

Max Rakitin

Publications

About

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>

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[○ @mrakitin](#) • [in @mrakitin](#) • [Google Scholar](#) • [ResearchGate](#)
[○ ORCID: 0000-0003-3685-852X](#)

Publications

62. Z. Lentz, R. Tang-Kong, M. Rakitin, T. Morris, and S. Miskovich, “ML-assisted beamline optimization at LCLS,” in *Proc. 20th Int. Conf. Accel. Large Exp. Phys. Control Syst. (ICALEPCS'25)*, ser. International Conference on Accelerator and Large Experimental Physics Control Systems, no. 20. JACoW Publishing, Geneva, Switzerland, Sep. 2025, paper FRAG001, pp. 1873–1877. <https://doi.org/10.18429/JACoW-ICALEPCS2025-FRAG001>
61. D. Gavrilov, T. Caswell, A. Sligar, and M. Rakitin, “Bluesky Queue Server for beamline control at NSLS-II,” in *Proc. 20th Int. Conf. Accel. Large Exp. Phys. Control Syst. (ICALEPCS'25)*, ser. International Conference on Accelerator and Large Experimental Physics Control Systems, no. 20. JACoW Publishing, Geneva, Switzerland, Sep. 2025, paper THPD053, pp. 1706–1710. <https://doi.org/10.18429/JACoW-ICALEPCS2025-THPD053>
60. Y. Hidaka, D. Allan, and M. Rakitin, “A new Python middle layer framework: Particle Accelerator Middle Layer (PAMILA),” in *Proc. 6th North American Particle Accel. Conf. (NAPAC2025)*, ser. North American Particle Accelerator Conference, no. 2025. JACoW Publishing, Geneva, Switzerland, Aug. 2025, paper MOP005, pp. 48–51. <https://doi.org/10.18429/JACoW-NAPAC2025-MOP005>
59. 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>

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, "Five-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*, vol. 31, no. 6, pp. 1609–1621, Nov. 2024. <https://doi.org/10.1107/S1600577524009342>
57. 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>
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, Feb. 2024, paper TUSDSC02, pp. 921–924. <https://doi.org/10.18429/JACoW-ICALEPCS2023-TUSDSC02>
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, Feb. 2024, paper MO3BCO05, pp. 165–170. <https://doi.org/10.18429/JACoW-ICALEPCS2023-MO3BCO05>
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, *Book "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, May 2023, paper THPA128, pp. 4266–4268. <https://doi.org/10.18429/JACoW-IPAC2023-THPA128>
 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. Rakin, 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. Rakin, 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. Rakin, 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. Rakin, 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. Rakin, 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. Rakin, 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. Rakin, 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. Rakin, "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. Rakin 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. Rakin, 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>
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>
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>
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, 2017, p. 103880S. <https://doi.org/10.1117/12.2274285>
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, 2017, p. 103880N. <https://doi.org/10.1117/12.2274403>

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, 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. 14 486–14 494, 2017. <https://doi.org/10.1039/C7CP00840F>
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>
11. 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 $\text{Al}_x\text{In}_{1-x}\text{N}$ 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>
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. <https://doi.org/10.1038/srep22873>
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. 26 283–26 288, 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 manual: 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>
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. <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>