

## CURRICULUM VITAE (August 31, 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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Scopus Author ID: 6701334785

#### Personal data:

Born on 03.03.1975 in Moscow, Russia.

Married, four children (two daughters, two sons).

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, 227 papers and book chapters, including 5 in *Nature*, 2 in *Science*, 1 in *Nature* patents, citation: *Materials*, 3 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 = 10717 (Web of Science) and 14676 (Google Scholar). Hirsch's h-index = 53 (Web of Science) and 60 (Google Scholar).

Talks: 343 in total, including 45 plenary/keynote, 291 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 Russian Highly Cited Researcher in Physics (Clarivate Analytics)

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 ( <i>J. Chem. Phys.</i> 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
2013	Elected Fellow of the Mineralogical Society of America
2012	Honorary Professor, Yanshan University, China
2012	1000 talents professor of People's Republic of China
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

### In Media:

Ranked among the most successful Russian scientists by Russian Newsweek (2008), and Forbes Russia (2011), and among 100 most influential Russians by 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 flight of the thought" (directed by V. Gerchikov, 2017).

### 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: <i>Geodynamics and Tectonophysics</i>
2011-present	Editorial Board member: <i>Scientific Reports (Nature Publishing Group)</i>
2009-present	Editorial Board member: <i>Journal of Superhard Materials</i>
2006-2010	Associate Editor: <i>American Mineralogist</i>
2005-2012	Organized 6 Special Issues (2005: <i>Z. Krist.</i> , 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 Over 60 journals, including *Nature*, *Science*; *Nature Chemistry*, *Nature Materials*;

(papers): *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. Boulfefel (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 govt.), 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., 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:

18. 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. *In press*.
17. 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.
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  $\gamma$ -B<sub>28</sub>, 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

## PAPERS IN REFEREED JOURNALS

209. Shorikov A.O., Roizen V.V., Oganov A.R., Anisimov V.I. (2018). The role of temperature and Coulomb correlations in stabilization of CsCl-phase in FeS under pressure. *Phys. Rev. B.*, in press.
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<sub>2</sub> and predicted stability of novel AuTe compound. *Proc. Natl. Acad. Sci.*, in press.
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<sub>2</sub>Si-Mg<sub>2</sub>Pb 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<sub>10</sub>, AcH<sub>12</sub>, AcH<sub>16</sub> 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 M3B2 and M5B3 borides. *Acta Materialia* **149**, 274-284.
195. Kvashnin A.G., Kruglov I.A., Semenok D.V., Oganov A.R. (2018). Iron superhydrides FeH<sub>5</sub> and FeH<sub>6</sub>: 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<sub>2</sub> system at high pressure. *Crystals* **8**, art. 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 *sp*<sup>3</sup>-CaCO<sub>3</sub> 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<sub>2</sub>. *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<sub>x</sub>Ny 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., Zh Gatti C., Deringer V., Dronskowski R., Zhou X.-F., Prakapenka V., Konopkova Z., Popo Boldyrev A.I., Wang H.T. (2017). A stable compound of helium and sodium at high pres *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 sp<sup>3</sup>-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<sub>2</sub>Te 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<sub>6</sub>O 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<sub>6</sub>O): new ground state of B<sub>6</sub>O. *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.* **B93**, 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* **B72**, 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<sub>2</sub> phases. *J. Phys. Chem.* **C120**, 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<sub>2</sub>(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<sub>2</sub>O<sub>5</sub> 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 (SnnHm) 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<sub>8</sub>O<sub>12</sub> 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.
146. Xie C.W., Oganov A.R., Dong D., Li D., Debela T.T., Liu N., Zeng Q.F. (2015). Rational design of inorganic dielectric materials with expected permittivity. *Sci. Rep.* **5**, 16769.
145. Yu S.Y., Zeng Q.F., Frapper G., Oganov A.R., Zhang L.T. (2015). Pressure-driven formation and stabilization of the superconductive chromium hydrides. *Sci. Rep.* **5**, 17764.
144. Zhang J., Oganov A.R., Li Z.F., Xue K.H., Wang Z.H., Dong H.F. (2015). Pressure-induced novel compounds in the Hf-O system from first-principles calculations. *Phys. Rev.* **B92**, 184104.
143. Li D.X., Oganov A.R., Dong X., Zhou X.F., Zhu Q., Qian G.R., Dong H.F., Li R.K. (2015). Nitrogen oxides under pressure: stability, ionization, polymerization, and superconductivity. *Sci. Rep.* **5**, 16311.
142. Zhu Q., Oganov A.R., Lyakhov A.O., Yu X.X. (2015). Generalized evolutionary metadynamics for sampling energy landscapes and its applications. *Phys. Rev.* **B92**, 024106.
141. Lobanov S.S., Zhu Q., Holtgrewe N., Prescher C., Prakapenka V.B., Oganov A.R., Goncharov A.F. (2015). Stable magnesium peroxide at high pressure. *Sci. Rep.* **5**, 13582.
140. Shen Y.Q., Oganov A.R., Qian G.R., Zhang J., Dong H.F., Zhu Q., Zhou Z.X. (2015). Novel lithium-nitrogen compounds at ambient and high pressures. *Sci. Rep.* **5**, 14204.
139. Rakitin M.S., Oganov A.R., Niu H.Y., Esfahani Davari M.M., Zhou X.F., Qian G.R., Solozhenko V.L. (2015). A novel phase of beryllium fluoride at high pressure. *Phys. Chem. Chem. Phys.* **17**, 26283-26288.
138. Wang Z.H., Zhou X.F., Zhang X.M., Zhu Q., Dong H.F., Zhao M.W., Oganov A.R. (2015). Phagraphene: a low-energy graphene allotrope composed of 5-6-7 carbon rings with distorted Dirac cones. *Nano Lett.* **15**, 6182-6186.
137. Yu X.H., Oganov A.R., Popov I.A., Boldyrev A.I. (2015). Spherical aromaticity in Ce<sub>6</sub>O<sub>8</sub>. *J. Comput. Chem.* DOI: 10.1002/jcc.24049

