CURRICULUM VITAE (January 5, 2018)

Artem R. Oganov

Professor, Skolkovo Institute of Science and Technology,
3 Nobel St., Moscow 143026, Russia

Director, International Center for Materials Discovery, Northwestern Polytechnical University,
Xi'an, 710072, China

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Personal data:
Born on 03.03.1975 in Moscow, Russia.
Married, three children (two daughters, one son).
Languages: English (fluent), Russian (native), German, French, Italian.

Academic Degrees:

2016	Doctor of Physical & Mathematical Sciences (Russian highest degree, by equivalence to Habilitation)
2007	Habilitation, Dept. of Materials, ETH Zurich, Switzerland
2002	PhD degree, University College London. Thesis "Computer Simulation Studies of Minerals"
1997	MSc in Crystallography (Moscow State University), *summa cum laude*

Employment:

2015-now	Professor, Skolkovo Institute of Science and Technology, Russia
2013-now	Head of Laboratory and Professor, Moscow Institute of Physics and Technology, Russia
2013-2017	Director, Center for Materials by Design, Stony Brook University
2010-2017	Professor, Stony Brook University
2008-2010	Associate Professor, Stony Brook University
2003-2008	Group Leader and Privatdozent, ETH Zurich
2002-2003	Research Fellow, University College London
1993-1995	External scientific collaborator, Russian Chemical Abstracts (VINITI)

Visiting Appointments: Adjunct Professor of Moscow State University since 2006, Northwestern Polytechnical University (China) since 2012, and Moscow Institute of Physics and Technology (Russia) since 2013. Since 2005 was an invited professor in Italy (Milan), France (Paris, Lille and Poitiers), China (Guilin, Beijing, Hong Kong, Kaifeng, Urumqi).

Career Summary:

Publications, patents, citation:	210 papers and book chapters, including 5 in *Nature*, 2 in *Science*, 1 in *Nature Materials*, 2 in *Nature Chemistry*, 2 in *Nature Communications*, 5 in *PNAS*, 11 in *PRL*, 1 in *Accounts of Chemical Research*, 1 in *Angew. Chem.*, 1 in *JACS*. 1 book, 5 patents. Total citation = 9347 (Web of Science) and 12783 (Google Scholar). Hirsch's h-index = 51 (Web of Science) and 57 (Google Scholar).
Talks:	339 in total, including 42 plenary/keynote, 285 invited, 12 contributed talks

Research Interests:
Interdisciplinary research centered on theory and simulation of materials – with applications to high-pressure physics, planetary sciences, materials science and chemistry.

Honors and Awards:

2017	Concord prize

2017	George Gamov award
2017	Elected Member of Academia Europaea (M.A.E.)
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	Elected Professor of the Russian Academy of Sciences
2015	Japan Society for Promotion of Science Invitation Fellow
2014	Listed among 100 most influential Russians today (Russian Reporter)
2013	Elected Fellow of the Mineralogical Society of America
2012	Honorary Professor, Yanshan University, China
2011	Ranked 6th most successful Russian scientist (Forbes Russia)
2010	Most cited paper award, *Earth and Planetary Science Letters* (2005-2010)
2008	Ranked 12th among all Russian scientists living abroad (Russian Newsweek)
2007	Most cited paper award, *Earth and Planetary Science Letters* (2004-2007)
2007	Research Excellence Medal of the European Mineralogical Union
2006	University Latsis Prize (25,000 CHF)
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
1998-2002	Russian President's Scholarship, British Government Scholarship, Graduate Scholarship of University College London

Select Professional Services:

