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Denis Gryaznov, Dr.

Education

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| *Oct 2002 – Sep 2006* | **Universität Stuttgart**Dr. rer. nat.(PhD) in Materials ResearchStuttgart, Germany |
| *Sep 1999 – Jun 2001* | **Transport and Telecommunication Institute**Master, Computer Modeling of Semiconductor TechnologiesRiga, Latvia |
| *Sep 1995 – Jun 1999* | **Riga Aviation University**Bachelor, Semiconductor TechnologiesRiga, Latvia |

Research Experience

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| *Oct 2009 – Dec 2013* | **PostDoc Position**Max Planck Institute for Solid State Research, Department of Physical Chemistry of Solids (prof. J. Maier)Stuttgart, Germany |
| *Oct 2006 – Sep 2009* | **PostDoc Position**EC Institute for Transuranium Elements, Materials ResearchKarlsruhe, Germany |
| *Jan 2004 – present* | Latvijas Universitāte, Senior Scientist, Theoretical Department, Institute of Solid State Physics, Riga, Latvia |
| *Aug 2002 – Sep 2006* | **PhD Student**Max Planck Institute for Solid State Research, Department of Physical Chemistry of Solids (prof. J.Maier), |
| *Sep 1998 – Apr 2002* | **Research Assistant**Baltic Scientific Instruments,Riga, Latvia |

Skills & Activities

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| *Skills* | Electronic Structure, Density Functional Theory, First-principles Calculations, Ab Initio Calculations, Quantum Chemistry, DFT Calculations, Ab Initio Methods, Ab Initio, VASP, Diffusion, Materials Chemistry, Cheminformatics and Computational Chemistry, Theoretical Chemistry, Computational Chemistry, Crystal, Phase Transitions, GaAs, Computational Materials Science, Quantum Mechanics, Molecular Dynamics, Physical Chemistry, Molecular Dynamics Simulation, Molecular Structure, Molecular Modeling, Material Modeling, Molecular Simulation, Computational Nanotechnology, Chemical Physics, Conceptual Density Functional Theory, Chemical Bonding, ADF, Normal mode analysis, Solid State Physics, Materials Science, Condensed Matter Physics, Atoms, Hydrogen Bonding |
| *Languages* | English, German, Latvian, Russian |
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Publication Highlights

Book Chapters

Yuri Zhukovskii, Dmitry Bocharov, Denis Gryaznov, Eugene Kotomin: *First Principles Simulations on Surface Properties and Oxidation of Nitride Nuclear Fuels*. IN: Advances in Nuclear Fuels, Edited by S.T. Revankar, 02/2012: pages 95-122; InTech Open Access Publishers, Rijeka, Croatia., ISBN: 978-953-51-0042-3

Journal Publications

Tor S Bjørheim, Marco Arrigoni, Denis Gryaznov, Eugene Kotomin, Joachim Maier: *Thermodynamic properties of neutral and charged oxygen vacancies in BaZrO3 based on first principles phonon calculations*. Physical Chemistry Chemical Physics 07/2015; 17:20765-20774. DOI:10.1039/c5cp02529j

Marco Arrigoni, Eugene Kotomin, Denis Gryaznov, Joachim Maier: *Confinement effects for the F center in non-stoichiometric BaZrO3 ultrathin films*. physica status solidi (b) 01/2015; 252(1):139-143. DOI:10.1002/pssb.201400116

Denis Gryaznov, Stefan Baumann, Eugene A. Kotomin, Rotraut Merkle: *Comparison of Permeation Measurements and Hybrid Density-Functional Calculations on Oxygen Vacancy Transport in Complex Perovskite Oxides*. The Journal of Physical Chemistry C 12/2014; 118(51):28542. DOI:10.1021/jp509206k

Denis Gryaznov, Mike W Finnis, Robert A Evarestov, Joachim Maier: *Oxygen vacancy formation energies in Sr-doped complex perovskites: Ab initio thermodynamic study*. Solid State Ionics 01/2014; 254:11. DOI:10.1016/j.ssi.2013.10.046

Evgeny Blokhin, Robert A. Evarestov, Denis Gryaznov, Eugene A. Kotomin, Joachim Maier: *Theoretical modeling of antiferrodistortive phase transition for SrTiO3 ultrathin films*. Physical Review B 12/2013; 88(24):241407. DOI:10.1103/PhysRevB.88.241407

Denis Gryaznov, Evgeny Blokhin, Alexandre Sorokine, Eugene A Kotomin, Robert A Evarestov, Annette Bussmann-Holder, Joachim Maier: *A Comparative Ab Initio Thermodynamic Study of Oxygen Vacancies in ZnO and SrTiO3: Emphasis on Phonon Contribution*. The Journal of Physical Chemistry C 06/2013; 117:13776. DOI:10.1021/jp400609e

A Weizman, D Fuks, E.A. Kotomin, D Gryaznov: *Ab initio study of phase competition in (La 1 − c ,Sr c )CoO 3 solid solutions*. Solid State Ionics 01/2013; DOI:10.1016/j.ssi.2012.09.007

D. Bocharov, D. Gryaznov, Yu. F. Zhukovskii, E. A. Kotomin: *Ab initio simulations of oxygen interaction with surfaces and interfaces in uranium mononitride*. Journal of Nuclear Materials 11/2012; 435(s 1–3). DOI:10.1016/j.jnucmat.2012.12.031

