

# Maksim Rakitin

## Curriculum vitae

NSLS-II,  
Brookhaven National Laboratory,  
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📄 [github.com/mrakitin](https://github.com/mrakitin)



### Personal details

Full name: Maksim S. Rakitin

Links: [BNL](#) | [LinkedIn](#) | [Google Scholar](#) | [ResearchGate](#) | [GitHub](#) | [SBU](#) | [IACS](#) | [SUSU](#)

### Experience

2015.12–Present **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>.
- **CRL simulator** — a code for simulation of a transfocator (compound refractive lenses (CRL) for X-ray focusing), <https://github.com/mrakitin/bnclrl>.
- **Image processing and data visualization**, <https://github.com/mrakitin/plotting>.

#### 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



Oganov's Lab

COMPUTATIONAL MATERIALS DISCOVERY LABORATORY

**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<sub>2</sub> and SiO<sub>2</sub> systems in a wide pressures range ([link](#)) 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> 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  $\text{\LaTeX}$ , 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 Autolt3, 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.

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## 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

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## 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 courses 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 13<sup>th</sup> 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

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## Languages

- English Full working proficiency, fluent
- Russian Native language

## Computer skills

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|-------------------------------------|---|
| <b>Atomistic simulation</b>         | VASP, WIEN2k, Quantum Espresso, CASTEP, SIESTA, CP2K, FHI-aims, QuantumWise<br>ATK, Tinker, GULP, LAMMPS, DMACRYS, Phonopy, TB-LMTO-ASA   |
| <b>Data analysis, visualization</b> | Python, NumPy, SciPy, Matplotlib, Matlab, Octave, OriginPro, gnuplot, VESTA, XCrystal, STM4, P4VASP, Molden, VMD, RasTop, etc.  |
| <b>Programming</b>                  | Python (including TkInter, PyQt, NumPy, SciPy, Matplotlib, PIL), C++, Fortran, Matlab, Octave, JavaScript, jQuery, AngularJS, WebGL, PHP, HTML5, bash, csh/tcsh, make, Perl, Autot3, REXX, SQL, JCL |
| <b>Parallelization</b>              | MPI, OpenMP   |
| <b>IDE</b>                          | PyCharm, Visual Studio, Eclipse, Aptana Studio, emacs, vim  |
| <b>Writing</b>                      | L <sup>A</sup> T <sub>E</sub> X, BibT <sub>E</sub> X, TeXlipse/Eclipse, JabRef, MS Word   |
| <b>OS</b>                           | Linux (CentOS, SuSE, RedHat, Fedora, Ubuntu, Debian, etc.), Mac OS X, AIX, Solaris, HP-UX, Windows, DOS, z/OS   |
| <b>Virtualization</b>               | Docker, Vagrant, VirtualBox, VMware   |
| <b>VCS</b>                          | GitHub, Git, SVN, CVS, Bazaar, Trac   |
| <b>Hobby projects</b>               | Weather in console — <a href="https://github.com/mrakitin/weather">https://github.com/mrakitin/weather</a>  |

## References

- Supervisor **Oleg Chubar**, Ph.D., Physicist, Beamline Support  
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 phone: +1 (631) 344-4525
- Collaborator **David L. Bruhwiler**, President / CEO, Ph.D.  
 Radiasoft LLC, Boulder, CO 80304  
 e-mail: [bruhwiler@radiasoft.net](mailto:bruhwiler@radiasoft.net)  
 phone: +1 (720) 502-3928
- Ph.D. adviser **Alexander A. Mirzoev**, Professor, Dr. of Sciences.  
 Department of General and Theoretical Physics, South Ural State University, Chelyabinsk, Russia  
 e-mail: [mirzoev@physics.susu.ac.ru](mailto:mirzoev@physics.susu.ac.ru)  
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- Colleague **Qiang Zhu**, Assistant Professor, Ph.D.  
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 phone: +1 (702) 895-1707  
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COMPUTATIONAL MATERIALS DISCOVERY LABORATORY

*Additional references available upon request.*

## Publications

- [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.
- [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.
- [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.
- [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.
- [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.
- [6] 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.
- [7] 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.
- [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 ( $\text{Sn}_n\text{H}_m$ ) under pressure," *Scientific Reports*, vol. 6, p. 22873, Mar. 2016.
- [9] Y. H. R. Chang, T. L. Yoon, T. L. Lim, and M. Rakitin, "Thorough investigations of the structural and electronic properties of  $\text{Al}_x\text{In}_{1-x}\text{N}$  ternary compound via *ab initio* computations," *Journal of Alloys and Compounds*, vol. 682, pp. 338–344, 2016.

## Conferences, talks, workshops and schools

- 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<sub>2</sub> and BeF<sub>2</sub> 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<sub>2</sub> and BeF<sub>2</sub> 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<sup>nd</sup> 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<sup>th</sup> All-Russian scientific-technical conference "Physical properties of metals and alloys"* 🌐, Yekaterinburg, Russia



- 2011.09 *International conference "Thermodynamics 2011"* 🌐, 📄, Athens, Greece
- 2011.05 *2<sup>nd</sup> 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<sup>rd</sup> International conference on theoretical physics "Kourovka-2010"* 🌐, 📄, Novouralsk, Russia
- 2009.11 *9<sup>th</sup> International conference "High-performance parallel computing on cluster systems"* 🌐, 📄, Vladimir, Russia
- 2009.10 *12<sup>th</sup> V.A. Fock All-Russian conference on quantum and computational chemistry* 🌐, Kazan, Russia
- 2007.04 *13<sup>th</sup> All-Russian students conference in physics* 🌐, 📄, Rostov-on-Don, Russia