CURRICULUM VITAE (April 23, 2017)

Artem R. Oganov

Professor, Department of Geosciences & Department of Physics and Astronomy
Director, Center for Materials by Design,
State University of New York at Stony Brook
Stony Brook 11794-2100, U.S.A.

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

ORCID: http://orcid.org/0000-0001-7082-9728
Scopus Author ID: 6701334785

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-now	Director, Center for Materials by Design, Stony Brook University
2010-now	Professor, Stony Brook University
2008-2010	Associate Professor, Stony Brook University
2003-2008	Group Leader and Privatdozent, ETH Zurich
2002-2003	Postdoc, 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, Urumqi).

Career Summary:

Publications, patents, citation:	199 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 = 7928 (Web of Science) and 10921 (Google Scholar). Hirsch's h-index = 46 (Web of Science) and 54 (Google Scholar).
Grants:	Over $15 million in federal and private grants in 2004-2016.
Talks:	313 in total, including 37 plenary/keynote, 264 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:

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	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:

2014	International Program Committee of the 2014 International Union of Crystallography meeting (Montreal, Canada, 5-12 August 2014)
2012-2017	Chairman, *ad interim* 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 13 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-	Graduate course "Crystal Chemistry", SBU
2010-	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-), Jin Zhang (2014-), Ivan Kruglov (2014-), Congwei Xie (2014-), Oleg Feya (2013-), Mahdi Davari (2013-), Shengnan Wang (2013-2016, now at UC Irvine), 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-), Elizaveta Pavlova (2015-), Julia Fomicheva (2015-, now at Ecole Polytech., Paris), Saeed Rakhmanian Koshkaki (2015-), 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.6., eds. R. Dronskowski, S. Kikkawa, A. Stein. In press.
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:

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. *Uspekhi Physics*, in press. https://doi.org/10.3367/UFNr.2017.03.038079 (Russian version) https://doi.org/10.3367/UFNe.2017.03.038079 (English version).
181. Esfahani Davari M.M., Zhu Q., Dong H.F., Oganov A.R., Wang S.N., Rakitin M.S., Zhou (2016). Novel magnesium borides and their superconductivity. In press.
180. Zeng Q.F., Yu S.Y., Frapper G., Oganov A.R., Li D. (2017). Evolution of chemical

bonding in hydrogen chlorides under 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.

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_6O_8. *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 $BaTiO_3$(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 $NaFe_2As_2$ 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 $Li_{15}Si_4$ synthesized under pressure. *Adv. Energy Mat.*, 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 CsFn 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_2 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 α-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 $Zr_xSi_{1-x}SiO_4$ dielectrics by evolutionary first-principles approaches. *Phys. Lett.* ***A*****378**, 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., Pilania 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 $MgAl_2O_4$ 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 β-Mg_2C_3: 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_3 and MnB_4. *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 $BaAl_2O_4$. *Physics Letters* ***A*****378**, 1867-1870.
109. Zhao Z., Wang S., Oganov A.R., Chen P.C., Liu Z., Mao W.L. (2014). High pressure behavior of Ag_2Se: structural transitions and metallization. *Phys. Rev.* ***B*****89**, 180102(R) (Rapid Communications).
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 Crystallographica* **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 Crystallographica* **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. B*88, 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. *Scientific Reports* **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. *Reviews in Mineralogy and Geochemistry* **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 Chemistry* **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 sp3-forms of carbon predicted by evolutionary metadynamics and analysis of their synthesizability using transition path sampling. *J. Superhard Materials* **34**, 350-359.
91. Zhu Q., Zeng Q., Oganov A.R. (2012). Systematic search for low-enthalpy sp^3 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". *Scientific Reports* **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 $NaNH_2$. *J. Phys. Chem. C*, **116**, 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 $CaRhO_3$ 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 $NaAlH_4$ 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, γ-B_{28}: 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_2. *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., Pertierra 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 $MgSiO_3$-Al_2O_3 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 $CaLi_2$. *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

$LiBeH_3$ 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_2N. *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. P*hys. 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_2. *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 γ-B_{28}. *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 Pressure Research* **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 $LiBeH_3$ 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 $MgCO_3$, $CaCO_3$ and CO_2 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. Mattter* **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 ζ-phase of oxygen and isosymmetric nature of the ε-ζ 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 Reports* **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_2 from classical and *ab initio* metadynamics. *Nature Materials* **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^{3+} incorporation in $MgSiO_3$ 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_2O_3 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 $CaSiO_3$ 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 $CaCO_3$: 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 $MgSiO_3$ 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 $CaIrO_3$-type phase in $MgSiO_3$ 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 $CaSiO_3$ 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 $MgSiO_3$ 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 $MgSiO_3$ 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 $MgSiO_3$ 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 $Nd_{0.75}Sm_{0.25}GaO_3$ – 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_2SiO_5 polymorphs. *Acta Crystallogr.* **A57**, 548-557.
8. Oganov A.R., Brodholt J.P., Price G.D. (2001). The elastic constants of $MgSiO_3$ 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 $MgSiO_3$ 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 $MgSiO_3$ perovskite. *Phys. Earth Planet. Int.* **122**, 277-288.
4. Oganov A.R., and Brodholt J.P. (2000). High-pressure phases in the Al_2SiO_5 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_2SiO_5 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.