136. Chen P.C., Wang N., Oganov A.R., Duan W.H. (2015). Effects of ferroelectric polarization on surface phase diagram: evolutionary algorithm study of BaTiO<sub>3</sub>(001) surface. *Phys. Rev.* **B92**, 085432.
135. Goncharov A.F., Holtgrewe N., Qian G.R., Hu C.H., Oganov A.R., Somayazulu M., Stavrou E., Pickard C.J., Berlie A., Yen F., Mahmood M., Lobanov S.S., Konopkova Z., Prakapenka V.B. (2015). The backbone NxH compounds at high pressures. *J. Chem. Phys.* **142**, 214308.
134. Stavrou E., Chen X.J., Oganov A.R., Wang A.F., Yan Y.J., Luo X.G., Chen X.H., Goncharov A.F. (2015). Formation of As-As interlayer bonding in the collapsed tetragonal phase of NaFe<sub>2</sub>As<sub>2</sub> under pressure. *Sci. Rep.* **5**, 9868.
133. Zhang J., Oganov A.R., Li X.F., Zeng Q.F., Dong H.F. (2015). Novel compounds in the Zr-O system, their crystal structures and mechanical properties. *Phys. Chem. Chem. Phys.* **17**, 17301-17310.
132. Yu S.Y., Zeng Q.F., Oganov A.R., Frapper G., Zhang L.T. (2015). Phase stability, mechanical properties and chemical bonding of titanium nitrides: A first-principles study. *Phys. Chem. Chem. Phys.* **17**, 11763-11769
131. Dong H.F., Oganov A.R., Zhu Q., Qian G.R. (2015). The phase diagram and hardness of carbon nitrides. *Sci. Rep.* **5**, 9870.
130. Li Y.L., Wang S.N., Oganov A.R., Gou H.Y., Smith J.S., Strobel T.A. (2015). Diverse chemistry of stable calcium carbides. *Nature Comm.* **6**, 6974.
129. Zeng Z.D., Zeng Q.F., Liu N., Oganov A.R., Zeng Q.S., Cui Y., Mao W.L. (2015). A new phase of Li<sub>15</sub>Si<sub>4</sub> synthesized under pressure. *Adv. Energy Mat.* **5**, 1500214.
128. Liu Y., Wang S.N., Oganov A.R., Zhu Q., Dong X., Kresse G. (2015). Prediction of new thermodynamically stable aluminum oxides. *Sci. Rep.* **5**, 9518.
127. Xu C.S., Xu B., Yang Y.R., Dong H.F., Oganov A.R., Wang S.Y., Duan W.H., Gu B.L., Bellaiche L. (2015). Prediction of a stable post-post-perovskite structure from first principles. *Phys. Rev.* **B91**, 020101 (Rapid Communications).
126. Zhu Q., Oganov A.R., Zeng Q.F. (2015). Formation of stoichiometric CsF<sub>n</sub> compounds. *Sci.Rep.* **5**, 7875.
125. Wang Q.G., Oganov A.R., Zhu Q., Zhou X.F. (2014). Novel reconstructions of the (110) surface of rutile TiO<sub>2</sub> predicted by an evolutionary method. *Phys. Rev. Lett.* **113**, 266101.
124. Zhou X.F., Oganov A.R., Shao X., Zhu Q., Wang H.T. (2014). Unexpected reconstruction of the  $\alpha$ -boron (111) surface. *Phys. Rev. Lett.* **113**, 176101.
123. Zhu Q., Oganov A.R., Zhou X.F. (2014). Crystal structure prediction and its application in Earth and materials sciences. *Topics in Current Chemistry* **345**, 223-256.