2017-	Academic Council, Russian Railways Corporation
2017-	Member of Russian Presidential Council for Science and Education
2017-	Consultant, Commission on Crystallography of Materials (International Union of Crystallography)
2017	Panelist at sessions "AI and Manufacturing" and "Global Innovation: a View from Russia" at World Economic Forum (Dalian, June 2017)
2017	Award Committee, RUSNANOPRIZE
2016-	Academic Council, Fersman Mineralogical Museum
2016-	Academic Council, Skolkovo Institute of Science and Technology
2014	International Program Committee of the 2014 International Union of Crystallography meeting (Montreal, Canada, 5-12 August 2014)
2011-2017	Chairman, Commission on Crystallography of Materials (International Union of Crystallography)
2010-2012	Scientific Advisory Committees, EHPRG-48 (Uppsala, Sweden, 2010), EHPRG-49 (Budapest, Hungary, 2011), EHPRG-50 (Thessaloniki, Greece, 2012) conferences.
2009-2012	Member of the University Senate, Stony Brook University
2004-2017	Organized 14 workshops (2004 – Lyon; 2011 – Poitiers; Xi'an; 2012 – Lausanne; Stony Brook; 2013 – Guilin; 2014 – Xi'an; Montreal; 2015 – Shiv Nadar University (India); Poitiers; Beijing; 2016 – Varenna; 2017 – Poitiers; Shanghai)

Courses taught:

2015-	Graduate course "Structure and Properties of Materials", Skoltech
2011-2012	Graduate course "Crystal Chemistry", SBU
2010-2017	Undergraduate/graduate course "Structure and Properties of Materials", SBU
2009	Graduate seminar "Electronic Structure Calculations in Crystallography", SBU
2009	Graduate course "Crystalline Solids", SBU
2009	Undergraduate course "Mineralogy", SBU
2004-2007	Undergraduate course "Mineralogical Crystallography", ETH Zurich

Editorial Activities and Refereeing:

2016-present	Editorial Board member: *Geodynamics and Tectonophysics*
2011-present	Editorial Board member: *Scientific Reports (Nature Publishing Group)*
2009-present	Editorial Board member: *Journal of Superhard Materials*
2006-2010	Associate Editor: *American Mineralogist*
2005-2012	Organized 6 Special Issues (2005: *Z. Krist.*, Special Issue "Computational Crystallography"; 2010: *J. Superhard Mat.*, Special Issue "Theory of Superhard

	Materials"; 2011: *J. Superhard Mat.*, Special Issue "Boron and Boron-rich Solids"; 2012: *J. Superhard Mat.*, Special Issue "Superhard Carbon"; 2014: *Acta Cryst.C*, Special Issue "Computational Materials Discovery"; 2014: *J. Superhard Mat.*, Special Issue "Novel Superhard Materials")
2010	Book Editor: „Modern Methods of Crystal Structure Prediction", Wiley-VCH.
Peer reviews (papers):	Over 60 journals, including *Nature, Science; Nature Chemistry, Nature Materials; Nature Geoscience; Phys. Rev. Lett.; Adv. Mat.; Inorg. Chem.*, etc.
(grants):	Referee for funding agencies in the US (NSF, DoE, CRDF), Asia (Hong Kong's Research Grants Council), Europe (ERC, Germany's DFG, France's ANR, Switzerland's SNF, Poland's National Science Center, Russia's RSF).

Research faculty mentored: Prof. Qiang Zhu (2013-2016, now Asst. Prof. at UNLV, USA), Prof. Andriy O. Lyakhov (2011-2013).

Postdocs supervised: Alexander Kvashnin (2015-), Haiyang Niu (2015-), Evgeny Tikhonov (2015-), Zhenhai Wang (2015-), Sergey Lepeshkin (2013-), Vladimir Baturin (2013-), Nikita Matsko (2013-), Dong Dong (2013-), Pavel Bushlanov (2013-), Maribel Nunez Valdez (2015-2016, now Prof. at Pottsdam U., Germany), Gabriele Saleh (2013-2016, now Res. Fellow at Trinity Coll. Dublin), Fei Qi (2013-2015, now Assoc. Prof. at Xidian Univ., China), Maksim Rakitin (2013-2015, now Res. Fellow at BNL, USA), Qinggao Wang (2013-2016, now Prof. at Henan U., China), Xiaohu Yu (2013-2015, now Assoc. Prof. at Henan Normal U., China), Huafeng Dong (2013-2015, now Assoc. Prof., Guangdong U. of Tech., China), Xiang-Feng Zhou (2012-2015, now Prof. at Nankai U., China), Salah E. Boulfelfel (2010-2012, now Res. Fellow at Georgia Tech, USA), Andriy O. Lyakhov (2007-2011), Yanming Ma (2006-2008, now Prof. at Jilin U., China).

