

# Max Rakitin

Bio

## Personal details

Name: Max Rakitin (a.k.a. Maksim S. Rakitin)

Summary: I am a group leader of the Data Acquisition and Detectors group of the Data Science and Systems Integration Division of NSLS-II, BNL.

News: "Computer, Is My Experiment Finished?" (September 16, 2022)

<https://www.bnl.gov/newsroom/news.php?a=220832>

"Seeing the Forest Through the Trees: Brookhaven Lab Scientists Develop New Computational Approach to Reduce Noise in X-ray Data." (April 18, 2022)

<https://www.bnl.gov/newsroom/news.php?a=219533>

Links: [BNL](#) • [SBU](#) • [SUSU](#)

[@mrakitin](#) • [@mrakitin](#) • [Google Scholar](#) • [ResearchGate](#)

[ORCID: 0000-0003-3685-852X](#)

## 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** (<https://www.appliedtech.ru/en/>), 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 translocator (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, <https://uspex-team.org/en/uspex/tools>.
- **USPEX manual** — <https://uspex-team.org/en/uspex/documentation>.
- Utilities for DFT simulations
- IBM Mainframe software projects

## Publications

59. H. Wijesinghe, A. Barbour, L. Wiegart, Carlin, J. Einstein-Curtis, P. Moeller, R. Nagler, R. O'Rourke, N. Cook, and M. Rakitin, "Bluesky and Raydata: An Integrated Platform for Adaptive Experiment Orchestration," *IEEE (Accepted)*, 2024.
58. A. Tayal, D. S. Coburn, D. Abel, M. Rakitin, O. Ivashkevych, J. Wlodek, D. Wierzbicki, W. Xu, E. Nazaretski, E. Stavitski, and D. Leshchev, "5-Analyzer Johann Spectrometer for Hard X-ray Photon-in-Photon-out Spectroscopy at the Inner Shell Spectroscopy Beamline at NSLS-II: Design, Alignment, and Data Acquisition," *Journal of Synchrotron Radiation (Accepted Manuscript)*, 2024. <https://submission.iucr.org/status?Qname=Rakitin&Qcnor=ok5123&Submit+query=Submit+Query>
57. T. W. Morris, M. Rakitin, A. Islegen-Wojdyla, Y. Du, B. Nash, P. Moeller, W. H. Li, M. Fedurin, A. C. Giles, D. Leshchev, E. Stavitski, A. L. Walter, and B. Romasky, "A General Bayesian Algorithm for the Autonomous Alignment of Beamlines," *Journal of Synchrotron Radiation (Accepted Manuscript)*, 2024. <https://submission.iucr.org/status?Qname=Rakitin&Qcnor=gy5067&Submit+query=Submit+Query>
56. H. Goel, O. Chubar, R. Li, L. Wiegart, M. Rakitin, and A. Fluerasu, "Efficient end-to-end simulation of time-dependent coherent X-ray scattering experiments," *Journal of Synchrotron Radiation*, vol. 31, no. 3, pp. 517–526, May 2024. <https://doi.org/10.1107/S1600577524001267>
55. N. M. Cook, A. M. Barbour, E. G. Carlin, J. A. Einstein-Curtis, R. Nagler, R. O'Rourke, M. Rakitin, L. Wiegart, and H. Wijesinghe, "Integrating Online Analysis with Experiments to Improve X-Ray Light Source Operations," in *Proc. 19th Int. Conf. Accel. Large Exp. Phys. Control Syst. (ICALEPCS'23)*, ser. International Conference on Accelerator and Large Experimental Physics Control Systems, no. 19. JACoW Publishing, Geneva, Switzerland, 02 2024, paper TUSDSC02, pp. 921–924. <https://jacow.org/icalpcs2023/papers/tusdsc02.pdf>
54. J. A. Einstein-Curtis, D. T. Abell, Y. Du, A. Giles, M. V. Keilman, J. Lynch, P. Moeller, T. Morris, B. Nash, I. V. Pogorelov, M. Rakitin, and A. L. Walter, "Online Models for X-ray Beamlines Using Sirepo-Bluesky," in *Proc. 19th Int. Conf. Accel. Large Exp. Phys. Control Syst. (ICALEPCS'23)*, ser. International Conference on Accelerator and Large Experimental Physics Control Systems, no. 19. JACoW Publishing, Geneva, Switzerland, 02 2024, paper MO3BCO05, pp. 165–170. <https://jacow.org/icalpcs2023/papers/mo3bco05.pdf>
53. P. M. Maffettone, D. B. Allan, A. Barbour, T. A. Caswell, D. Gavrilov, M. D. Handwell, T. Morris, D. Olds, M. Rakitin, S. I. Campbell, and B. Ravel, *Methods and Applications of Autonomous Experimentation. Chapter 8: "Artificial Intelligence Driven Experiments at User Facilities"*, 1st ed. Chapman & Hall/CRC Computational Science, 2023, ch. Chapter 8. <https://doi.org/10.1201/9781003359593>
52. M. Rakitin, R. Bode, T. W. Morris, A. C. Giles, A. L. Walter, J. K. Lynch, J. Maldonado, Y. Du, B. Romasky, M. Fedurin, P. Moeller, and B. Nash, "Recent updates of the Sirepo-Bluesky library for virtual beamline representation," in *Advances in Computational Methods for X-Ray Optics VI*, O. Chubar and T. Tanaka, Eds., vol. 12697, International Society for Optics and Photonics. SPIE, 2023, p. 126970D. <https://doi.org/10.1117/12.2678030>
51. T. W. Morris, Y. Du, M. Fedurin, A. C. Giles, P. Moeller, B. Nash, M. Rakitin, B. Romasky, A. L. Walter, N. Wilson, and A. Wojdyla, "Latent Bayesian optimization for the autonomous alignment of synchrotron beamlines," in *Advances in Computational Methods for X-Ray Optics VI*, O. Chubar and T. Tanaka, Eds., vol. 12697, International Society for Optics and Photonics. SPIE, 2023, p. 126970B. <https://doi.org/10.1117/12.2677895>
50. B. Nash, M. S. Rakitin, D. T. Abell, M. Keilman, P. Moeller, I. Pogorelov, Y. Du, A. Giles, J. Lynch, T. W. Morris, A. L. Walter, and N. Goldring, "Reduced model representations of synchrotron radiation and a software framework for beamline control," in *Advances in Computational Methods for X-Ray Optics VI*, O. Chubar and T. Tanaka, Eds., vol. PC12697, International Society for Optics and Photonics. SPIE, 2023, p. PC1269703. <https://doi.org/10.1117/12.2676921>