122. Yu S.Y., Zeng Q.F., Oganov A.R., Hu C.H., Frapper G., Zhang L.T. (2014). Exploration of stable compounds, crystal structures, and superconductivity in the Be-H system. *AIP Advances* **4**, 107118.
121. Zhang J., Zeng Q.F., Oganov A.R., Dong D., Y.F. Li (2014). High throughput exploration of ZrxSi<sub>1-x</sub>SiO<sub>4</sub> dielectrics by evolutionary first-principles approaches. *Phys. Lett.* **A378**, 3549-3554.
120. Zhu Q., Sharma V., Oganov A.R., Ramprasad R. (2014). Predicting polymeric crystal structures by evolutionary algorithms. *J. Chem. Phys.* **141**, 154102.
119. Wang D.H., Zhou H.Y., Hu C.H., Oganov A.R., Zhong Y., Rao G.H. (2014). BaC: a thermodynamically stable layered superconductor. *Phys. Chem. Chem. Phys.* **16**, 20780-20784.
118. Sharma V., Wang C., Zhu Q., Pilia G., Oganov A.R., Ramprasad R. (2014). First-principles design of advanced polymer dielectrics. *Nat. Comm.* **5**, art. 4845.
117. Xie C.W., Zeng Q.F., Oganov A.R., Dong D. (2014). Discovering low-permittivity materials: evolutionary search for novel MgAl<sub>2</sub>O<sub>4</sub> polymorphs. *Appl. Phys. Lett.* **105**, 022907.
116. Raza Z., Errea I., Oganov A.R., Saitta A.M. (2014). Superconducting metallic skutterudite-type phosphorus nitride at high pressure from first-principles calculations. *Sci. Rep.* **4**, 5889.
115. Qian G.R., Lyakhov A.O., Zhu Q., Oganov A.R., Dong X. (2014). Novel hydrogen hydrate structures under pressure. *Sci.Rep.* **4**, 5606.
114. Strobel T., Kurakevych O., Kim D.Y., Le Godec Y., Crichton W., Guignard G., Guignot N., Cody G., Oganov A.R. (2014). Synthesis of  $\beta$ -Mg<sub>2</sub>C<sub>3</sub>: a monoclinic high-pressure polymorph of magnesium sesquicarbide. *Inorg. Chem.* **53**, 7020-7027.
113. Zhu Q., Feya O.D., Boulfelfel S.E., Oganov A.R. (2014). Metastable host-guest structure of carbon. *J. Superhard Mater.* **36**, 246-256.
112. Solozhenko V.L., Kurakevych O.O., Kurnosov A., Oganov A.R. (2014). Boron phosphide under pressure: in situ study by Raman scattering and X-ray diffraction. *J. Appl. Phys.* **116**, 033501.
111. Niu H., Chen X.Q., Ren W., Zhu Q., Oganov A.R., Li D., Li Y. (2014). Variable-composition structure prediction and experimental verification of MnB<sub>3</sub> and MnB<sub>4</sub>. *Phys. Chem. Chem. Phys.* **16**, 15866-15873.
110. Xie C.W., Zeng Q.F., Dong D., Gao S., Cai Y., Oganov A.R. (2014). First-principles calculations of the dielectric and vibrational properties of ferroelectric and paraelectric BaAl<sub>2</sub>O<sub>4</sub>. *Phys. Lett.* **A378**, 1867-1870.