PhD students supervised: Heng Zhang (2016-), Pengyan Xue (2016-), Anastasia Naumova (2015-), Artem Samtsevich (2015-), Valery Royzen (2015-), Zahed Allahyari (2014-), Ivan Kruglov (2014-), Congwei Xie (2014-), Oleg Feya (2013-),Jin Zhang (2014-2017, now postdoc at Stony Brook University), Mahdi Davari (2013-2017, now postdoc at Stony Brook University), Shengnan Wang (2013-2016, now at Amazon), Guangrui Qian (2011-2015, now at IBM, China), Qiang Zhu (2009-2014, now Asst. Prof. at UNLV, USA), Yu Xie (2007-2010, now Res. Fellow at Oak Ridge Natl. Lab, USA), Feiwu Zhang (2005-2008, now Professor in Inst. Geochemistry, Chinese Acad. Sci.), Colin W. Glass (2006-2009, now at Stuttgart Comp. Center), Donat Adams (2004-2007, now Res. Fellow at EMPA, Switzerland), Kai H. Hassdenteufel (2003-2006, now teacher in Switzerland), Daniel Y. Jung (2004-2008, now at ETH Zurich).

MSc/BSc students supervised: Arslan Mazitov (2015-), Sergey Pozdnyakov (2017-), Efim Mazhnik (2017-), Nikita Rybin (2017-). Maria Kravets (2017-), Elizaveta Pavlova (2015-), Saeed Rakhmanian Koshkaki (2015-2017), Pavel Dolgirev (2014-2016), Valery Royzen (2013-2015), Anastasia Naumova (2014-2015), Igor Blinov (2013-2015), Hongfei Xu (2012-2014), Yue Liu (2012-2013), Sandro Schönborn (2008), Colin W. Glass (2005-2006, now at Stuttgart Comp. Center), Daniel Y. Jung (2003-2004, now at ETH Zurich), Alina V. Gutina (1997-1998).

Visiting scientists: Ali Berberov (Moscow University of Oil and Gas, Russia, 2014, now at Gazprom Research), Dongxu Li (Assoc. Prof., Huaqiao University, China, 2013-2014), Yanqing Shen (Lecturer, Harbin Institute of Technology, China, 2013-2014), Pengcheng Chen (Tsinghua University, China, 2013-2014, now works in Chinese govmt.), Qianku Hu (Henan Polytechnic University, China, 2013-2014, now Asst. Prof.), Xiao Dong (Nankai University, China, 2012-2014, now Res. Fellow at HPSTAR, Beijing), Qingfeng Zeng (Assoc. Prof., Northwestern Polytechnical University, Xi'an, China, 2011-2012), Chaohao Hu (Prof., Guilin University of Electronic Technology, China, 2011-2012), Jose Perez (Prof., University of Cartagena, Spain, 2011), Weiwei Zhang (China Agricultural University, Beijing, 2011-2013, now Prof. at China Agr. Univ.), Yanchao Wang (Jilin University, China, 2009-2010, now postdoc at Jilin U., China), Miguel Martinez Canales (University of Bilbao, Spain, 2009, now Res. Fellow at U. of Edinburgh), Love Koci (University of Uppsala, Sweden, 2007), Steeve Greaux (University of Paris Est, France, 2005, now at Ehime U., Japan).

Sabbatical visitors: Prof. Artem Masunov (University of Central Florida, USA, 2013-2014), Prof. Alberto Garcia (University of Basque Country, Spain, 2006, now at Natl. Inst. Mater. Sci, Barcelona)

List of publications of Artem R. Oganov.

BOOKS:

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:

17. Dong X., Oganov A.R. (2017). Electrides and their high-pressure chemistry. In: *Correlations in Condensed Matter Under Extreme Conditionst,* ed. G.N.N. Angilella & A. La Magna, Springer Verlag. Pp. 69-84.
16. 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.
15. Oganov A.R., Lyakhov A.O., Zhu Q. (2014). Theory of superhard materials. *In: Comprehensive Hard Materials Review*, Elsevier, v.3, 59-79.
14. Oganov A.R. (2011). Discovery of γ-B_{28}, 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.
13. 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.
12. 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.
11. 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.
10. 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.
9. 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.
8. Oganov A.R., Ma Y., Lyakhov A.O., Valle M., Gatti C. (2010). Evolutionary crystal structure prediction as a method for the discovery of minerals and materials. *Rev. Mineral. Geochem.* **71**, 271-298.
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

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*, in press.

