

April 15, 2010

## CURRICULUM VITAE

Prof. Artem R. Oganov

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State University of New York at Stony Brook,  
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**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:**

11/2008-now Associate Professor and Head of Laboratory, Stony Brook University  
2007-2008 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)

**Visiting Appointments:**

3/2006-present Adjunct Professor, Moscow State University, Russia  
2009 Invited Professor, Guilin University of Electronic Technology, China  
2009 Invited Professor, Ecole Polytechnique de Lille, France  
2008 Invited Professor, Chinese University of Hong Kong  
2006-2007 Invited Professor, Universite de Paris Est (Marne-la-Vallée), France  
2005 Invited Professor, University of Milan (Italy)

**Research Output:**

Publications, 85 papers, reviews and book chapters, including 5 in *Nature*, 4 in *PNAS*, 1 in *Nature*  
patents, citation: *Materials*, 6 in *PRL*. 1 international patent. Hirsch’s h-index = 21.  
Talks: 124 in total, including 14 plenary/keynote, 93 invited, 12 contributed  
Coverage of Numerous press items in many languages, including:  
research in **In English:** *Physics Today* (09/2006), *Nature* (06/07), *Chemistry World* (02/2009),  
popular media: *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:**

Multidisciplinary 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,

**Honors and Awards:**

2008	Rated 12 <sup>th</sup> 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)
2005	Offered Assistant Professorship at Princeton University (USA), declined
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

**Professional 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
2003-2008	Representative of ETH Zurich in COMPRES (Consortium for Materials Properties Research in Earth Sciences)
9/2004	Organiser of the CECAM/Psi-k workshop "First-Principles Simulations: Perspectives and Challenges in Mineral Sciences" (Lyon, France)

**Editorial Activities and Refereeing:**

2009-present	Member of the Editorial Board: <i>Journal of Superhard Materials</i>
2006-2010	Associate Editor: <i>American Mineralogist</i>
5-6/2005	Guest Editor: <i>Zeitschrift für Kristallographie</i>
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	32 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):	German Research Foundation (DFG), French National Research Agency (ANR), Petroleum Research Fund (American Chemical Society), US National Science Foundation, Swiss National Science Foundation

**Pedagogical Activities:**

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 course GEO306/546, Stony Brook University
2004-2007	"Mineralogical Crystallography" (2 hours/week lectures, 1 hour/week seminars) 2 <sup>nd</sup> 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)

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

#### Grants:

2010	Prediction and synthesis of new polymorphs of molecular crystals	3'600'000 RUB
Russian Ministry of Science and Education		
2010	Crystal Structure Design of New Superhard Materials	200'000 RMB
National Science Foundation of China		
2009-2010	Towards development of the evolutionary methodology for structure prediction (and Prediction of the Atomic Structure of Interfaces)	192'000 USD
Intel Corporation		
2007-2009	Crystal Structure Prediction at the Quantum Monte Carlo Level	141'119 CHF
Swiss National Science Foundation		
2006-2011	Computing Facilities for Evolutionary Crystal Structure Prediction	200'000 CHF
ETH Zurich Research Commission		
2006-2009	Development and Application of Evolutionary Algorithms for Crystal Structure Prediction	309'355 CHF
Swiss National Science Foundation		
2006-2009	Design of Pentagonal and Heptagonal Boron-based Quasicrystals	153'000 CHF
ETH Zurich Research Commission		
2006-2009	The Role of Post-perovskite Phase Transition in the Mantle Dynamics	139'172 CHF
Swiss National Science Foundation		
2005-2008	Mineral Physics of Earth's D'' layer	146'000 CHF
ETH Zurich Research Commission		
2004-2007	High-Pressure Physics of Mantle-Forming Minerals	143'336 CHF
ETH Zurich Research Commission		
2004	Workshop "First-Principles Simulations: Perspectives and Challenges in Mineral Sciences"	31'000 CHF
Psi-k, CECAM, German Crystallographic Society (DGK)		
2004-2006	Computing facilities for mineral physics	200'000 CHF
Laboratory of Crystallography, ETH Zurich		
2008-present	Crystal structure prediction	2'000'000

Skif MSU supercomputer, Moscow State University, Russia		CPU hours/year
2007-present	Crystal structure prediction: development of the methodology, and applications	1'000'000 CPU hours/year
2003-2008	Computational mineral physics and crystallography	Total of ~4'000'000 CPU hours

