Maksim S. Rakitin

Curriculum vitae

Personal details

Full name: Maksim S. Rakitin

Links: ○ BNL • SBU • IACS • SUSU

○ • • • ResearchGate

Experience

2017.11–present

Assistant Computational Scientist, *DAMA group, NSLS-II, Brookhaven National Laboratory*, Upton, NY (https://www.bnl.gov).

Supervisor: Dr. Stuart Campbell

Projects:

- **Bluesky** — a library for experiment control and collection of scientific data and metadata, http://nsls-ii.github.io/bluesky.
- **Databroker** — a simple, user-friendly interface for retrieving stored data and metadata from multiple sources, http://nsls-ii.github.io/databroker.
- Other related software projects.

Responsibilities:

- Scientific software development & maintenance.
- NSLS-II beamlines support.

2015.12–2017.10

Research Associate (Postdoc), *NSLS-II, Brookhaven National Laboratory*, Upton, NY (https://www.bnl.gov).

Supervisor: Dr. Oleg Tchoubar (Chubar)

Projects:

- **Synchrotron Radiation Workshop (SRW)** — computer code for X-ray source and optics simulations, https://github.com/mrakitin/SRW.
- **Sirepo** — a cloud-based framework for SRW, https://github.com/radiasoft/sirepo.
- **Image processing and data visualization**, https://github.com/mrakitin/plotting and https://github.com/mrakitin/experiments.
- **CRL simulator** — a code for simulation of a transfocator (compound refractive lenses (CRL) for X-ray focusing), https://github.com/mrakitin/bnlcrl.

Responsibilities:

- Adding new functionality to Sirepo (*e.g.*, new optical elements, new reports, implementation of dynamical access of crystal data and optical constants from external servers).
- Adding new functionality to SRW (*e.g.*, new optical elements).
- Creation of new SRW/Sirepo "virtual beamline" scripts/examples.
- Creation and update of Sirepo & SRW wiki documentation.
- SRW & Sirepo users community support via GitHub issues, email communication, *etc.*
- Deployment of SRW & Sirepo to NSLS-II servers for usage by beamline scientists.
- Computational support for NSLS-II beamlines — carrying out required SRW & Sirepo simulations.
- Assistance with scan plans preparation using **Bluesky** data collection framework and **ophyd** package for controlling motors, detectors, *etc.*
- Participation in X-ray experiments (SRX, ESM, SMI, CHX beamlines of NSLS-II) — carrying out measurements and bulk data analysis, processing & visualization using Python (NumPy, SciPy, Matplotlib, PIL, *etc.*; raw data and images, NumPy arrays, HDF5 datasets).
- Implementation of a library of samples for coherent scattering experiments in SRW and Sirepo (collaborative project with CFN).
- Assisting with development of the Hartmann mask optical element in SRW and its implementation in Sirepo (collaborative project with the Metrology group of NSLS-II).
- Tutorship of summer students.

2013.10–2015.12

Postdoctoral Associate (Postdoc), *Prof. Oganov's lab, Department of Geosciences, Stony Brook University*, Stony Brook, NY (http://stonybrook.edu, http://uspex.stonybrook.edu).

Supervisor: Prof. Artem R. Oganov

Projects:

- Refactoring of USPEX code and porting it from Matlab to Python using modern programming techniques.
- *Ab initio* investigation of BeF_2 and SiO_2 systems in a wide pressures range (paper) using USPEX, VASP, Quantum Espresso, Phonopy.
- Prediction of secondary structures of proteins from knowledge of sequences of amino acids. Development of USPEX interface for Tinker.

Responsibilities:

- Main developer of the project on rewriting USPEX in Python with use of NumPy, SciPy, TkInter, *etc.* Web-based API creation.
- New releases of Matlab/Octave version (USPEX 9.4.1, 9.4.2, 9.4.3, 9.4.4), new features, bug fixes, maintenance.
- Development and maintenance of USPEX continuous integration system (automatic nightly builds + testing).