49. L. Huang, T. Wang, O. Chubar, G. Dovillaire, A. He, M. Rakitin, Y. Yang, A. M. Kiss, and M. Idir, "Investigation of x-ray Hartmann wavefront sensing: from simulation to the initial experiment test," in *Advances in Computational Methods for X-Ray Optics VI*, O. Chubar and T. Tanaka, Eds., vol. PC12697, International Society for Optics and Photonics. SPIE, 2023, p. PC1269705. <https://doi.org/10.1117/12.2675754>
48. H. Goel, O. Chubar, L. Wiegart, A. Fluerasu, R. Li, A. He, M. Rakitin, M. Lin, P. Moeller, and R. Nagler, "GPU accelerated simulations of time-dependent coherent x-ray scattering experiments," in *Advances in Computational Methods for X-Ray Optics VI*, O. Chubar and T. Tanaka, Eds., vol. 12697, International Society for Optics and Photonics. SPIE, 2023, p. 1269709. <https://doi.org/10.1117/12.2677888>
47. N. Cook, E. Carlin, R. Nagler, R. O'Rourke, A. Barbour, M. Rakitin, and L. Wiegart, "An online analysis platform for improving x-ray light source operations," in *Proc. IPAC'23*, ser. IPAC'23 - 14th International Particle Accelerator Conference, no. 14. JACoW Publishing, Geneva, Switzerland, 05 2023, paper THPA128, pp. 4266–4268. <https://indico.jacow.org/event/41/contributions/2732>
46. M. Rakitin, S. Campbell, D. Allan, T. Caswell, D. Gavrilov, M. Hanwell, and S. Wilkins, "Next generation experimental data access at NSLS-II," *Journal of Physics: Conference Series*, vol. 2380, no. 1, p. 012100, Dec. 2022. <https://doi.org/10.1088/1742-6596/2380/1/012100>
45. B. Nash, D. Abell, R. Nagler, P. Moeller, M. Keilman, I. Pogorelov, N. Goldring, M. Rakitin, J. Lynch, A. Giles, A. Walter, J. Maldonado, T. Morris, S. Bak, and Y. Du, "Combining diagnostics, modeling, and control systems for automated alignment of the TES beamline," *Journal of Physics: Conference Series*, vol. 2380, no. 1, p. 012103, Dec. 2022. <https://doi.org/10.1088/1742-6596/2380/1/012103>
44. H. Goel, O. Chubar, L. Wiegart, A. Fluerasu, R. Li, A. He, M. Rakitin, P. Moeller, and R. Nagler, "Developments in SRW Code and Sirepo Framework Supporting Simulation of Time-Dependent Coherent X-ray Scattering Experiments," *Journal of Physics: Conference Series*, vol. 2380, no. 1, p. 012126, Dec. 2022. <https://doi.org/10.1088/1742-6596/2380/1/012126>
43. T. W. Morris, M. Rakitin, A. Giles, J. Lynch, A. L. Walter, B. Nash, D. Abell, P. Moeller, I. Pogorelov, and N. Goldring, "On-the-fly optimization of synchrotron beamlines using machine learning," in *Optical System Alignment, Tolerancing, and Verification XIV*, J. Sasián and R. N. Youngworth, Eds., vol. 12222, International Society for Optics and Photonics. SPIE, 2022, p. 122220M. <https://doi.org/10.1117/12.2644996>
42. L. Huang, T. Wang, O. Chubar, G. Dovillaire, A. He, M. Rakitin, and M. Idir, "Simulation of X-ray Hartmann wavefront sensing with the Synchrotron Radiation Workshop," *Opt. Express*, Oct. 2022. <https://doi.org/10.1364/oe.470197>