## Selected invited talks of Artem R. Oganov

Invited seminars at universities (Oxford, London, Princeton, Zurich, Basel, Bayreuth, Heidelberg, Torino, Milano, Stony Brook, Vi Paris, Kiel, Copenhagen, Munich, Bayreuth, Ann Arbor, Cornell, Yerevan), companies and research institutions (CEA at Bruyeres-le Carnegie Institution of Washington, USA; Institute of Geophysics in Rome, Italy; Mitsubishi Corporation Research Department in Y Swiss Supercomputer Centre, Switzerland).

Crystal structure prediction from first principles	Advanced Crystallography at High Pressure, July 19-22, 2009, Harbin Institute of Technology, Harbin, China	19-22/07/2009
Theoretical prediction of high-pressure structures	"High-pressure crystallography", Erice Crystallographic School, Erice, Italy	4-14/06/2009
Evolutionary crystal structure prediction and its applications to materials at extreme conditions	IUCr Meeting, Osaka, Japan	23-31/08/2008
Computational mineral physics: Exploring matter inside planets (public lecture)	Chinese University of Hong Kong	15/05/2008
Discovering new minerals in the deep Earth (EMU medal lecture)	EMU Award Lecture, EGU Meeting, Vienna, Austria	17/04/2008
Evolutionary crystal structure prediction: Finding the global energy minima for periodic solids	Metastability and rare events, Erwin Schroedinger Institute Meeting, Vienna, Austria	18-22/02/2008
Evolutionary crystal structure prediction: methodology and its applications in materials design and study of matter at extreme conditions	Chemisch Physikalische Gesellschaft, Vienna, Austria	20/11/2007
Evolutionary crystal structure prediction: a novel approach to materials design	Workshop "Theory Meets Industry", Vienna, Austria	12/06/2007
Matter at Extreme Conditions: Exploring New Chemistry and Interiors of Planets	ETH Latsis Prize Lecture, Geneva, Switzerland	8/11/2006
USPEX – an Evolutionary Algorithm for Crystal Structure Prediction	HPC (High-Performance Computing) Europe Workshop, Oxford, U.K.	25/09/2006
Crystal Structure Prediction: New Methodology and Geologically Important Results	International Mineralogical Association Congress, Kobe, Japan	23-28/07/2006
Crystal Structure Prediction with <i>Ab Initio</i> Evolutionary Algorithms	Electronic Structure 2006 conference, Columbus, Ohio,	25/06/2006
USPEX – an Evolutionary Algorithm for Crystal Structure Prediction	IDC HPC (High-Performance Computing) Conference, Zurich	1-2/06/2006
Recent Developments in Computational Mineral Physics	Royal Society Meeting - The Deep Earth: The Structure and Evolution of the Interior of our Planet, London	23-24/11/2005
Post-perovskite Phase of MgSiO <sub>3</sub> : the Discovery, its Geophysical Implications and Current State of Knowledge	2005 Psi-k conference, Schwaebisch Gmuend, Germany	20/09/2005
Rediscovering Nature with Supercomputers: from Microscopic Scale to Planetary Structures	CRAY XT3 Inauguration Keynote Lecture, CSCS, Manno, Switzerland	15/09/2005
Theoretical and Experimental Evidence for a Post-perovskite Phase of MgSiO <sub>3</sub> in Earth's D" Layer	APS (American Physical Society) March meeting, Los Angeles, USA,	21/03/2005
<i>Ab Initio</i> Phase Diagrams of Minerals	CECAM/Psi-k workshop "First-Principles Simulations: Perspectives and Challenges in Mineral Sciences", Lyon	28/09/2004
Phase Diagrams of Minerals from Density-Functional Perturbation Theory	European Crystallographic Meeting, Budapest, Hungary	29/08/2004
New Phenomena and Ideas in Inorganic Structural Chemistry	XV International Conference on X-ray Diffraction and Crystal Chemistry of Minerals, St. Petersburg, Russia	15-19/09/2003