109. Zhao Z., Wang S., Oganov A.R., Chen P.C., Liu Z., Mao W.L. (2014). Tuning the crystal structure and electronic states of Ag<sub>2</sub>Se: structural transitions and metallization under pressure. *Phys. Rev.* **B89**, 180102.
108. Baturin V.S., Lepeshkin S.V., Matsko N.L., Oganov A.R., Uspenskii Yu.A. (2014). Prediction of the atomic structure and stability for the ensemble of silicon nanoclusters passivated by hydrogen. *Europhys. Lett.* **106**, art. 37002.
107. Zhou X.F., Dong X., Oganov A.R., Zhu Q., Tian Y.J., Wang H.T. (2014). Semimetallic two-dimensional boron allotrope with massless Dirac fermions. *Phys. Rev. Lett.* **112**, 085502.
106. Xie Y., Li Q., Oganov A.R., Wang H. (2014). Superconductivity of lithium-doped hydrogen under high pressure. *Acta Cryst.* **C70**, 104-111.
105. Zeng Q.F., Oganov A.R., Lyakhov A.O., Xie C.W., Zhang X.D., Zhang J., Zhu Q., Wei B.Q., Grigorenko I., Zhang L.T., Cheng L.F. (2014). Evolutionary search for new high-k dielectric materials: methodology and applications to hafnia-based oxides. *Acta Cryst.* **C70**, 76-84.
104. Finkelstein G.J., Dera P.K., Jahn S., Oganov A.R., Holl C.M., Meng Y., Duffy T.S. (2014). Phase transitions and equation of state of forsterite to 90 GPa from single-crystal X-ray diffraction and molecular modeling. *Am. Mineral.* **99**, 35-43.
103. Zhang W.W., Oganov A.R., Goncharov A.F., Zhu Q., Boulfelfel S.E., Lyakhov A.O., Somayazulu M., Prakapenka V.B., Konopkova Z. (2013). Unexpected stoichiometries of stable sodium chlorides. *Science* **342**, 1502-1505.
102. Zeng Q.F., Peng J.H., Oganov A.R., Zhu Q., Xie C.W., Zhang X.D., Dong D., Zhang L., Cheng L.F. (2013). Prediction of stable hafnium carbides: their stoichiometries, mechanical properties, and electronic structure. *Phys. Rev.* **B88**, 214107.
101. Zhu Q., Li L., Oganov A.R., Allen P.B. (2013). Evolutionary method for prediction of surface reconstructions with variable stoichiometry. *Phys. Rev.* **B87**, 195317.
100. Qian G.R., Dong X., Zhou X.-F., Tian Y., Oganov A.R., Wang H.-T. (2013). Variable cell nudged elastic band method for studying solid-solid structural phase transitions. *Comp. Phys. Comm.* **183**, 2111-2118.
99. Zhu Q., Oganov A.R., Lyakhov A.O. (2013). Novel stable compounds in the Mg-O system under high pressure. *Phys. Chem. Chem. Phys.* **15**, 7796-7700.
98. Hu C.H., Oganov A.R., Zhu Q., Qian G.R., Frapper G., Lyakhov A.O., Zhou H.Y. (2013). Pressure-induced stabilization and insulator-superconductor transition of BH. *Phys. Rev. Lett.* **110**, 165504.
97. Hu M., Zhao Z.S., Tian F., Oganov A.R., Wang Q.Q., Xiong M., Fan Q.Z., Wen B., He J.L., Yu D.L., Wang H.-T., Xu B., Tian Y.J. (2013). Compressed carbon nanotubes: a family of new multifunctional carbon allotropes. *Sci. Rep.* **3**, 1331.
96. Oganov A.R., Hemley R.J., Hazen R.M., Jones A.P. (2013). Structure, Bonding, and Mineralogy of Carbon at Extreme Conditions. *Rev. Mineral. Geochem.* **75**, 47-77.
95. Lyakhov A.O., Oganov A.R., Stokes H.T., Zhu Q. (2013). New developments in evolutionary structure prediction algorithm USPEX. *Comp. Phys. Comm.* **184**, 1172-1182.
94. Zhu Q., Jung D.Y., Oganov A.R., Gatti C., Glass C.W., Lyakhov A.O. (2013). Stability of xenon oxides at high pressures. *Nature Chem.* **5**, 61-65.
93. Zhou X.-F., Oganov A.R., Qian G.R., Zhu Q. (2012). First-principles determination of the structure of magnesium borohydride. *Phys. Rev. Lett.* **109**, 245503.
92. Boulfelfel S.E., Zhu Q., Oganov A.R. (2012). Novel sp<sup>3</sup>-forms of carbon predicted by evolutionary metadynamics and analysis of their synthesizability using transition path sampling. *J. Superhard Mater.* **34**, 350-359.
91. Zhu Q., Zeng Q., Oganov A.R. (2012). Systematic search for low-enthalpy sp<sup>3</sup> carbon allotropes using evolutionary metadynamics. *Phys. Rev.* **B85**, 201407.
90. Zhu Q., Oganov A.R., Glass C.W., Stokes H.T. (2012). Structure prediction for molecular crystals using evolutionary algorithms: methodology and applications. *Acta Cryst.* **B68**, 215-226 (Feature Article).
89. Boulfelfel S.E., Oganov A.R., Leoni S. (2012). Understanding the nature of “superhard graphite”. *Sci. Rep.* **2**, art. 471.
88. Zhong Y., Zhou H.Y., Hu C.-H., Wang D.-H., Oganov A.R. (2012). Theoretical study on high-pressure phases, electronic structure, and vibrational properties of NaNH<sub>2</sub>. *J. Phys. Chem.* **C116**, 8387-8393.
87. Zhu Q., Oganov A.R., Lyakhov A.O. (2012). Evolutionary metadynamics: a novel method to predict crystal structures. *Cryst. Eng. Comm.* **14**, 3596-3601.
86. Bazhanova Z.G., Oganov A.R., Gianola O. (2012). Fe-C-H system at pressures of the Earth’s inner core. *Physics-USpekhi* **55**, 489-497.

