CURRICULUM VITAE (May 2, 2016)

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

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:

2013	Doctor of Technical Sciences (Russian highest degree, by equivalence to Habilitation)
2007	Habilitation (Venia Legendi), 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, Moscow Institute of Physics and Technology
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).

Career Summary:

Publications, patents, citation:	178 papers and book chapters, including 5 in *Nature*, 2 in *Science*, 1 in *Nature Materials*, 1 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 = 6563 (Web of Science) and 8916 (Google Scholar). Hirsch's h-index = 41 (Web of Science) and 48 (Google Scholar).
Grants:	Over $15 million in federal and private grants in 2004-2016.
Talks:	280 in total, including 34 plenary/keynote, 234 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:

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
2004-2012	Organized 10 workshops (2004 – Lyon; 2011 – Poitiers; 2011 – Xi'an; 2012 – Lausanne; 2012 – Stony Brook; 2013 – Guilin; 2014 – Xi'an; 2015 – Shiv Nadar University; 2015 – Poitiers; 2015 – Beijing)

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:

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), Europe (ERC, Germany's DFG, France's ANR, Switzerland's SNF, Russia's RSF).

Faculty mentored: Prof. Qiang Zhu (2013-), 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-), Gabriele Saleh (2013-), Fei Qi (2013-2015), Maksim Rakitin (2013-2015), Qinggao Wang (2013-2016), Xiaohu Yu (2013-2015), Huafeng Dong (2013-2015), Xiang-Feng Zhou (2012-2015), Salah E. Boulfelfel (2010-2012), Andriy O. Lyakhov (2007-2011), Yanming Ma (2006-2008).

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), Guangrui Qian (2011-2015), Qiang Zhu (2009-2014), Yu Xie (2007-2010), Feiwu Zhang (2005-2008), Colin W. Glass (2006-2009), Donat Adams (2004-2007), Kai H. Hassdenteufel (2003-2006), Daniel Y. Jung (2004-2008).

MSc/BSc students supervised: Julia Sklyueva (2015-), Arslan Mazitov (2015-), Elizaveta Pavlova (2015-), Julia Fomicheva (2015-), Qing-Long Liu (2015-), Saeed Rakhmanian Koshkaki (2015-), Pavel Dolgirev (2014-), 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), Daniel Y. Jung (2003-2004), Alina V. Gutina (1997-1998).

Visiting scientists: Ali Berberov (Moscow University of Oil and Gas, Russia, 2014), Dongxu Li (Huaqiao University, China, 2013-2014), Yanqing Shen (Harbin Institute of Technology, China, 2013-2014), Pengcheng Chen (Tsinghua University, China, 2013-2014), Qianku Hu (Henan Polytechnic University, China, 2013-2014), Xiao Dong (Nankai University, China, 2012-2014), Qingfeng Zeng (Northwestern Polytechnical University, Xi'an, China, 2011-2012), Chaohao Hu (Guilin University of Electronic Technology, China, 2011-2012), Jose Perez (University of Cartagena, Spain, 2011), Weiwei Zhang (China Agricultural University, Beijing, 2011-2013), Yanchao Wang (Jilin University, China, 2009-2010), Miguel Martinez Canales (University of Bilbao, Spain, 2009), Love Koci (University of Uppsala, Sweden, 2007), Steeve Greaux (University of Paris Est, France, 2005).

Sabbatical visitors: Prof. Artem Masunov (University of Central Florida, USA, 2013-2014), Prof. Alberto Garcia (University of Basque Country, Spain, 2006)

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:

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. (2016). 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:

162. 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*, in press.
161. 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.*, in press.
160. Wang Q.G., Oganov A.R., Zhu Q., Feya O.D., Ma D.W. (2016). Unexpectedly rich structures of rutile TiO2(011)-(2×1) and driving forces behind their formations: an *ab initio* evolutionary study. *Phys. Chem. Chem. Phys.*, in press.
159. 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.*, in press.
158. 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.*, in press.
157. 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.*, in press.
156. 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.
155. 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.
154. 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.
153. 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.

152. 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.

151. 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.

150. 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.

149. 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.

148. 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.

147. 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.

146. 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.

145. 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.

144. 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.

143. 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.

142. 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.

141. 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.

140. 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**.**

139. 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.

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.

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