Theory of Minerals at High and Ultrahigh Pressures: Structure, Properties, Dynamics, and Phase Transitions	School 'High Pressure Crystallography', Erice, Italy	13/06/2003
Quantum Geophysics: What can Quantum Mechanics Tell us about the Deep Earth?	Award Lecture, European Union of Geosciences Meeting, Nice, France	9/04/2003
New Metastable $\text{Al}_2\text{SiO}_5$ Polymorphs: Unexpected Results of Theoretical Calculations	International Union of Crystallography congress, Geneva, Switzerland	13/08/2002
Molecular Dynamics: Basic Theory, Methodology, and Simulations of Elasticity of Crystals	Workshop 'Crystal Physics: measuring, calculating and predicting physical properties of crystals', Rigi, Switzerland	1-5/08/2002
Equations of State of Solids	Summer School 'Energy Modelling in Minerals', Budapest, Hungary	2/07/2002

## 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:

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., Ma Y., Wang Y., 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. *Reviews in Mineralogy and Geochemistry* **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:

74. Jung D.Y., Vinograd V.L., Fabrichnaya O.B., Oganov A.R., Schmidt M.W., Winkler B. (2010). Thermodynamics of mixing in MgSiO<sub>3</sub>-Al<sub>2</sub>O<sub>3</sub> perovskite and ilmenite from *ab initio* calculations. *Earth Planet. Sci. Lett.*, in press.
73. Xie Y., Oganov A.R., Ma Y. (2010). Novel structures and high pressure superconductivity of CaLi<sub>2</sub>. *Phys. Rev. Lett.*, in press.
72. Oganov A.R., Lyakhov A.O. (2010). Towards the theory of hardness of materials. *J. Superhard Mater.*, in press.
71. 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.*, doi:10.1073/pnas.0910335107.
70. Gao G., Oganov A.R., Li Z., Li P., Cui T., Bergara A., Ma Y., Iitaka T., Zou G. (2010).