41. T. Konstantinova, L. Wiegart, M. Rakitin, A. M. DeGennaro, and A. M. Barbour, "Machine Learning for analysis of speckle dynamics: quantification and outlier detection," *Phys. Rev. Research*, vol. 4, p. 033228, Sep. 2022. <https://doi.org/10.1103/PhysRevResearch.4.033228>
40. D. Leshchev, M. Rakitin, B. Luvizotto, R. Kadyrov, B. Ravel, K. Attenkofer, and E. Stavitski, "The Inner Shell Spectroscopy beamline at NSLS-II: a facility for in situ and operando X-ray absorption spectroscopy for materials research," *Journal of Synchrotron Radiation*, vol. 29, no. 4, Jul. 2022. <https://doi.org/10.1107/S160057752200460X>
39. D. Hidas, A. M. Kiss, M. Rakitin, J. Sinsheimer, T. Tanabe, and M. Musardo, "High precision real-time insertion device and monochromator synchronization at NSLS-II," *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*, vol. 1031, p. 166505, Mar. 2022. <https://doi.org/10.1016/j.nima.2022.166505>
38. B. Nash, D. T. Abell, D. L. Bruhwiler, E. G. Carlin, Y. Du, J. P. Edelen, A. Giles, M. V. Keilman, J. Lynch, J. Maldonado, P. Moeller, R. Nagler, I. V. Pogorelov, M. S. Rakitin, A. Walter, and S. D. Webb, "X-Ray Beamline Control with Machine Learning and an Online Model," in *Proc. ICALEPCS'21*, ser. International Conference on Accelerator and Large Experimental Physics Control Systems, no. 18. JACoW Publishing, Geneva, Switzerland, Dec. 2021, pp. 695–699. <https://doi.org/10.18429/JACoW-ICALEPCS2021-WEPV024>
37. N. M. Cook, A. M. Barbour, E. G. Carlin, P. Moeller, R. Nagler, B. Nash, M. S. Rakitin, and L. Wiegart, "An Integrated Data Processing and Management Platform for X-Ray Light Source Operations," in *Proc. ICALEPCS'21*, ser. International Conference on Accelerator and Large Experimental Physics Control Systems, no. 18. JACoW Publishing, Geneva, Switzerland, Nov. 2021, pp. 1059–1063. <https://doi.org/10.18429/JACoW-ICALEPCS2021-FRBR02>
36. R. Jain, D. Abel, M. Rakitin, M. Sullivan, D. T. Lodowski, M. R. Chance, and E. R. Farquhar, "New high-throughput endstation to accelerate the experimental optimization pipeline for synchrotron X-ray footprinting," *Journal of Synchrotron Radiation*, vol. 28, no. 5, pp. 1321–1332, Sep. 2021. <https://doi.org/10.1107/S1600577521005026>
35. L. Yang, E. Lazo, J. Byrnes, S. Chodankar, S. Antonelli, and M. Rakitin, "Tools for supporting solution scattering during the COVID-19 pandemic," *Journal of Synchrotron Radiation*, vol. 28, no. 4, pp. 1237–1244, Jul. 2021. <https://doi.org/10.1107/S160057752100521X>
34. M. S. Rakitin and A. A. Mirzoev, "Ab initio Simulation of Dissolution Energy and Bond Energy of Hydrogen with 3sp, 3d, and 4d Impurities in bcc Iron," *Phys. Solid State*, vol. 63, no. 7, pp. 1065–1068, Jul. 2021. <https://doi.org/10.1134/S1063783421070180>

