncharov A.F., Stavrou E., Lobanov S., Saleh G., Qian G.R., Zhu Q., Gatti C., Deringer V., Dronskowski R., Zhou X.-F., Prakapenka V., Konopkova Z., Popov I., Boldyrev A.I., Wang H.T. (2017). A stable compound of helium and sodium at high pressure. *Nature Chemistry* **9**, 440-445.
172. Stavrou E., Lobanov S.V., Dong H.F., Oganov A.R., Prakapenka V.B., Konopkova Z., Goncharov A.F. (2016). Synthesis of ultra-incompressible sp3-hybridized carbon nitride with 1:1 stoichiometry. *Chem. Mater.* **28**, 6925-6033.
171. Lepeshkin S., Baturin V., Tikhonov E., Matsko N., Uspenskii Y., Naumova A., Feya O., Schoonen M.A., Oganov A.R. (2016). Super-oxidation of silicon nanoclusters: magnetism and reactive oxygen species at the surface. *Nanoscale* **8**, 1816-1820.
170. Zhu J., Oganov A.R., Feng W.X., Yao Y.G., Zhang S.J., Yu X.H., Zhu J.L., Yu R.C., Jin C.Q., Dai X., Fang Z., Zhao Y.S. (2016). Pressure-induced Ag2Te polymorphs in conjunction with topological non-trivial to metal transition. *AIP Advances* **6**, 085003.
169. Saleh G., Oganov A.R. (2016). Pressure-induced stabilization of carbonic acid and other compounds in the C-H-O phase diagram. *Sci. Rep.* **6**, 32486.
168. Dong H.F., Oganov A.R., Wang Q.G., Wang S.N., Wang Z.H., Zhang J., Davari Esfahani M.M., Zhou X.F., Wu F.G., Zhu Q. (2016). Prediction of a new ground state of superhard compound B6O at ambient conditions. *Sci. Rep.* **6**, 31288.
167. Matsko N.L., Tikhonov E.V., Baturin V.S., Lepeshkin S.V., Oganov A.R. (2016). The impact of electron correlations on the energetics and stability of silicon nanoclusters. *J. Chem. Phys.***145**, 074313.
166. Dolgirev P.E., Kruglov I.A., Oganov A.R. (2016). Machine learning scheme for fast extraction of interatomic potentials and chemistry. *AIP Advances* **6**, 085318.

165. An Q., Reddy K.M., Dong H.F., Chen M.-W., Oganov A.R., Goddard, W.A. III. (2016). Nanotwinned boron suboxide (B6O): new ground state of B6O. *Nano Letters* **16**, 4236-4242.
164. Goncharov A.F., Lobanov S.S., Kruglov I.A., Zhao X.M., Chen X.J., Oganov A.R., Konopkova Z., Prakapenka V.B. (2016). Hydrogen sulfide at high pressure: change in stoichiometry. *Phys. Rev. **B*93**, 174105.
163. Qian G.R., Niu H.Y., Hu C.H., Oganov A.R., Zeng Q.F., Zhou H.Y. (2016). Prediction of unique diversity of stable hydronitrogens, and implication for planetary and materials sciences. *Sci. Rep.* **6**, 25947.
162. Reilly A.M., Cooper R.I., …,Oganov A.R., …Groom C.R. (2016). Report on the sixth blind test of organic crystal structure prediction methods. *Acta Cryst **B*72**, 439-459.
161. Yu S.Y., Huang B., Jia X.J., Oganov A.R., Zeng Q.F., Zhang L.T., Frapper G. (2016). Exploring the real ground-state structures of molybdenum-nitrogen MoN2 phases. *J. Phys. Chem. **C*120**, 11060-11067.
160. Zhang W.W., Oganov A.R., Zhu Q., Lobanov S., Stavrou E., Goncharov A.F. (2016). Stability of numerous novel potassium chlorides at high pressure. *Sci. Rep.* **6**, 26265.
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