- Crystal structures and superconductivity of stannane under high pressure. *Proc. Natl. Acad. Sci.* **107**, 1317-1320.
69. Zhang F., Oganov A.R. (2010). Iron silicides at pressures of the Earth's inner core. *Geophys. Res. Lett.* **37**, art. L02305.
  68. 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., Zhou H.Y., Hafner J. (2009). Insulating states of LiBeH<sub>3</sub> under extreme compression. *Phys. Rev.* **B79**, 134116.
  64. Li Q., Ma Y., Oganov A.R., Wang H.B., Wang H., Xu Y., Cui T., Mao H.-K., Zou G. (2009). Superhard monoclinic polymorph of carbon. *Phys. Rev. Lett.* **102**, 175506.
  63. Wang H., Li Q., Li Y., Cui T., Oganov A.R., Ma Y. (2009). Ultra-incompressible phases of tungsten dinitride predicted from first principles. *Phys. Rev.* **B79**, 132109.
  62. Schönborn S., Goedecker S., Roy S., Oganov A.R. (2009). The performance of minima hopping and evolutionary algorithms for cluster structure prediction. *J. Chem. Phys.* **130**, 144108.
  61. Xu Y., Tse J.S., Oganov A.R., Cui T., Wang H., Ma Y., Zou G. (2009). Superconducting high-pressure phase of cesium iodide. *Phys. Rev.* **B79**, 144110.
  60. Li Q., Wang M., Oganov A.R., Cui T., Ma Y., Zou G. (2009). Rhombohedral superhard structure of BC<sub>2</sub>N. *J. Appl. Phys.* **105**, 053514.
  59. Oganov A.R., Valle M. (2009). How to quantify energy landscapes of solids. *J. Chem. Phys.* **130**, 104504.
  58. Ma Y., Eremets M.I., Oganov A.R., Xie Y., Trojan I., Medvedev S., Lyakhov A.O., Valle M., Prakapenka V. (2009). Transparent dense sodium. *Nature* **458**, 182-185.
  57. Martinez-Canales M., Oganov A.R., Lyakhov A., Ma Y., Bergara A. (2009). Novel structures of silane under pressure. *Phys. Rev. Lett.* **102**, 087005.
  56. Ma Y., Oganov A.R., Xie Y., Li Z., Kotakoski J. (2009). Novel high pressure structures of polymeric nitrogen. *Phys. Rev. Lett.* **102**, 065501.
  55. Ma Y., Wang Y., Oganov A.R. (2009). Absence of superconductivity in the novel high-pressure polymorph of MgB<sub>2</sub>. *Phys. Rev.* **B79**, 054101.
  54. Oganov A.R., Chen J., Gatti C., Ma Y.-Z., Ma Y.-M., Glass C.W., Liu Z., Yu T., Kurakevych O.O., Solozhenko V.L. (2009). Ionic high-pressure form of elemental boron. *Nature* **457**, 863-867.
  53. Solozhenko V.L., Kurakevych O.O., Oganov A.R. (2008). On the hardness of a new boron phase, orthorhombic  $\gamma$ -B<sub>28</sub>. *J. Superhard Mater.* **30**, 428-429.
  52. Errea I., Martinez-Canales M., Oganov A.R., Bergara A. (2008). Fermi surface nesting and phonon instabilities in simple cubic calcium. *High 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<sub>3</sub> using *ab initio* total-energy calculations and evolutionary simulations. *J. Chem. Phys.* **129**, art. 234105.
  50. Valle M., Oganov A.R. (2008). Crystal structure classifier for an evolutionary algorithm structure predictor. *IEEE Symposium on Visual Analytics Science and Technology* (October 21 - 23, Columbus, Ohio, USA), pp. 11- 18.
  49. Gao G., Oganov A.R., Bergara A., Martinez-Canalez M., Cui T., Iitaka T., Ma Y., Zou G. (2008). Superconducting high pressure phase of germane. *Phys. Rev. Lett.* **101**, 107002.
  48. Oganov A.R., Ono S., Ma Y., Glass C.W., Garcia A. (2008). Novel high-pressure structures of MgCO<sub>3</sub>, CaCO<sub>3</sub> and CO<sub>2</sub> and their role in the Earth's lower mantle. *Earth Planet. Sci. Lett.* **273**, 38-47.
  47. Ma Y., Oganov A.R., Xie Y. (2008). High pressure structures of lithium, potassium, and rubidium predicted by *ab initio* evolutionary algorithm. *Phys. Rev.* **B78**, 014102.
  46. Ono S., Oganov A.R., Brodholt J.P., Vocablo L., Wood I.G., Lyakhov A., Glass C.W., Côté A.S., Price G.D. (2008). High-pressure phase transformations of FeS: novel phases at conditions of planetary cores. *Earth Planet. Sci. Lett.* **272**, 481-487.
  45. Koci L., Ma Y., Oganov A.R., Souvatzis P., Ahuja R. (2008). Anomalous elastic behavior of superconducting metals V, Nb, Ta, Mo, and W at high pressure. *Phys. Rev.* **B77**, 214101.
  44. Oganov A.R., Glass C.W. (2008). Evolutionary crystal structure prediction as a tool in materials design. *J. Phys.: Cond. Matter* **20**, art. 064210 (invited paper).