- Development of tests for USPEX interface with VASP, GULP, LAMMPS, CASTEP, Quantum Espresso, SIESTA, CP2K, QuantumWise ATK, DMACRYS, Tinker, FHI-aims.
- Development and maintenance of online utilities http://han.ess.sunysb.edu and http://uspex-team.org using JavaScript, jQuery, PHP, HTML, JSON, REST API, WebGL, XML, SVN, interfaces to Python, Fortran, Matlab programs, *etc.*
- Installation, configuration, and maintenance of Trac system and SVN.
- Creation and maintenance of USPEX manual in LaTeX, PDF, HTML formats.
- USPEX community support.

2008.10–2013.09

Researcher, *Department of General and Theoretical Physics, South Ural State University*, Chelyabinsk, Russia (http://susu.ac.ru).

Supervisor: Prof. Alexander A. Mirzoev

Projects:

- Performing research on investigating influence of hydrogen on structure and properties of iron-based alloys using DFT methods (WIEN2k).

Responsibilities:

- Development of bash/Python utilities for monitoring WIEN2k calculations in PBS/Torque and SLURM queues and for processing data of calculations, developing mail notification system for the calculations.
- Installation of WIEN2k on a PC and on the university supercomputers (SKIF Ural, SKIF Aurora, Tornado).
- Teaching and consulting students how to use WIEN2k both on a PC and on supercomputers.

2007.06–2013.10

QA Engineer, QA Team Leader, *Applied Technologies Ltd.*, Chelyabinsk, Russia (http://www.appliedtech.ru), a partner of Rocket Software Inc., USA (http://www.rocketsoftware.com)

Supervisor: Valery Ermakov, CEO

Projects:

- Tivoli Enterprise Portal (August 2011 – October 2013) — QA team leader. Responsibilities: software testing on Windows, Linux, Linux on z, z/OS operating systems, GUI testing automation using IBM Rational Functional Tester, creation of TEP Automated Testing System (TATS) for automatic data verification using Python, REST API, JSON, XML, PHP, HTML, JavaScript, jQuery in six TEP-enabled products:
  - Tivoli Advanced Reporting and Management for DFSMShsm;
  - Tivoli Advanced Audit for DFSMShsm;
  - Tivoli Advanced Catalog Management for z/OS;
  - Tivoli Advanced Backup and Recovery for z/OS;
  - Tivoli Advanced Allocation Management;
  - Tivoli Automated Tape Allocation Manager for z/OS.

  Regular voice and video conversations with colleagues from the US.

- Tivoli Storage Manager for z/OS Media (February 2011 – August 2011) — QA engineer. Responsibilities: software testing on Windows, Linux on z, Solaris, AIX, z/OS operating systems with IBM DB2 databases, testing automation using IBM-developed tools, bash, batch.

- IBM Tivoli Advanced Allocation Management (January 2009 – January 2011) — QA engineer. Responsibilities: software testing on z/OS, testing automation using bash, JCL, REXX. Regular voice and video conversations with colleagues from the US.

- Rocket Servergraph Data Protection Expert (June 2007 – December 2008) — QA engineer. Responsibilities: software testing on Windows, Linux, Solaris, HP-UX, AIX operating systems with PostgreSQL databases, GUI testing automation using AutoIt3, automation of data verification using Perl and SQL. Regular voice and video conversations with colleagues from the US.

2006–2007 **System administrator**, *Department of General and Theoretical Physics, South Ural State University*, Chelyabinsk, Russia (http://susu.ac.ru)
Administer, secure and support Windows and Linux systems. Support HTTP server (Apache), proxy server (Squid). Help others to troubleshoot operating system, software, hardware and other issues. Also support the testing system for students.

