# Maksim S. Rakitin

*Bio*

## Personal details

Full name: Maksim S. Rakitin
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## Education and training

2008.10–2012.09 **Ph.D. in Condensed Matter Physics (defended on September 19, 2012)**
*South Ural State University (National Research University), Chelyabinsk, Russia*

2006.09–2008.06 **M.S. in Applied Mathematics and Physics (June 13, 2008)**
*South Ural State University (SUSU), Chelyabinsk, Russia*

2002.09–2006.06 **B.S. in Applied Mathematics and Physics (June 20, 2006), summa cum laude**
*South Ural State University (SUSU), Chelyabinsk, Russia*

## Research and professional expertise

2017.11–present **Associate Computational Scientist**, *DAMA group, NSLS-II, Brookhaven National Laboratory*, Upton, NY (https://www.bnl.gov)

2015.12–2017.10 **Research Associate (Postdoc)**, *NSLS-II, Brookhaven National Laboratory*, Upton, NY (https://www.bnl.gov)

2013.10–2015.12 **Postdoctoral Associate (Postdoc)**, *Department of Geosciences, Stony Brook University*, Stony Brook, NY (https://stonybrook.edu, https://uspex-team.org/en)

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 (https://www.rocketsoftware.com)

## Software projects

- **Bluesky** — a library for experiment control and collection of scientific data and metadata, https://blueskyproject.io/bluesky.
- **Ophyd** — a device abstraction library, https://blueskyproject.io/ophyd.
- **Databroker** — a simple, user-friendly interface for retrieving stored data and metadata from multiple sources, https://blueskyproject.io/databroker.
- **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.
- **Databroker extractor** — image processing and data visualization, https://github.com/mrakitin/databroker-extractor.
- **CRL simulator** — a code for simulation of a transfocator (compound refractive lenses (CRL) for X-ray focusing), https://github.com/mrakitin/bnlcrl.
- **USPEX** — a code for evolutionary crystal structure prediction, https://uspex-team.org/en.

- **USPEX online utilities** — a set of pre- and post-processing tools for crystal structure simulations, http://han.ess.sunysb.edu.
- **USPEX manual** — http://han.ess.sunysb.edu/uspex_manual.
- Utilities for DFT simulations
- IBM Mainframe software projects

## Publications


32. S. Campbell, D. B. Allan, A. Barbour, D. Olds, M. Rakitin, R. Smith, and S. B. Wilkins, "Outlook for artificial intelligence and machine learning at the nsls-ii," *Machine Learning: Science and Technology*, 2020.
31. O. Chubar, L. Wiegart, S. Antipov, R. Celestre, R. Coles, A. Fluerasu, and M. Rakitin, "Analysis of hard x-ray focusing by 2D diamond CRL," in *Advances in Computational Methods for X-Ray Optics V* (O. Chubar and K. Sawhney, eds.), vol. 11493, pp. 119 – 127, International Society for Optics and Photonics, SPIE, 2020.
30. O. Chubar, R. A. Coles, L. Wiegart, A. Fluerasu, M. Rakitin, J. Condie, P. Moeller, and R. Nagler, "Simulations of coherent scattering experiments at storage ring synchrotron radiation sources in the hard x-ray range," in *Advances in Computational Methods for X-Ray Optics V* (O. Chubar and K. Sawhney, eds.), vol. 11493, pp. 201 – 208, International Society for Optics and Photonics, SPIE, 2020.
29. A. He, O. Chubar, M. Rakitin, L. Samoylova, C. Fortmann-Grote, S. Yakubov, and A. Buzmakov, "Parallel performance of "Synchrotron Radiation Workshop" code: partially coherent calculations for storage rings and time-dependent calculations for XFELs," in *Advances in Computational Methods for X-Ray Optics V* (O. Chubar and K. Sawhney, eds.), vol. 11493, pp. 78 – 87, International Society for Optics and Photonics, SPIE, 2020.
28. M. S. Rakitin, A. Giles, K. Swartz, J. Lynch, P. Moeller, R. Nagler, D. B. Allan, T. A. Caswell, L. Wiegart, O. Chubar, and Y. Du, "Introduction of the Sirepo-Bluesky interface and its application to the optimization problems," in *Advances in Computational Methods for X-Ray Optics V* (O. Chubar and K. Sawhney, eds.), vol. 11493, pp. 209 – 226, International Society for Optics and Photonics, SPIE, 2020.
27. B. Nash, O. Chubar, D. Bruhwiler, M. Rakitin, P. Moeller, R. Nagler, and N. Goldring, "Undulator radiation brightness calculations in the Sirepo GUI for SRW," in *Advances in Laboratory-based X-Ray Sources, Optics, and Applications VII* (A. Murokh and D. Spiga, eds.), vol. 11110, pp. 79–92, International Society for Optics and Photonics, SPIE, 2019.
26. B. Nash, N. Goldring, D. L. Bruhwiler, O. Tchoubar, A. He, M. Rakitin, R. Nagler, and P. Moeller, "Phase IIA Final Technical Report for "Development of software framework for x-Ray optics simulation and modeling"," 7 2019.
25. D. Allan, T. Caswell, S. Campbell, and M. Rakitin, "Bluesky's Ahead: A Multi-Facility Collaboration for an a la Carte Software Project for Data Acquisition and Management," *Synchrotron Radiation News*, vol. 32, no. 3, pp. 19–22, 2019.
24. L. Wiegart, M. Rakitin, Y. Zhang, A. Fluerasu, and O. Chubar, "Towards the simulation of partially coherent x-ray scattering experiments," *AIP Conference Proceedings*, vol. 2054, no. 1, p. 060079, 2019.
23. B. Nash, O. Chubar, N. Goldring, D. L. Bruhwiler, P. Moeller, R. Nagler, and M. Rakitin, "Detailed x-ray brightness calculations in the sirepo GUI for SRW," *AIP Conference Proceedings*, vol. 2054, no. 1, p. 060080, 2019.
22. M. S. Rakitin, P. Moeller, R. Nagler, B. Nash, D. L. Bruhwiler, D. Smalyuk, M. Zhernenkov, and O. Chubar, "*Sirepo*: an open-source cloud-based software interface for X-ray source and optics simulations," *Journal of Synchrotron Radiation*, vol. 25, pp. 1877–1892, Nov 2018.
21. A. Blednykh, B. Bacha, G. Bassi, W. Cheng, O. Chubar, A. Derbenev, R. Lindberg, M. Rakitin, V. Smaluk, M. Zhernenkov, Y.-c. K. Chen-Wiegart, and L. Wiegart, "New aspects of longitudinal instabilities in electron storage rings *(DOE Science Highlight)*," *Scientific Reports*, vol. 8, no. 1, p. 11918, 2018.
20. O. Chubar, C. Kitegi, Y.-C. K. Chen-Wiegart, D. Hidas, Y. Hidaka, T. Tanabe, G. Williams, J. Thieme, T. Caswell, M. Rakitin, L. Wiegart, A. Fluerasu, L. Yang, S. Chodankar, and M. Zhernenkov, "Spectrum-Based Alignment of In-Vacuum Undulators in a Low-Emittance Storage Ring," *Synchrotron Radiation News*, vol. 31, no. 3, pp. 4–8, 2018.
19. M. Rakitin, A. A. Mirzoev, and D. A. Mirzaev, "First-Principles and Thermodynamic Simulation of Elastic Stress Effect on Energy of Hydrogen Dissolution in Alpha Iron," *Russian Physics Journal*, vol. 60, pp. 2136–2143, Apr 2018.
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.

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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.

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