

February 15, 2012

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.

Personal data:

Born on 03.03.1975 in Moscow, Russia.

Languages: English (fluent), Russian (native), German, French, Italian.

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), *summa cum laude*

Career History:

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| 1/2010-now | Full 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) |

Visiting Appointments: Adjunct Professor of Moscow State University since 2006. Since 2005 was an invited professor in Milan (Italy), Paris, Lille and Poitiers (France), Guilin and Hong Kong (China).

Research Output:

Publications, 100 papers, reviews and book chapters, including 5 in *Nature*, 5 in *PNAS*, 6 in *PRL*, 1 patents, citation: in *Nature Materials*, 1 in *Accounts of Chemical Research*. 1 book, 1 patent. Total citation = 2759. Hirsch’s h-index = 28.

Talks: 159 in total, including 21 plenary/keynote, 126 invited, 12 contributed

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:

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| 2011 | Rated 6 th most successful Russian scientist (Forbes Russia) |
| 2010 | Most cited paper award, <i>Earth and Planetary Science Letters</i> (2005-2010) |
| 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) |
| 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:

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| 2011 | Co-organizer of Crystal Structure Prediction workshops in Poitiers, France (23-30 June 2011) and Xi'an, China (2-6 August 2011) |
| 2009- | Member of the University Senate, Stony Brook University |
| 2010- | Member of the Scientific Advisory Committees, EHPRG-48 (Uppsala, Sweden, 2010) and EHPRG-49 (Budapest, Hungary, 2011) conferences. |
| 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 | Organiser of the CECAM/Psi-k workshop "First-Principles Simulations: Perspectives and Challenges in Mineral Sciences" (Lyon, France) |
| Refereeing: | Referee for over 40 journals, including <i>Nature</i> , <i>Science</i> , etc. Referee for scientific projects in the US, Germany, France, Switzerland, Russia. |

Editorial Activities and Refereeing:

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| 2011-present | Member of the Editorial Board: <i>Scientific Reports (Nature Publishing Group)</i> |
| 2011-present | Member of the Editorial Board: <i>Central European Journal of Geosciences, Journal of Geology and Geosciences</i> |
| 2009-present | Member of the Editorial Board: <i>Journal of Superhard Materials</i> |
| 2006-2010 | Associate Editor: <i>American Mineralogist</i> |
| 6/2011 | Editor: <i>Journal of Superhard Materials</i> , Special Issue "Boron and boron-rich solids" |
| 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") |

Pedagogical Activities:

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| 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) 2 nd 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), Berkeley (2009) |

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| 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 |
| | Dr. Weiwei Zhang (China Agricultural University, Beijing) | 2010-2011 |
| | Dr. Jose Perez (Technical University of Cartagena, Spain) | 2011 |
| | Prof. Chaohao Hu (Guilin University of Electronic | 2011-2012 |

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| | Technology, China) | |
| | Prof. Qingfeng Zeng (Northwestern Polytechnical University, Xi'an, China) | 2011-2012 |
| Postdoctoral fellows: | Dr. Yanming Ma | 2006-2008 |
| | Dr. Andriy Lyakhov | 2007-now |
| | Dr. Salah E. Boulfelfel | 2010-now |
| PhD students: | Guangrui Qian | 2011-2016 |
| | Lonia Friedlander | 2010-2015 |
| | Qiang Zhu | 2009-2014 |
| | Yu Xie | 2007-2010 |
| | Heinrich Orsini-Rosenberg (co-supervised with W. Steurer) | 2007-2008 |
| | 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 |
| | Judith Gabel | 2010-2011 |
| 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 |
| | Petr Sokolov (University Paris XIII, France) | 2010 |

Invited talks:

- Numerous conferences in physics, chemistry, earth sciences and materials science.
- 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, Poitiers, Moscow, Novosibirsk)
- 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; Max Planck Institute for Solid State Research; Russian Institute of High-Pressure Physics; 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:

- 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:

- Oganov A.R. (2012). Theory of superhard materials. Invited review for handbook *Comprehensive Hard Materials Review*, Elsevier. In press.
- Oganov A.R. (2011). Discovery of γ -B₂₈, a Novel Boron Allotrope with Partially Ionic Bonding. MRS Fall 2010 Meeting Book "Boron and borides", in press.
- 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.
- 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.
- 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.
- 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.
- 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.
- 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.
- 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).
- 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.
- 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.
- 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.
- 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.
- 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.
- 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:

- Shirako Y., Kojitani H., Oganov A.R., Fujino K., Miura H., Mori D., Inaguma Y., Yamaura K., Akaogi M. (2012). Crystal structure of CaRhO₃ 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 NaAlH₄ from first principles. *Appl. Phys. Lett.* **100**, 061905.
82. Oganov A.R., Solozhenko V.L., Gatti C., Kurakevych O.O., Le Godec Y. (2011). The high-pressure phase of boron, γ -B₂₈: disputes and conclusions of 5 years after discovery. *J. Superhard Materials* **33**, 363-379.
81. Lyakhov A.O., Oganov A.R. (2011). Evolutionary search for superhard materials applied to forms of carbon and TiO₂. *Phys. Rev.* **B84**, 092103.
80. 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.
79. 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.
78. Wen X.D., Hand L., Labet V., Yang T., Hoffmann R., Ashcroft N.W., Oganov A.R., Lyakhov A.O. (2011). The stacking of graphanes under pressure. *Proc. Natl. Acad. Sci.* **108**, 6833-6837.
77. Oganov A.R., Lyakhov A.O., Valle M. (2011). How evolutionary crystal structure prediction works - and why. *Acc. Chem. Res.* **44**, 227-237.
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 MgSiO₃-Al₂O₃ 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 CaLi₂. *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 LiBeH₃ 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 BC₂N. *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 MgB₂. *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 -B₂₈. *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 LiBeH₃ 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-Canales 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 MgCO₃, CaCO₃ and CO₂ 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.
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