43. Martoňák R., Donadio D., Oganov A.R., Parrinello M. (2007). 4- to 6- coordinated silica: transformation pathways from metadynamics. *Phys. Rev.* **B76**, art. 014120.
42. Ma Y.-M., Oganov A.R., Glass C.W. (2007). Structure of the metallic  $\zeta$ -phase of oxygen and isosymmetric nature of the  $\varepsilon$ - $\zeta$  phase transition: *Ab initio* simulations. *Phys. Rev.* **B76**, art. 064101.
41. Martoňák R., Oganov A.R., Glass C.W. (2007). Crystal structure prediction and simulations of structural transformations: metadynamics and evolutionary algorithms. *Phase Transitions* **80**, 277-298.
40. Hassdenteufel K.H., Oganov A.R., Steurer W., Katrich S. (2007). *Ab initio* study of the W-phase of Al-Co-Ni, an approximant of the decagonal Al-Co-Ni quasicrystal. *Phys. Rev.* **B75**, art. 144115.
39. Xie Y., Tse J.S., Cui T., Oganov A.R., He Z., Ma Y., Zou G. (2007). Electronic and phonon instabilities in face-centered cubic alkali metals under pressure. *Phys. Rev.* **B75**, art. 064102.
38. Dorogokupets P.I., Oganov A.R. (2007). Ruby, metals, and MgO as alternative pressure scales: A semiempirical description of shock-wave, ultrasonic, x-ray, and thermochemical data at high temperatures and pressures. *Phys. Rev.* **B75**, art. 024115.
37. Glass C.W., Oganov A.R., Hansen N. (2006). USPEX – evolutionary crystal structure prediction. *Comp. Phys. Comm.* **175**, 713-720.
36. Zhang F., Oganov A.R. (2006). Valence and spin states of iron impurities in mantle-forming silicates. *Earth Planet. Sci. Lett.* **249**, 436-443.
35. Pushcharovsky D.Yu., Oganov A.R. (2006). Structural transformations of minerals in deep geospheres: a review. *Crystallography 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<sub>2</sub> 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<sup>3+</sup> incorporation in MgSiO<sub>3</sub> post-perovskite at high pressures. *Earth Planet. Sci. Lett.* **248**, 54-61.
30. Ono S., Oganov A.R., Koyama T., Shimizu H. (2006). Stability and compressibility of high-pressure phase of Al<sub>2</sub>O<sub>3</sub> up to 200 GPa: implications for electrical conductivity at the base of the lower mantle. *Earth Planet. Sci. Lett.* **246**, 326-335.
29. Adams D.J., Oganov A.R. (2006). *Ab initio* molecular dynamics study of CaSiO<sub>3</sub> perovskite at *P-T* conditions of Earth's lower mantle. *Phys. Rev.* **B73**, 184106.
28. Boldyreva E.V., Ahsbahs H., Chernyshev V.V., Ivashevskaya S.N., Oganov A.R. (2006). Effect of hydrostatic pressure on the crystal structure of sodium oxalate: X-ray diffraction study and *ab initio* simulations. *Z. Krist.* **221**, 186-197.
27. Ghose S., Krisch M., Oganov A.R., Beraud A., Bossak A., Gulve R., Seelaboyina R., Yang H., Saxena S.K. (2006). Lattice dynamics of MgO at high pressure: theory and experiment. *Phys. Rev. Lett.* **96**, art. 035507.
26. Oganov A.R., Glass C.W., Ono S. (2006). High-pressure phases of CaCO<sub>3</sub>: crystal structure prediction and experiment. *Earth Planet. Sci. Lett.* **241**, 95-103.
25. Oganov A.R., Martoňák R., Laio A., Raiteri P., Parrinello M. (2005). Anisotropy of Earth's D'' layer and stacking faults in the MgSiO<sub>3</sub> post-perovskite phase. *Nature* **438**, 1142-1144.
24. Oganov A.R., S. Ono (2005). The high-pressure phase of alumina and implications for Earth's D'' layer. *Proc. Natl. Acad. Sci.* **102**, 10828-10831.
23. Ono S., Oganov A.R. (2005). *In situ* observations of phase transition between perovskite and CaIrO<sub>3</sub>-type phase in MgSiO<sub>3</sub> and pyrolitic mantle composition. *Earth Planet. Sci. Lett.* **236**, 914-932.
22. Jung D.Y., Oganov A.R. (2005). *Ab initio* study of the high-pressure behaviour of CaSiO<sub>3</sub> perovskite. *Phys. Chem. Minerals* **32**, 146-153.
21. Oganov A.R., Price G.D., Scandolo S. (2005). *Ab initio* theory of planetary materials. *Z. Krist.* **220**, 531-548.
20. Oganov A.R., Price G.D. (2005). *Ab initio* thermodynamics of MgSiO<sub>3</sub> perovskite at high pressures and temperatures. *J. Chem. Phys.* **122**, art. 124501.
19. Alfreðsson 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  $\text{MgSiO}_3$  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  $\text{MgSiO}_3$  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  $\text{Nd}_{0.75}\text{Sm}_{0.25}\text{GaO}_3$  – 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  $\text{Al}_2\text{SiO}_5$  polymorphs. *Acta Crystallogr.* **A57**, 548-557.
  8. Oganov A.R., Brodholt J.P., Price G.D. (2001). The elastic constants of  $\text{MgSiO}_3$  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  $\text{MgSiO}_3$  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  $\text{MgSiO}_3$  perovskite. *Phys. Earth Planet. Int.* **122**, 277-288.
  4. Oganov A.R., and Brodholt J.P. (2000). High-pressure phases in the  $\text{Al}_2\text{SiO}_5$  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  $\text{Al}_2\text{SiO}_5$  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.