## Maksim S. Rakitin

## **Publications**

## **About**

Name: Maksim S. Rakitin

Summary: I am a computational scientist at NSLS-II, BNL. I help beamline staff and users run scientific experiments and perform data analysis. I write code in Python to integrate hardware (motors, cameras, detectors, etc.) and 3rd-party software systems with the Bluesky data acquisition framework. I am developing the Sirepo-Bluesky library that integrates Bluesky and the Sirepo browser-based interface to scientific modeling codes to enable access to "virtual" beamlines. I am a proponent of well-tested, modular, reusable, sustainable, and easily accessible code. I am fluent with modern CI systems (GitHub Actions, MS Azure Pipelines, etc.) I use Docker/Podman (including the creation of images), Linux (RHEL8, CentOS, Ubuntu, etc.), vagrant/VirtualBox on a daily basis. I am maintaining over 100 conda-forge feedstocks (Python, Python with C-extensions, C/C++, Fortran). I lead the continuous integration efforts to deploy and test the conda environments with the Bluesky software stack. I am enthusiastic about new technologies and AI/ML projects. I am a PI on an AI/ML LDRD project and a PI for two SBIR subcontracts with Radiasoft LLC (total funds of 1M+).

Links: OBNL • SBU • SUSU

○ 😱 @mrakitin • 🛅 @mrakitin • 🕿 Google Scholar • 💌 ResearchGate • 📵 ORCID

## **Publications**

- 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://link.aps.org/doi/10.1103/PhysRevResearch.4.033228
- 39. 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
- 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
- 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

Last updated:

- Experimental Physics Control Systems, no. 18. JACoW Publishing, Geneva, Switzerland, Dec. 2021, pp. 695–699. https://doi.org/10.18429/JACoW-ICALEPCS2021-WEPV024
- 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
- 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. 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
- 33. 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
- 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
- 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
- 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*

Last updated:

- 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
- 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
- D. Allan, T. Caswell, S. Campbell, and M. Rakitin, "Bluesky's Ahead: 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
- 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
- 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. https://doi.org/10.1063/1.5084711
- 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
- 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
- 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
- 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, 2017, p. 1038805. https://doi.org/10.1117/12.2274285
- 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, 2017, p. 103880N. https://doi.org/10.1117/12.2274403
- 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, 2017, p. 103880Z. https://doi.org/10.1117/12.2274264
- 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. https://doi.org/10.1039/C7CP00840F
- 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
- 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, ser. International Particle Accelerator Conference, no. 8. Geneva, Switzerland: JACoW, May 2017, paper WEPIK117, pp. 3224-3226. https://doi.org/10.18429/JACoW-IPAC2017-WEPIK117
- 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  $Al_x ln_{1-x} N$  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
- 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. https://doi.org/10.1038/srep22873
- 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. https://doi.org/10.1039/C5CP04010H
- 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 Universal Structure Predictor: Evolutionary Xtallography, 2013–2015. https://uspex-team.org/en/uspex/documentation
- 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. https://doi.org/10.1080/00268976.2011.645895
- 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. https://vestnik.susu.ru/mmph/issue/viewFile/46/22#page=114
- 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. https://vestnik.susu.ru/mmph/issue/viewFile/46/22#page=77
- 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. https://vestnik.susu.ru/metallurgy/issue/archive
- 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. https://vestnik.susu.ru/mmph/issue/viewFile/36/12#page=103