Eugene A. Kotomin, Yuri F. Zhukovkii, Dmitry Bocharov, Denis Gryaznov: *Ab initio modelling of UN grain boundary interfaces*. IOP Conference Series Materials Science and Engineering 11/2012; 38(1). DOI:10.1088/1757-899X/38/1/012058

Robert Evarestov, Evgeny Blokhin, Denis Gryaznov, Eugene A. Kotomin, Rotraut Merkle, Joachim Maier: *Jahn-Teller effect in the phonon properties of defective SrTiO\_ {3} from first principles*. Physical review. B, Condensed matter 05/2012; 85(17). DOI:10.1103/PhysRevB.85.174303

Denis Gryaznov, Eugene Heifets, Eugene Kotomin: *The first-principles treatment of the electron-correlation and spin-orbital effects in uranium mononitride nuclear fuels*. Physical Chemistry Chemical Physics 04/2012; 14(13):4482-90. DOI:10.1039/c2cp40297a

E.A. Kotomin, Yuri F. Zhukovskii, D. Bocharov, D. Gryaznov: *Ab initio modelling of UN grain boundary interfaces*. IOP Conference Series Materials Science and Engineering 01/2012; 38:012058.

D Bocharov, D Gryaznov, Yu F Zhukovskii, E A Kotomin: *Ab initio modeling of oxygen impurity atom incorporation into uranium mononitride surface and sub-surface vacancies*. Journal of Nuclear Materials 07/2011; 416:200-204.

D Bocharov, D Gryaznov, Yu F Zhukovskii, E A Kotomin: *DFT calculations of point defects on UN(001) surface*. Surface Science 02/2011; 605:396-400.

E A Kotomin, V Alexandrov, D Gryaznov, R A Evarestov, J Maier: *Confinement effects for ionic carriers in SrTiO3 ultrathin films: First-principles calculations of oxygen vacancies*. Physical Chemistry Chemical Physics 01/2011; 13(3):923-6. DOI:10.1039/c0cp01060j

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Denis Gryaznov, Eugene Heifets, David Sedmidubsky: *Density Functional Theory Calculations On Magnetic Properties Of Actinide Compounds*. Physical Chemistry Chemical Physics 10/2010; 12(38):12273-8. DOI:10.1039/c0cp00372g

D Bocharov, D Gryaznov, Yu. F. Zhukovskii, E.A. Kotomin: *DFT calculations of point defects on UN (001) surface*. Surface Science 08/2010; 605(3-4). DOI:10.1016/j.susc.2010.11.007

Dmitry Bocharov, Denis Gryaznov, Yuri F. Zhukovskii, Eugene A. Kotomin: *Ab initio modeling of oxygen impurity atom incorporation into uranium mononitride surface and subsurface vacancies*. Journal of Nuclear Materials 08/2010; 416(1-2). DOI:10.1016/j.jnucmat.2010.11.090

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D. Gryaznov, S. Rashkeev, E. A. Kotomin, E. Heifets, Y. Zhukovskii: *Helium Behavior in Oxide Nuclear Fuels: First Principles Modeling*. Nuclear Instruments and Methods in Physics Research Section B Beam Interactions with Materials and Atoms 01/2010; 268(19). DOI:10.1016/j.nimb.2010.05.054

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D Gryaznov, J Fleig, J Maier: *Finite Element Simulation of Diffusion Into Polycrystalline Materials*. Solid State Sciences 06/2008; 10(6). DOI:10.1016/j.solidstatesciences.2008.03.030

E.A. Kotomin, D. Gryaznov, R. W. Grimes, D. Parfitt, Yu.F. Zhukovskii, Yu.A. Mastrikov, P. Van Uffelen, V. V. Rondinella, R.J.M. Konings: *First-principles modelling of radiation defects in advanced nuclear fuels*. Nuclear Instruments and Methods in Physics Research Section B Beam Interactions with Materials and Atoms 06/2008; 266(12-13):2671-2675. DOI:10.1016/j.nimb.2008.03.226

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D. Gryaznov, J. Fleig, Joachim Maier: *Numerical Study of Grain Boundary Diffusion in Nanocrystalline Materials*. Defect and Diffusion Forum 01/2005; 237-240:1043-1048. DOI:10.4028/www.scientific.net/DDF.237-240.1043

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V Gostilo, D Gryaznov, I Lisjutin: *Technological limitations and processing-generated defects at the development of pixel and strip arrays*. Nuclear Instruments and Methods in Physics Research Section A Accelerators Spectrometers Detectors and Associated Equipment 07/2002; 487:13-18. DOI:10.1016/S0168-9002(02)00938-5

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D. V. Gryaznov, A. V. Loupilov: *Characteristics of InP γ-Detectors*. Instruments and Experimental Techniques 01/2001; 44(4):462-465. DOI:10.1023/A:1017996115937

D. V. Gryaznov, A. V. Lupilov: *An X-ray Detection Unit Based on GaAs Detector*. Instruments and Experimental Techniques 11/2000; 43(6):815-817. DOI:10.1023/A:1026640505886

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Denis Gryaznov, Juergen Fleig, Joachim Maier: *Numerical Study of Grain Boundary Diffusion: Size Effects*. Diffusion Fundamentals 2; 01/2005

V. Gostilo, C. Budtz-Jorgensen, I. Kuvvetli, D. Gryaznov, I. Lisjutin, A. Loupilov: *Development of drift-strip detectors based on CdZnTe*. Nuclear Science Symposium Conference Record, 2001 IEEE; 02/2001