85. Shirako Y., Kojitani H., Oganov A.R., Fujino K., Miura H., Mori D., Inaguma Y., Yamaura K., Akaogi M. (2012). Crystal structure of CaRhO<sub>3</sub> polymorph: High-pressure intermediate phase between perovskite and post-perovskite. *Am. Mineral.* **97**, 159–163.
84. Zhou X.-F., Dong X., Zhao Z., Oganov A.R., Tian Y., Wang H.-T. (2012). High-pressure phases of NaAlH<sub>4</sub> from first principles. *Appl. Phys. Lett.* **100**, 061905.
83. Oganov A.R., Solozhenko V.L., Gatti C., Kurakevych O.O., Le Godec Y. (2011). The high-pressure phase of boron,  $\gamma$ -B<sub>28</sub>: disputes and conclusions of 5 years after discovery. *J. Superhard Materials* **33**, 363-379.
82. Lyakhov A.O., Oganov A.R. (2011). Evolutionary search for superhard materials applied to forms of carbon and TiO<sub>2</sub>. *Phys. Rev.* **B84**, 092103.
81. Zhou X.-F., Oganov A.R., Dong X., Zhang L., Tian Y., Wang H.-T. (2011). Superconducting high pressure phase of platinum hydride. *Phys. Rev.* **B84**, 054543.
80. Zhu Q., Oganov A.R., Salvado M., Perterra P., Lyakhov A.O. (2011). Denser than diamond: ab initio search for superdense carbon allotropes. *Phys. Rev.* **B83**, 193410.
79. Wen X.D., Hand L., Labet V., Yang T., Hoffmann R., Ashcroft N.W., Oganov A.R., Lyakhov A.O. (2011). Graphane sheets and crystals under pressure. *Proc. Natl. Acad. Sci.* **108**, 6833-6837.
78. Oganov A.R., Lyakhov A.O., Valle M. (2011). How evolutionary crystal structure prediction works - and why. *Acc. Chem. Res.* **44**, 227-237.
77. 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.
76. Gao G., Oganov A.R., Wang H., Li P., Ma Y., Cui T., Zou G. (2010). Dissociation of methane under high pressure. *J. Chem. Phys.* **133**, 144508.
75. Valle M., Oganov A.R. (2010). Crystal fingerprints space. A novel paradigm to study crystal structures sets. *Acta Cryst.* **A66**, 507-517.
74. Lyakhov A.O., Oganov A.R., Valle M. (2010). How to predict very large and complex crystal structures. *Comp. Phys. Comm.* **181**, 1623-1632.
73. Oganov A.R., Lyakhov A.O. (2010). Towards the theory of hardness of materials. *J. Superhard Mater.* **32**, 143-147.
72. Jung D.Y., Vinograd V.L., Fabrichnaya O.B., Oganov A.R., Schmidt M.W., Winkler B. (2010). Thermodynamics of mixing in MgSiO<sub>3</sub>-Al<sub>2</sub>O<sub>3</sub> perovskite and ilmenite from *ab initio* calculations. *Earth Planet. Sci. Lett.* **295**, 477-486.
71. Xie Y., Oganov A.R., Ma Y. (2010). Novel structures and high pressure superconductivity of CaLi<sub>2</sub>. *Phys. Rev. Lett.* **104**, 177005.
70. Oganov A.R., Ma Y.M., Xu Y., Errea I., Bergara A., Lyakhov A.O. (2010). Exotic behavior and crystal structures of calcium under pressure. *Proc. Natl. Acad. Sci.* **107**, 7646-7651.
69. Gao G., Oganov A.R., Li Z., Li P., Cui T., Bergara A., Lyakhov A.O., Ma Y., Iitaka T., Zou G. (2010). Crystal structures and superconductivity of stannane under high pressure. *Proc. Natl. Acad. Sci.* **107**, 1317-1320.
68. Zhang F., Oganov A.R. (2010). Iron silicides at pressures of the Earth's inner core. *Geophys. Res. Lett.* **37**, art. L02305.
67. Zurek E., Hoffmann R., Ashcroft N.W., Oganov A.R., Lyakhov A.O. (2009). A little bit of lithium does a lot for hydrogen. *Proc. Natl. Acad. Sci.* **106**, 17640-17643.
66. Oganov A.R., Solozhenko V.L. (2009). Boron: a hunt for superhard polymorphs. *J. Superhard Materials* **31**, 285-291.
65. Hu C.H., Oganov A.R., Lyakhov A.O., Zhou H.Y., Hafner J. (2009). Insulating states of LiBeH<sub>3</sub> under extreme compression. *Phys. Rev.* **B79**, 134116.
64. Li Q., Ma Y., Oganov A.R., Wang H.B., Wang H., Xu Y., Cui T., Mao H.-K., Zou G. (2009). Superhard monoclinic polymorph of carbon. *Phys. Rev. Lett.* **102**, 175506.
63. Wang H., Li Q., Li Y., Cui T., Oganov A.R., Ma Y. (2009). Ultra-incompressible phases of tungsten dinitride predicted from first principles. *Phys. Rev.* **B79**, 132109.
62. Schönborn S., Goedecker S., Roy S., Oganov A.R. (2009). The performance of minima hopping and evolutionary algorithms for cluster structure prediction. *J. Chem. Phys.* **130**, 144108.
61. Xu Y., Tse J.S., Oganov A.R., Cui T., Wang H., Ma Y., Zou G. (2009). Superconducting high-pressure phase of cesium iodide. *Phys. Rev.* **B79**, 144110.
60. Li Q., Wang M., Oganov A.R., Cui T., Ma Y., Zou G. (2009). Rhombohedral superhard structure of BC<sub>2</sub>N. *J. Appl. Phys.* **105**, 053514.
59. Oganov A.R., Valle M. (2009). How to quantify energy landscapes of solids. *J. Chem. Phys.* **130**, 104504.
58. Ma Y., Eremets M.I., Oganov A.R., Xie Y., Trojan I., Medvedev S., Lyakhov A.O., Valle M., Prakapenka V. (2009). Transparent dense sodium. *Nature* **458**, 182-185.