Education

2008.10–2012.09 **Ph.D. in Condensed Matter Physics (defended on September 19, 2012)**
South Ural State University (National Research University), Chelyabinsk, Russia
Thesis: Study of impurities influence on the hydrogen dissolution energy in the bcc iron
Scientific adviser: Prof. A.A. Mirzoev, Dr. of Sciences

2006.09–2008.06 **M.S. in Applied Mathematics and Physics (June 13, 2008)**
South Ural State University (SUSU), Chelyabinsk, Russia
Thesis: Computer simulation of influence of structural relaxation and impurities on dissolution energy of H in Fe
Scientific adviser: Prof. A.A. Mirzoev, Dr. of Sciences
GPA: 3.85 / 4.0

2002.09–2006.06 **B.S. in Applied Mathematics and Physics (June 20, 2006), summa cum laude**
South Ural State University (SUSU), Chelyabinsk, Russia
Thesis: Binding energy of hydrogen in bcc iron lattice
Scientific adviser: Prof. A.A. Mirzoev, Dr. of Sciences
GPA: 3.69 / 4.0

Honors, awards and certificates

2012 Certificate of summer school on computer simulations and massive calculations in modern physics with invited lectors from the US (Chelyabinsk, Russia)

2010 Certificate of summer school on computational material sciences (San-Sebastian, Spain)

2010 Scholarship of the University President (Chelyabinsk, Russia)

2009 Certificate of cources on high-performance computational systems (Nizhny Novgorod, Russia)

2009–2010 State contract (grant) on Federal Programme "Scientific and pedagogical staff for an innovative Russia" (Moscow, Russia)

2007 Diploma of the 13th All-Russian Physics Students Conference for the talk "Computer simulation of hydrogen atom in bcc iron" (Rostov-on-Don, Russia)

2006 Summa cum laude in Bachelor's studies (Chelyabinsk, Russia)

2006 Scholarship of the President of Russia

Languages

English Full working proficiency, fluent

Russian Native language

Computer skills

Atomistic simulation VASP, WIEN2k, Quantum Espresso, CASTEP, SIESTA, CP2K, FHI-aims, QuantumWise ATK, Tinker, GULP, LAMMPS, DMACRYS, Phonopy, TB-LMTO-ASA

Data analysis, visualization Python, NumPy, SciPy, Matplotlib, Bokeh, D3.js, Matlab, Octave, OriginPro, gnuplot, VESTA, XCrysDen, STM4, P4VASP, Molden, VMD, RasTop, *etc.*

Programming Python (including TkInter, PyQT, NumPy, SciPy, Matplotlib, PIL), C++, Fortran, Matlab, Octave, JavaScript, jQuery, AngularJS, WebGL, PHP, HTML5, bash, csh/tcsh, make, Perl, AutoIt3, REXX, SQL, JCL

Parallelization MPI, OpenMP

IDE PyCharm, Visual Studio, Eclipse, Aptana Studio, emacs, vim

Writing LaTeX, BibTeX, TeXlipse/Eclipse, plasTeX, JabRef, MS Word

OS Linux (CentOS, SuSE, RedHat, Fedora, Ubuntu, Debian, Raspbian, *etc.*), Mac OS X, AIX, Solaris, HP-UX, Windows, DOS, z/OS

Virtualization Docker, Vagrant, VirtualBox, VMware

VCS GitHub, Git, SVN, CVS, Bazaar, Trac

Hobby projects

- Raspberry Pi-based web server — https://mrakitin.xyz (production HTTPS web server configuration — Nginx+uWSGI+Flask with Jinja2 templates)
- Weather in console — https://github.com/mrakitin/weather

References

Supervisor **Oleg Chubar**, Ph.D., Physicist, Beamline Support
NSLS-II/Photon Science Division, Brookhaven National Laboratory, Upton, NY 11973
chubar@bnl.gov +1 (631) 344–4525

Colleague **Mikhail Zhernenkov**, Ph.D., Associate Physicist, NSLS-II SMI Beamline Scientist
NSLS-II/Photon Science Division, Brookhaven National Laboratory, Upton, NY 11973
zherne@bnl.gov +1 (631) 344–5158

Collaborator **David L. Bruhwiler**, President / CEO, Ph.D.
RadiaSoft LLC, Boulder, CO 80304
bruhwiler@radiasoft.net +1 (720) 502–3928

Collaborator **Robert Nagler**, CTO
RadiaSoft LLC, Boulder, CO 80304
nagler@radiasoft.net

Colleague **Qiang Zhu**, Assistant Professor, Ph.D.
Department of Physics and Astronomy, University of Nevada Las Vegas, NV 89154-4002
qiang.zhu@unlv.edu +1 (702) 895–1707

Ph.D. adviser **Alexander A. Mirzoev**, Professor, Dr. of Sciences.
Department of General and Theoretical Physics, South Ural State University, Chelyabinsk, Russia
mirzoev@physics.susu.ac.ru +7 (351) 265–4713

Additional references available upon request.