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 sp^3-$CaCO_3$ 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 RuO_2. *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 Mg_xN_y 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 (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 Ag_2Te 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 B_6O 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 (B_6O): new ground state of B_6O. *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 MoN_2 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.
159. Wang Q.G., Oganov A.R., Zhu Q., Feya O.D., Ma D.W. (2016). Unexpectedly rich structures of rutile TiO_2(011)-(2×1) and driving forces behind their formations: an *ab initio* evolutionary study. *Phys. Chem. Chem. Phys.* **18**, 19549-19556.
158. Xie C.W., Oganov A.R., Dong D., Zeng Q.F. (2016). A first-principles study of the structural and mechanical properties of stable zirconium carbides. *Phys. Chem. Chem. Phys.* **18**, 12299-12306.
157. Zhu Q., Shtukenberg A., Carter D., Yu T.Q., Yang J.X., Chen M., Raiteri P., Oganov A.R., Pokroy B., Polishchuk I., Bygrave P., Day G., Rohl A., Tuckerman M., Kahr B. (2016). Resorcinol Crystallization from the Melt: A New Ambient Phase and New "Riddles". *J. Am. Chem. Soc.* **138**, 4881-4889.
156. Woerner B.R., Qian G.R., Oganov A.R., Stephens P.W., Dharmagunawardhane H.A.N., Sinclair A., Parise J.B. (2016). Combined theoretical and in situ scattering strategies for optimized discovery and recovery of high-pressure phases: A case study of the GaN-Nb_2O_5 system. *Inorg. Chem.* **55**, 3384-3392.
155. Davari Esfahani M.M., Wang Z.H., Oganov A.R., Dong H.F., Zhu Q., Wang S.N., Rakitin M.S., Zhou X.F. (2016). Superconductivity of novel tin hydrides (Sn_nH_m) under pressure. *Sci. Rep.* **6**, 22873.
154. Wang Q.G., German K.E., Oganov A.R., Dong H.F., Feya O.D., Zubavichus Y.V., Murzin V. (2016). Explaining stability of transition metal carbides – and why TcC does not exist. *RSC Advances* **6**, 16197-16202.
153. Zhou X.F., Oganov A.R., Wang Z.H., Popov I.A., Boldyrev A.I., Wang H.T. (2016). Two-

dimensional magnetic boron. *Phys. Rev.* **B93**, 085406.

152. Wang S.N., Oganov A.R., Qian G.R., Zhu Q., Dong H.F., Davari Esfahani M.M. (2016). Novel superhard B-C-O phases predicted from first principles. *Phys. Chem. Chem. Phys.* **18**, 1859-1863.
151. Saleh G., Oganov A.R. (2016). Alkali subhalides: High-pressure stability and interplay between metallic and ionic bonds. *Phys. Chem. Chem. Phys.* **18**, 2840-2849.
150. Yu X.H., Oganov A.R., Popov I.A., Qian G.R., Boldyrev I.A. (2016). Antiferromagnetic stabilization in Ti_8O_{12} cluster. *Angew. Chem. Int. Ed.* **55**, 1699-1703.
149. Zhu Q., Oganov A.R., Zeng Q.F., Zhou X.F. (2016). Structure prediction and its applications in computational materials design. *Chem. Model.* **12**, 219-248.
148. Mannix A.J., Zhou X.F., Kiraly B., Wood J.D., Alducin D., Myers B., Liu X.L., Fisher B.L., Santiago U., Guest J.R., Yacaman M.J., Ponce-Pedraza A., Oganov A.R., Hersam M.C., Guisinger N.P. (2015). Synthesis of borophene: An anisotropic, two-dimensional boron allotrope. *Science* **350**, 1513-1516.
147. Niu H.Y., Oganov A.R., Chen X.Q., Li D.Z. (2015). Novel stable compounds in the Mg-Si-O system under exoplanet pressures and their implications in planetary science. *Sci. Rep.* **5**, 18347.
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