Maksim S. Rakitin

Bio

Personal details

Full name: Maksim S. Rakitin
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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 **Assistant 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 (http://stonybrook.edu, http://uspex.stonybrook.edu)

2007.06–2013.10 **QA Engineer, QA Team Leader**, *Applied Technologies Ltd.*, Chelyabinsk, Russia (http://www.appliedtech.ru), a partner of Rocket Software Inc., USA (http://www.rocketsoftware.com)

Software projects

- **Bluesky** — a library for experiment control and collection of scientific data and metadata, http://nsls-ii.github.io/bluesky.
- **Databroker** — a simple, user-friendly interface for retrieving stored data and metadata from multiple sources, http://nsls-ii.github.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 transfocator (compound refractive lenses (CRL) for X-ray focusing), https://github.com/mrakitin/bnlcrl.
- **USPEX** — a code for evolutionary crystal structure prediction, .
- **USPEX online utilities** — a set of pre- and post-processing tools for crystal structure simulations, http://han.ess.sunysb.edu.

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- **USPEX manual** — http://han.ess.sunysb.edu/uspex_manual.
- Utilities for DFT simulations
- IBM Mainframe software projects

Publications

19. M. S. Rakitin, P. Moeller, R. Nagler, D. L. Bruhwiler, D. Smalyuk, and O. Chubar, "Sirepo — software framework for X-ray source and optics simulations **(under preparation)**," *Journal of Synchrotron Radiation*, 2017.
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, p. 103880R, 2017.
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, p. 1038811, 2017.
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, p. 1038805, 2017.
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, p. 103880N, 2017.
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, p. 103880Z, 2017.
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.
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*, no. 8 in International Particle Accelerator Conference, (Geneva, Switzerland), pp. 1663–1665, JACoW, May 2017.
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*, no. 8 in International Particle Accelerator Conference, (Geneva, Switzerland), pp. 3224–3226, JACoW, May 2017.
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.
9. Y. H. R. Chang, T. L. Yoon, T. L. Lim, and M. Rakitin, "Thorough investigations of the structural and electronic properties of $Al_xIn_{1-x}N$ ternary compound via *ab initio* computations," *Journal of Alloys and Compounds*, vol. 682, pp. 338–344, 2016.
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.
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. 26283–26288, 2015.
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.
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.
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.
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.
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.
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.