Publications

19. M. S. Rakitin, P. Moeller, R. Nagler, D. L. Bruhwiler, D. Smalyuk, and O. Chubar, "Sirepo — software framework for X-ray source and optics simulations **(under preparation)**," *Journal of Synchrotron Radiation*, 2017.

18. M. S. Rakitin, O. Chubar, P. Moeller, R. Nagler, and D. L. Bruhwiler, "Sirepo: a web-based interface for physical optics simulations - its deployment and use at NSLS-II **(invited paper)**," in *Proc. SPIE, Advances in Computational Methods for X-Ray Optics IV (23 August 2017)*, vol. 10388, p. 103880R, 2017.

17. O. Chubar, M. Rakitin, Y.-C. Chen-Wiegart, A. Fluerasu, and L. Wiegart, "Simulation of experiments with partially coherent x-rays using Synchrotron Radiation Workshop," in *Proc. SPIE, Advances in Computational Methods for X-Ray Optics IV (23 August 2017)*, vol. 10388, p. 1038811, 2017.

16. O. Chubar, M. Rakitin, Y.-C. Chen-Wiegart, Y. S. Chu, A. Fluerasu, D. Hidas, and L. Wiegart, "Main functions, recent updates, and applications of Synchrotron Radiation Workshop code **(invited paper)**," in *Proc. SPIE, Advances in Computational Methods for X-Ray Optics IV (23 August 2017)*, vol. 10388, p. 1038805, 2017.

15. L. Wiegart, M. Rakitin, A. Fluerasu, and O. Chubar, "X-ray optical simulations supporting advanced commissioning of the coherent hard x-ray beamline at NSLS-II," in *Proc. SPIE, Advances in Computational Methods for X-Ray Optics IV (23 August 2017)*, vol. 10388, p. 103880N, 2017.

14. M. Idir, M. Rakitin, B. Gao, J. Xue, L. Huang, and O. Chubar, "Alignment of KB mirrors with at-wavelength metrology tool simulated using SRW," in *Proc. SPIE, Advances in Computational Methods for X-Ray Optics IV (23 August 2017)*, vol. 10388, p. 103880Z, 2017.

13. M. M. Davari Esfahani, Q. Zhu, H. Dong, A. R. Oganov, S. Wang, M. S. Rakitin, and X.-F. Zhou, "Novel magnesium borides and their superconductivity," *Phys. Chem. Chem. Phys.*, vol. 19, pp. 14486–14494, 2017.

12. O. V. Chubar, T. A. Caswell, Y. Chen-Wiegart, A. Fluerasu, Y. Hidaka, D. A. Hidas, C. A. Kitegi, M. S. Rakitin, T. Tanabe, J. Thieme, L. Wiegart, and G. Williams, "Analysis and Correction of in-Vacuum Undulator Misalignment Effects in a Storage Ring Synchrotron Radiation Source," in *Proc. of International Particle Accelerator Conference (IPAC'17), Copenhagen, Denmark, 14–19 May, 2017*, no. 8 in International Particle Accelerator Conference, (Geneva, Switzerland), pp. 1663–1665, JACoW, May 2017.

11. A. Blednykh, B. Bacha, G. Bassi, O. V. Chubar, M. S. Rakitin, V. V. Smaluk, and M. Zhernenkov, "A Comprehensive Study of the Microwave Instability," in *Proc. of International Particle Accelerator Conference (IPAC'17), Copenhagen, Denmark, 14–19 May, 2017*, no. 8 in International Particle Accelerator Conference, (Geneva, Switzerland), pp. 3224–3226, JACoW, May 2017.

10. D. A. Mirzaev, A. A. Mirzoev, and M. S. Rakitin, "Alloying effects on thermodynamic characteristics of hydrogen in bcc iron," *Bulletin of the South Ural State University, Ser. Metallurgy*, vol. 16, no. 4, pp. 40–53, 2016. Original Russian Text.