57. Martinez-Canales M., Oganov A.R., Lyakhov A., Ma Y., Bergara A. (2009). Novel structures of silane under pressure. *Phys. Rev. Lett.* **102**, 087005.
56. Ma Y., Oganov A.R., Xie Y., Li Z., Kotakoski J. (2009). Novel high pressure structures of polymeric nitrogen. *Phys. Rev. Lett.* **102**, 065501.
55. Ma Y., Wang Y., Oganov A.R. (2009). Absence of superconductivity in the novel high-pressure polymorph of MgB<sub>2</sub>. *Phys. Rev.* **B79**, 054101.
54. Oganov A.R., Chen J., Gatti C., Ma Y.-Z., Ma Y.-M., Glass C.W., Liu Z., Yu T., Kurakevych O.O., Solozhenko V.L. (2009). Ionic high-pressure form of elemental boron. *Nature* **457**, 863-867.
53. Solozhenko V.L., Kurakevych O.O., Oganov A.R. (2008). On the hardness of a new boron phase, orthorhombic  $\gamma$ -B<sub>28</sub>. *J. Superhard Mater.* **30**, 428-429.
52. Errea I., Martinez-Canales M., Oganov A.R., Bergara A. (2008). Fermi surface nesting and phonon instabilities in simple cubic calcium. *High Press. Res.* **28**, 443-448.
51. Hu C.H., Oganov A.R., Wang Y.M., Zhou H.Y., Lyakhov A., Hafner J. (2008). Crystal structure prediction of LiBeH<sub>3</sub> using ab initio total-energy calculations and evolutionary simulations. *J. Chem. Phys.* **129**, art. 234105.
50. Valle M., Oganov A.R. (2008). Crystal structure classifier for an evolutionary algorithm structure predictor. IEEE Symposium on Visual Analytics Science and Technology (October 21 - 23, Columbus, Ohio, USA), pp. 11- 18.
49. Gao G., Oganov A.R., Bergara A., Martinez-Canalez M., Cui T., Iitaka T., Ma Y., Zou G. (2008). Superconducting high pressure phase of germane. *Phys. Rev. Lett.* **101**, 107002.
48. Oganov A.R., Ono S., Ma Y., Glass C.W., Garcia A. (2008). Novel high-pressure structures of MgCO<sub>3</sub>, CaCO<sub>3</sub> and CO<sub>2</sub> and their role in the Earth's lower mantle. *Earth Planet. Sci. Lett.* **273**, 38-47.
47. Ma Y., Oganov A.R., Xie Y. (2008). High pressure structures of lithium, potassium, and rubidium predicted by ab initio evolutionary algorithm. *Phys. Rev.* **B78**, 014102.
46. Ono S., Oganov A.R., Brodholt J.P., Vocadlo L., Wood I.G., Lyakhov A., Glass C.W., Côté A.S., Price G.D. (2008). High-pressure phase transformations of FeS: novel phases at conditions of planetary cores. *Earth Planet. Sci. Lett.* **272**, 481-487.
45. Koci L., Ma Y., Oganov A.R., Souvatzis P., Ahuja R. (2008). Anomalous elastic behavior of superconducting metals V, Nb, Ta, Mo, and W at high pressure. *Phys. Rev.* **B77**, 214101.
44. Oganov A.R., Glass C.W. (2008). Evolutionary crystal structure prediction as a tool in materials design. *J. Phys.: Cond. Matter* **20**, art. 064210 (invited paper).
43. Martoňák R., Donadio D., Oganov A.R., Parrinello M. (2007). 4- to 6- coordinated silica: transformation pathways from metadynamics. *Phys. Rev.* **B76**, art. 014120.
42. Ma Y.-M., Oganov A.R., Glass C.W. (2007). Structure of the metallic  $\zeta$ -phase of oxygen and isosymmetric nature of the  $\varepsilon$ - $\zeta$  phase transition: Ab initio simulations. *Phys. Rev.* **B76**, art. 064101.
41. Martoňák R., Oganov A.R., Glass C.W. (2007). Crystal structure prediction and simulations of structural transformations: metadynamics and evolutionary algorithms. *Phase Transitions* **80**, 277-298.
40. Hassdenteufel K.H., Oganov A.R., Steurer W., Katrich S. (2007). Ab initio study of the W-phase of Al-Co-Ni, an approximant of the decagonal Al-Co-Ni quasicrystal. *Phys. Rev.* **B75**, art. 144115.
39. Xie Y., Tse J.S., Cui T., Oganov A.R., He Z., Ma Y., Zou G. (2007). Electronic and phonon instabilities in face-centered cubic alkali metals under pressure. *Phys. Rev.* **B75**, art. 064102.
38. Dorogokupets P.I., Oganov A.R. (2007). Ruby, metals, and MgO as alternative pressure scales: A semiempirical description of shock-wave, ultrasonic, x-ray, and thermochemical data at high temperatures and pressures. *Phys. Rev.* **B75**, art. 024115.
37. Glass C.W., Oganov A.R., Hansen N. (2006). USPEX – evolutionary crystal structure prediction. *Comp. Phys. Comm.* **175**, 713-720.
36. Zhang F., Oganov A.R. (2006). Valence and spin states of iron impurities in mantle-forming silicates. *Earth Planet. Sci. Lett.* **249**, 436-443.
35. Pushcharovsky D.Yu., Oganov A.R. (2006). Structural transformations of minerals in deep geospheres: a review. *Crystallography Rep.* **51**, 767-777.
34. Dorogokupets P.I., Oganov A.R. (2006). Equations of state of Al, Au, Cu, Pt, Ta and W and the revised ruby pressure scale. *Doklady Earth Sciences* **410**, 1091-1095.
33. Martoňák R., Donadio D., Oganov A.R., Parrinello M. (2006). Crystal structure transformations in SiO<sub>2</sub> from classical and ab initio metadynamics. *Nature Mater.* **5**, 623-626.
32. Oganov A.R., Glass C.W. (2006). Crystal structure prediction using ab initio evolutionary techniques: principles and applications. *J. Chem. Phys.* **124**, art. 244704.
31. Zhang F., Oganov A.R. (2006). Mechanisms of Al<sup>3+</sup> incorporation in MgSiO<sub>3</sub> post-perovskite at high pressures. *Earth Planet. Sci. Lett.* **248**, 54-61.

