

September 2, 2010

CURRICULUM VITAE**Prof. Artem R. Oganov**

Department of Geosciences, Department of Physics and Astronomy, and New York Center for Computational Science, State University of New York at Stony Brook, Stony Brook 11794-2100, U.S.A.

Education and Degrees:

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), with top honours

Career History:

1/2010-now Professor and Head of Laboratory, Stony Brook University
 11/2008-1/2010 Associate Professor and Head of Laboratory, Stony Brook University
 8/2007-11/2008 Privatdozent and Group Leader, ETH Zurich
 2003-2007 Senior Researcher, Lecturer and Group Leader, ETH Zurich
 2002-2003 Research Fellow, University College London
 1993-1995 External scientific collaborator, Russian Chemical Abstracts (VINITI)

Invited Professorships: University of Milan (2005), Universite de Paris Est (2006-2007), Chinese University of Hong Kong (2008), Polytech’Lille (2009), Guilin University of Electronic Technology (2009). Adjunct Professor of Moscow State University (2006-present).

Research Output:

Publications, 89 papers, reviews and book chapters, including 5 in *Nature*, 4 in *PNAS*, 6 in *PRL*, 1 patents, citation: in *Nature Materials*. 1 international patent. **Total citation = 1779**. Hirsch’s h-index = 23.

Talks: 131 in total, including 15 plenary/keynote, 104 invited, 12 contributed

Coverage of research in popular media: Numerous press items in many languages, including:
In English: *Physics Today* (09/2006), *Nature* (06/07), *Chemistry World* (02/2009), *Science* (02/2009), *New York Times* (02/2009), *Nature Chemistry* (04/2009), *Nature* (05/2009), *New Scientist* (09/2009), *Nature Materials* (01/2010).
In French: *La Recherche* (01/2005, 01/2010).
In German: *Neue Zürcher Zeitung* (07/2006, 02/2009), *Tages Anzeiger* (07/2004), *Spektrum der Wissenschaft* (01/2007), *Spiegel* (02/2009).
In Russian: *Kommersant* (02/2007), *Troitsky Variant* (05/2008), *Voice of America* (02/2009), *Izvestia* (02/2009), *Chemistry and Life* (04/2009).
Radio Interviews: *SWR Radio* (07/2004, 01/2006, in German), *Nature Chemistry Podcast* (02/2009).

Research Interests:

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

Computational methodology: Development of simulation methods for crystal structure prediction, thermodynamic and transport properties, phase transformations

Materials Science: Computational materials design for environmental and industrial applications

Earth and Planetary Sciences: Prediction of structures, phase diagrams and properties of planet-forming materials, geochemistry at extreme conditions

Physics and Chemistry: Structure (atomic, electronic) and dynamics of condensed matter, theory of chemical bonding, rules determining stability of materials

Honors and Awards:

2008	Rated 12 th among all Russian scientists living abroad (Russian Newsweek)
2007	Most cited paper award, <i>Earth and Planetary Science Letters</i> (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
1993-1999	5 consecutive Soros Foundation scholarships. Also Lomonosov, Vinogradov and twice Shubnikov scholar

Selected Services:

2009-	Member of the University Senate, Stony Brook University
2010	Member of the Scientific Advisory Committee, EHPRG-48 conference, Uppsala, Sweden, September 2010.
2006-2008	Executive Committee member, User Group of Swiss National Supercomputing Centre
2005-2008	Elected vice-chairman of the Special Interest Group "Mineralogical Crystallography" of the European Crystallographic Association
9/2004	Organizer of the CECAM/Psi-k workshop "First-Principles Simulations: Perspectives and Challenges in Mineral Sciences" (Lyon, France)

Selected Editorial and Refereeing Activities:

2009-present	Member of the Editorial Board: <i>Journal of Superhard Materials</i>
2006-2010	Associate Editor: <i>American Mineralogist</i>
3/2010	Editor: <i>Journal of Superhard Materials</i> , Special Issue "Theory of Superhard Materials"
5-6/2005	Editor: <i>Zeitschrift für Kristallographie</i> , Special Issue "Computational Crystallography"
2010	Book Editor: „Modern methods of crystal structure prediction“, Wiley-VCH.
2004	Book Editor: "First-principles simulations: perspectives and challenges in mineral [German Crystallographic Society, 2004]
2002	Book referee for Oxford University Press (M.T. Dove "Structure and Dynamics")
2009	Scientific reviewer, Swiss National Supercomputing Centre
Peer reviews	Over 30 journals, including <i>Nature</i> , <i>Science</i> ; <i>Nature Chemistry</i> , <i>Nature Materials</i> ;
(papers):	<i>Physical Review Letters</i> ; <i>Reports on Progress in Physics</i> ; <i>Journal of Chemical Physics</i> ; <i>Physical Review B</i> ; <i>Applied Physics Letters</i> ; <i>Journal of Computational Physics</i> ; <i>Geophysical Research Letters</i> ; <i>Earth and Planetary Science Letters</i> ; <i>Inorganic Chemistry</i> .
(grants):	US National Science Foundation, US Department of Energy (Basic Energy Sciences), American Chemical Society (Petroleum Research Fund), German Research Foundation (DFG), French National Research Agency (ANR), Swiss National Science Foundation

Pedagogical Activities:

2011-	"Crystal Chemistry" (3 hours/week) Graduate course GEO517, Stony Brook University
2010-	"Structure and properties of materials" (3 hours/week) Undergraduate/graduate course GEO312/512, Stony Brook University
2009	"Electronic Structure Calculations in Crystallography" (3 hours/week) Graduate seminar GEO618, Stony Brook University
2009	"Crystalline Solids" (4 hours/week lectures, 4 hours/week labs) Graduate course GEO531, Stony Brook University
2009	"Mineralogy" (4 hours/week lectures, 4 hours/week labs) Undergraduate/graduate course GEO306/546, Stony Brook University
2004-2007	"Mineralogical Crystallography" (2 hours/week lectures, 1 hour/week seminars)

2nd year undergraduate course, ETH Zurich
 2005-now Invited professor short courses at Moscow State University, University of Milano,
 University of Paris Est, Chinese University of Hong Kong
 Lecturer at Summer Schools:
 Budapest (2002), Gargnano (2003), Heidelberg (2005), Nancy (2005), Erice (2003, 2009)

Sabbatical guests:	Prof. Alberto Garcia (University of Bilbao, Spain)	2006
Visiting scientists:	Miguel Martinez Canales (University of Bilbao, Spain)	2009
	Love Koci (University of Uppsala, Sweden)	2007
	Steeve Greaux (University of Paris Est, France)	2005
	Yanchao Wang (Jilin University, China)	2009-2010
Postdoctoral fellows:	Dr. Yanming Ma	2006-2008
	Dr. Andriy Lyakhov	2007-now
	Dr. Salah Eddine Boulfefel	2010-now
PhD students:	Yu Xie (co-supervised with Y. Ma)	2007-now
	Qiang Zhu	2009-2014
	Heinrich Orsini-Rosenberg (co-supervised with W. Steurer)	2007-now
	Donat Adams	2004-2007
	Daniel Y. Jung	2004-2008
	Feiwu Zhang	2005-2008
	Colin W. Glass	2006-2009
	Kai H. Hassdenteufel (co-supervised with W. Steurer)	2003-2006
Diploma students:	Alina V. Gutina	1997-1998
	Daniel Y. Jung	2003-2004
	Colin W. Glass	2005-2006
	Sandro Schönborn (co-supervised with S. Goedecker)	2008
PhD examiner:	Davina Sihachakr (University of Paris XI, France, 2005), Steeve Greaux (University of Marne-la-Vallee, France, 2006), Benoit Dubacq (University of Grenoble, France, 2008), Yuanyuan Zheng (University Lille 1, France, 2009), Ibrahim Khalil Benazzouz (University Lille 1, France, 2010)	

Invited talks:

Invited seminars at universities (Oxford, London, Princeton, Zurich, Basel, Bayreuth, Heidelberg, Torino, Milano, Stony Brook, Vienna, Grenoble, Paris, Kiel, Copenhagen, Munich, Bayreuth, Ann Arbor, Las Vegas, Cornell, Yerevan, Hong Kong, Changchun, Lille, Moscow, Novosibirsk).

Invited lectures at companies and research institutions (Mitsubishi Corp., Yokohama, Japan; Swiss Supercomputer Centre; Carnegie Institution of Washington, USA; CEA at Bruyeres-le-Chatel, France; Italian Institute of Geophysics and Volcanology; Russian Academy of Sciences; Chinese Academy of Sciences; Austrian Society of Chemical Physics; Institute of the Physics of the Globe, Paris).

List of publications of Artem R. Oganov.

BOOKS:

1. Oganov A.R. (Editor). *Modern Methods of Crystal Structure Prediction*. Wiley-VCH, in press (2010).

REVIEWS AND CHAPTERS IN BOOKS:

13. 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), Wiley-VCH. *In press*.
12. Oganov A.R. (2010). Crystal structure prediction, a formidable problem. In *Modern Methods of Crystal Structure Prediction* (ed. A.R. Oganov), Wiley-VCH. *In press*.
11. Oganov A.R. (2010). Boron under pressure: phase diagram and novel high-pressure phase. In "Boron rich solids", eds. N. Orlovskaya and M. Lugovy. *In press*.
10. Lyakhov A.O., Oganov A.R., Valle M. (2010). Crystal structure prediction using evolutionary approach. In "Modern methods of crystal structure prediction", ed. A.R. Oganov. Wiley-VCH. *In press*.
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". Lecture Notes of the Erice school, *in press*.
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:

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 $\text{MgSiO}_3\text{-Al}_2\text{O}_3$ 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. *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_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 $\gamma\text{-B}_{28}$. *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. 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 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 SiO₂ 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 Al³⁺ incorporation in MgSiO₃ 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 Al₂O₃ 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 CaSiO₃ 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 CaCO₃: 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 MgSiO₃ 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 CaIrO₃-type phase in MgSiO₃ 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 CaSiO₃ 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 MgSiO₃ 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 MgSiO₃ 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 MgSiO₃ 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}GaO₃ – 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 Al₂SiO₅ polymorphs. *Acta Crystallogr.* **A57**, 548-557.
8. Oganov A.R., Brodholt J.P., Price G.D. (2001). The elastic constants of MgSiO₃ 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 MgSiO₃ 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 MgSiO₃ perovskite. *Phys. Earth Planet. Int.* **122**, 277-288.
4. Oganov A.R., and Brodholt J.P. (2000). High-pressure phases in the Al₂SiO₅ 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 Al₂SiO₅ 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.