9. Y. H. R. Chang, T. L. Yoon, T. L. Lim, and M. Rakitin, "Thorough investigations of the structural and electronic properties of $Al_xIn_{1-x}N$ ternary compound via *ab initio* computations," *Journal of Alloys and Compounds*, vol. 682, pp. 338–344, 2016.

8. M. M. Davari Esfahani, Z. Wang, A. R. Oganov, H. Dong, Q. Zhu, S. Wang, M. S. Rakitin, and X.-F. Zhou, "Superconductivity of novel tin hydrides (Sn_nH_m) under pressure," *Scientific Reports*, vol. 6, p. 22873, Mar. 2016.

7. M. S. Rakitin, A. R. Oganov, H. Niu, M. M. Davari Esfahani, X.-F. Zhou, G.-R. Qian, and V. L. Solozhenko, "A novel phase of beryllium fluoride at high pressure," *Phys. Chem. Chem. Phys.*, vol. 17, pp. 26283–26288, 2015.

6. A. R. Oganov, C. W. Glass, A. O. Lyakhov, Q. Zhu, G.-R. Qian, H. T. Stokes, M. S. Rakitin, M. Davari, P. Bushlanov, Z. Allahyari, and S. Lepeshkin, *USPEX manual: Universal Structure Predictor: Evolutionary Xtallography*, 2013–2015.

5. D. A. Mirzaev, A. A. Mirzoev, K. Y. Okishev, and M. S. Rakitin, "Theory of hydrogen solubility in binary iron alloys based on *ab initio* calculation results," *Molecular Physics*, vol. 110, no. 11-12, pp. 1299–1304, 2012.

4. A. V. Ursaeva, M. S. Rakitin, G. E. Ruzanova, and A. A. Mirzoev, "*Ab initio* study of hydrogen interaction with point defects in bcc iron," *Bulletin of the South Ural State University: Math., Mech. and Phys.*, vol. 4, no. 10, pp. 114–119, 2011. Original Russian Text.

3. A. A. Mirzoev, D. A. Mirzaev, and M. S. Rakitin, "Impurities influence on dissolution of hydrogen in bcc iron," *Bulletin of the South Ural State University: Math., Mech. and Phys.*, vol. 4, no. 10, pp. 77–83, 2011. Original Russian Text.

2. M. S. Rakitin, A. A. Mirzoev, and D. A. Mirzaev, "Change of electronic structure in iron containing interstitial atoms of hydrogen," *Bulletin of the South Ural State University: Metallurgy*, vol. 14, no. 13, pp. 67–71, 2010. Original Russian Text.

1. A. A. Mirzoev, M. M. Yalalov, and M. S. Rakitin, "Dependence of TB-LMTO calculations accuracy on k-points number: effect of iterations mixing parameter using Broyden scheme," *Bulletin of the South Ural State University: Math., Phys. and Chem.*, vol. 6, no. 6, pp. 103–105, 2005. Original Russian Text.

Conferences, talks, workshops and schools

2017.11 *Sirepo — an open-source browser interface for X-ray source and optics simulations*, ORNL Visualization Hackathon, Oak Ridge National Laboratory, Oak Ridge, TN

2017.10 *Sirepo — an open-source cloud-based software interface for X-ray source and optics simulations*, NSLS-II Lunchtime seminar, Brookhaven National Laboratory, Upton, NY

2017.08 **Invited talk** — *Sirepo: a web-based interface for physical optics simulations — its deployment and use at NSLS-II*, SPIE Optical Engineering + Applications, San Diego, CA

2017.05 *2017 NSLS-II & CFN Users' Meeting*, Brookhaven National Laboratory, Upton, NY

2016.12 *Collaboration meeting with RadiaSoft LLC* RadiaSoft LLC, Boulder, CO

2016.12 *Early Career Researcher Symposium 2016*, Brookhaven National Laboratory, Upton, NY

2016.10 *Software for Optical Simulations (SOS) Workshop*, ICTP, Trieste, Italy

2016.05 *2016 NSLS-II & CFN Joint Users' Meeting*, Brookhaven National Laboratory, Upton, NY