30. Ono S., Oganov A.R., Koyama T., Shimizu H. (2006). Stability and compressibility of high-pressure phase of Al<sub>2</sub>O<sub>3</sub> up to 200 GPa: implications for electrical conductivity at the base of the lower mantle. *Earth Planet. Sci. Lett.* **246**, 326-335.
29. Adams D.J., Oganov A.R. (2006). Ab initio molecular dynamics study of CaSiO<sub>3</sub> perovskite at P-T conditions of Earth's lower mantle. *Phys. Rev.* **B73**, 184106.
28. Boldyreva E.V., Ahsbahs H., Chernyshev V.V., Ivashevskaya S.N., Oganov A.R. (2006). Effect of hydrostatic pressure on the crystal structure of sodium oxalate: X-ray diffraction study and ab initio simulations. *Z. Krist.* **221**, 186-197.
27. Ghose S., Krisch M., Oganov A.R., Beraud A., Bossak A., Gulve R., Seelaboyina R., Yang H., Saxena S.K. (2006). Lattice dynamics of MgO at high pressure: theory and experiment. *Phys. Rev. Lett.* **96**, art. 035507.
26. Oganov A.R., Glass C.W., Ono S. (2006). High-pressure phases of CaCO<sub>3</sub>: crystal structure prediction and experiment. *Earth Planet. Sci. Lett.* **241**, 95-103.
25. Oganov A.R., Martoňák R., Laio A., Raiteri P., Parrinello M. (2005). Anisotropy of Earth's D'' layer and stacking faults in the MgSiO<sub>3</sub> post-perovskite phase. *Nature* **438**, 1142-1144.
24. Oganov A.R., S. Ono (2005). The high-pressure phase of alumina and implications for Earth's D'' layer. *Proc. Natl. Acad. Sci.* **102**, 10828-10831.
23. Ono S., Oganov A.R. (2005). In situ observations of phase transition between perovskite and CaIrO<sub>3</sub>-type phase in MgSiO<sub>3</sub> and pyrolitic mantle composition. *Earth Planet. Sci. Lett.* **236**, 914-932.
22. Jung D.Y., Oganov A.R. (2005). Ab initio study of the high-pressure behaviour of CaSiO<sub>3</sub> perovskite. *Phys. Chem. Minerals* **32**, 146-153.
21. Oganov A.R., Price G.D., Scandolo S. (2005). Ab initio theory of planetary materials. *Z. Krist.* **220**, 531-548.
20. Oganov A.R., Price G.D. (2005). Ab initio thermodynamics of MgSiO<sub>3</sub> perovskite at high pressures and temperatures. *J. Chem. Phys.* **122**, art. 124501.
19. Alfredsson M., Dobson D.P., Oganov A.R., Catlow C.R.A., Brodholt J.P., Parker S.C., Price G.D. (2005). Crystal morphology and surface structures of the orthorhombic MgSiO<sub>3</sub> perovskite. *Phys. Chem. Minerals* **31**, 671-682.
18. Oganov A.R., Gillan M.J., Price G.D. (2005). Structural stability of silica at high pressures and temperatures. *Phys. Rev.* **B71**, art. 064104.
17. Oganov A.R., Ono S. (2004). Theoretical and experimental evidence for a post-perovskite phase of MgSiO<sub>3</sub> in Earth's D'' layer. *Nature* **430**, 445-448.
16. Oganov A.R. & Dorogokupets P.I. (2004). Intrinsic anharmonicity in thermodynamics and equations of state of solids. *J. Phys.: Cond. Matter.* **16**, 1351-1360.