33. T. Konstantinova, L. Wiegart, M. Rakitin, A. M. DeGennaro, and A. M. Barbour, "Noise reduction in X-ray photon correlation spectroscopy with convolutional neural networks encoder-decoder models," *Sci Rep*, vol. 11, no. 1, Jul. 2021. <https://doi.org/10.1038/s41598-021-93747-y>
32. S. I. Campbell, D. B. Allan, A. M. Barbour, D. Olds, M. S. Rakitin, R. Smith, and S. B. Wilkins, "Outlook for artificial intelligence and machine learning at the NSLS-II," *Machine Learning: Science and Technology*, vol. 2, no. 1, p. 013001, Mar. 2021. <https://doi.org/10.1088/2632-2153/abbd4e>
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, International Society for Optics and Photonics. SPIE, Aug. 2020, pp. 119–127. <https://doi.org/10.1117/12.2568980>
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, International Society for Optics and Photonics. SPIE, Aug. 2020, pp. 201–208. <https://doi.org/10.1117/12.2568833>
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, International Society for Optics and Photonics. SPIE, Aug. 2020, pp. 78–87. <https://doi.org/10.1117/12.2567448>
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, International Society for Optics and Photonics. SPIE, Aug. 2020, pp. 209–226. <https://doi.org/10.1117/12.2569000>
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, International Society for Optics and Photonics. SPIE, 2019, pp. 79–92. <https://doi.org/10.1117/12.2530663>
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", " Jul. 2019. <https://www.osti.gov/biblio/1532614>
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. <https://doi.org/10.1080/08940886.2019.1608121>
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. <https://doi.org/10.1063/1.5084710>
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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, no. 6, pp. 1877–1892, Nov. 2018. <https://doi.org/10.1107/S1600577518010986>
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. <https://doi.org/10.1038/s41598-018-30306-y>
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. <https://doi.org/10.1080/08940886.2018.1460173>
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, no. 12, pp. 2136–2143, Apr. 2018. <https://doi.org/10.1007/s11182-018-1337-2>
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, 2017, p. 103880R. <https://doi.org/10.1117/12.2274031>
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, 2017, p. 1038811. <https://doi.org/10.1117/12.2274481>

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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*, ser. International Particle Accelerator Conference, no. 8. Geneva, Switzerland: JACoW, May 2017, paper TUPAB140, pp. 1663–1665. <https://doi.org/10.18429/JACoW-IPAC2017-TUPAB140>
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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. <https://doi.org/10.14529/met160405>
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. <https://doi.org/10.1016/j.jallcom.2016.04.281>
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