2015.11 *Sensitivity, Error and Uncertainty Quantification for Atomic, Plasma, and Material Data*, IACS, Stony Brook University, Stony Brook, NY

2015.10 *Collaboration Meeting on "Simulation and Modeling for SR Sources and X-Ray Optics"*, NSLS-II, Brookhaven National Laboratory, Upton, NY

2015.07 **Invited talk** — *Crystal and protein structure modeling, software development and applications*, Brookhaven National Laboratory, Upton, NY

2015.06 *Advances in Functional Materials — Conference 2015*, Stony Brook University, Stony Brook, NY

2015.06 *Recent progress in USPEX development*, Group seminar, Stony Brook University, Stony Brook, NY

2015.04 **Invited talk** — *Crystal structure prediction from first principles*, Humboldt-Universität zu Berlin, Institut für Physik, Berlin, Germany

2015.04 *Oracle R, Advanced & predictive Analytics Workshop*, Stony Brook University, Stony Brook, NY

2015.02 *MATLAB & Simulink for Project-Based Learning using LEGO MINDSTORMS EV3*, Stony Brook University, Stony Brook, NY

2015.01 *IACS workshop "Intro to Python"*, Stony Brook University, Stony Brook, NY

2014.11 *Novel phase of beryllium fluoride at high pressure*, Group seminar, Stony Brook University, Stony Brook, NY

2014.11 **Invited tutor** — *Theory and Computation for Interface Science and Catalysis: Fundamentals, Research and Hands on Engagement using VASP*, Brookhaven National Laboratory, Upton, NY

2014.10 *MATLAB and Simulink Complimentary Technical Sessions at Stony Brook University*, Stony Brook, NY

2014.09 *Proteins structure prediction using USPEX*, Group seminar, Stony Brook University, Stony Brook, NY

2014.09 *USPEX tests for Tinker: Different amino-acids XYZ-20, ALA-40, CASP10, REMD*, Group seminar, Stony Brook University, Stony Brook, NY

2014.07 *Introduction to Python*, Group seminar, Stony Brook University, Stony Brook, NY

2014.04 *SiO_2 and BeF_2 phase transformation under pressure. Proteins simulation with Tinker interface for USPEX*, Group seminar, Stony Brook University, Stony Brook, NY

2014.03 *CECAM workshop "Simulation of biomolecular interactions with inorganic and organic surfaces as a challenge for future nanotechnologies"*, Toulouse, France

2014.03 *USPEX mini-workshop*, Group seminar, Stony Brook University, Stony Brook, NY

2014.02 *SiO_2 and BeF_2 phase transformation under pressure*, Group seminar, Stony Brook University, Stony Brook, NY

2013.11 *Study of impurities influence on the hydrogen dissolution energy in the bcc iron*, Group seminar, Stony Brook University, Stony Brook, NY

2013.08 *2^{nd} summer school on computer simulations in modern physics*, Chelyabinsk, Russia

2012.08 *Summer school on computer simulations and massive calculations in modern physics*, Chelyabinsk, Russia

2011.10 *6^{th} All-Russian scientific-technical conference "Physical properties of metals and alloys"*, Yekaterinburg, Russia

2011.09 *International conference "Thermodynamics 2011"*, Athens, Greece

2011.05 *2^{nd} All-Russian youth school-conference "Modern problems of metal science"*, Pitsunda, Abkhazia

2010.07 *International symposium "Metal-hydrogen systems. Fundamentals and applications"*, Moscow, Russia

2010.06 *International summer school "Computational Materials Science"*, San Sebastian, Spain

2010.03 *All-Russian conference "Parallel computing technologies 2010"*, Ufa, Russia

2010.02 *33^{rd} International conference on theoretical physics "Kourovka-2010"*, Novouralsk, Russia

2009.11 *9^{th} International conference "High-performance parallel computing on cluster systems"*, Vladimir, Russia

2009.10 *12th V.A. Fock All-Russian conference on quantum and computational chemistry*, Kazan, Russia

2007.04 *13th All-Russian students conference in physics*, Rostov-on-Don, Russia