15. Dorogokupets P.I. & Oganov A.R. (2004). Intrinsic anharmonicity in equations of state of solids and minerals. *Doklady Earth Sciences* **395**, 238-241.
14. Senyshyn A., Oganov A.R., Vasylechko L., Ehrenberg H., Bismayer U., Berkowski M., Matkovskii A. (2004). Crystal structure and thermal expansion of the perovskite – type Nd<sub>0.75</sub>Sm<sub>0.25</sub>GaO<sub>3</sub> – powder diffraction and lattice dynamical studies. *J. Phys.: Cond. Matter.* **16**, 253-265.
13. Dorogokupets P.I. & Oganov A.R. (2003). Equations of state of Cu and Ag and the revised ruby pressure scale. *Doklady Earth Sciences* **391A**, 854-857.
12. Oganov A.R. & Dorogokupets P.I. (2003). All-electron and pseudopotential study of MgO: Equation of state, anharmonicity, and stability. *Phys. Rev.* **B67**, art. 224110.
11. Oganov A.R., Gillan M.J., Price G.D. (2003). Ab initio lattice dynamics and structural stability of MgO. *J. Chem. Phys.* **118**, 10174-10182.
10. Brodholt J.P., Oganov A.R., Price G.D. (2002). Computational mineral physics and physical properties of perovskite. *Phil. Trans. Royal Soc. London* **A360**, 2507-2520.
9. Oganov A.R., Price G.D., Brodholt J.P. (2001). Theoretical investigation of metastable Al<sub>2</sub>SiO<sub>5</sub> polymorphs. *Acta Crystallogr.* **A57**, 548-557.
8. Oganov A.R., Brodholt J.P., Price G.D. (2001). The elastic constants of MgSiO<sub>3</sub> perovskite at pressures and temperatures of the Earth's mantle. *Nature* **411**, 934-937.
7. Oganov A.R., Brodholt J.P., Price G.D. (2001). Ab initio elasticity and thermal equation of state of MgSiO<sub>3</sub> perovskite. *Earth and Planetary Science Letters* **184**, 555-560.
6. Oganov A.R., Organova N.I., Urusov V.S. (2001). Nature of Al-Si anti-ordering in a two-phase feldspar from the Pektusan volcano. *Geochem. Int.* **39**, 1160-1171.
5. Oganov A.R., Brodholt J.P., Price G.D. (2000). Comparative study of quasiharmonic lattice dynamics, molecular dynamics and Debye model in application to MgSiO<sub>3</sub> perovskite. *Phys. Earth Planet. Int.* **122**, 277-288.
4. Oganov A.R., and Brodholt J.P. (2000). High-pressure phases in the Al<sub>2</sub>SiO<sub>5</sub> system and the problem of Al-phase in Earth's lower mantle: ab initio calculations. *Phys. Chem. Minerals* **27**, 430-439.

3. Urusov V.S., Eremin N.N., Oganov A.R. (1999). Modeling of structures and properties of oxide crystals by minimization of the atomization energy. *Crystallography. Rep.* **44**, 356-365.
2. Urusov V.S., Oganov A.R., Eremin N.N. (1998). Computer simulation of structure, properties and stability of Al<sub>2</sub>SiO<sub>5</sub> polymorphs. I. Ionic approximation. *Geochem. Int.* **36**, 397-414.
1. Oganov A.R. (1996). A finding of rhombohedral pyrite crystals. *Proc. Russ. Min. Soc.*, No.1, 65-69.