

Max Rakin

Bio

Personal details

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

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>

"EPICS Collaboration Meeting (workshop organizer)" (September 16–20, 2024)
<https://conference.sns.gov/event/448/timetable/?view=standard>

Links: [○ BNL](#) • [● mrakin.github.io](#) • [● SBU](#) • [● SUSU](#)
[○ @mrakin](#) • [● @mrakin](#) • [● 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
 Brookhaven National Laboratory

Computational Scientist (RS-3 → RS-5), Data Acquisition and Detectors Group (formerly Data Acquisition, Management, and Analysis (DAMA) Group), Data Science and Systems Integration (DSSI) Division, NSLS-II, Brookhaven National Laboratory, Upton, NY (<https://www.bnl.gov>)

- 2024.06–present: **Computational Scientist (RS-5), Group Leader**
- 2023.01–2024.06: **Computational Scientist (RS-5), Deputy Group Leader**
- 2021.03–2023.01: **Associate Computational Scientist (RS-4), Supervisor**
- 2019.10–2021.03: **Associate Computational Scientist**
- 2017.11–2019.09: **Assistant Computational Scientist**

2023.06–2024.05
 MAT3RA

Consultant, Exabyte Inc. (Mat3ra), Remote (<https://www.mat3ra.com>). Materials modeling platform.

2015.12–2017.10

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

2013.10–2015.12
 Stony Brook University

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>.
- **Blop** — a Bayesian optimization library for autonomous experiment control, <https://blueskyproject.io/blop>.
- **edrxs** — an open-source toolkit for resonant inelastic X-ray scattering simulations, <https://github.com/EDRIXS/edrxs>. Contributions: packaging, design of team refactoring, and testing of a new implementation based on **PETSc** and **SLEPc** at NERSC.
- **Synchrotron Radiation Workshop (SRW)** — computer code for X-ray source and optics simulations, <https://github.com/ochubar/SRW>.
- **Sirepo** — a cloud-based framework for SRW, <https://github.com/radiasoft/sirepo>.
- **Sirepo-Bluesky** — an interface library between the Bluesky data acquisition framework and the Sirepo simulation framework, <https://github.com/NSLS-II/sirepo-bluesky>.
- **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, <https://uspex-team.org/en/uspex/tools>.
- **USPEX manual** — <https://uspex-team.org/en/uspex/documentation>.
- Utilities for DFT simulations
- IBM Mainframe software projects

Selected Publications

8. H. Wijesinghe, A. Barbour, L. Wiegart, E. 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," in *SC24-W: Workshops of the International Conference for High Performance Computing, Networking, Storage and Analysis*, 2024, pp. 2162–2167. <https://doi.org/10.1109/SCW63240.2024.00271>
7. T. W. Morris, M. Rakitin, Y. Du, M. Fedurin, A. C. Giles, D. Leshchev, W. H. Li, B. Romasky, E. Stavitski, A. L. Walter, P. Moeller, B. Nash, and A. Islegen-Wojdyla, "A general Bayesian algorithm for the autonomous alignment of beamlines," *Journal of Synchrotron Radiation*, vol. 31, no. 6, pp. 1446–1456, Nov. 2024. <https://doi.org/10.1107/S1600577524008993>
6. 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>
5. 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>
4. 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>
3. 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>
2. 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>
1. 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. 26 283–26 288, 2015. <https://doi.org/10.1039/C5CP04010H>