

# Maksim S. Rakitin

## Publications

### Personal details

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### Publications

12. 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.
11. 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.*, pp. —, 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  $\text{Al}_x\text{In}_{1-x}\text{N}$  ternary compound via *ab initio* computations," *Journal of Alloys and Compounds*, vol. 682, pp. 338–344, 2016.
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.
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.

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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.