

# Maksim S. Rakitin

## Publications

### Personal details

Full name: Maksim S. Rakitin

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

[ORCID](#) • [LinkedIn](#) • [Graduate](#) • [ResearchGate](#)

### Publications

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. 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* modeling of the dissolution energy and binding energy of hydrogen with 3sp-, 3d- 4d-impurities in bcc iron," *Solid State Physics*, vol. 63, no. 7, p. 830, Apr. 2021, Original Russian Text. <https://doi.org/10.21883/ftt.2021.07.51031.034>
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, 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, 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, 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, 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.
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. Zhernenkova, 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. Zhernenkova, 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. Zhernenkova, "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. 1038805. <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 ( $\text{Sn}_n\text{H}_m$ ) 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>