

Roman R. Kapaev

General information:

- birth date: 5 December 1995
- birth place: Kogalym, Russia

Education

- **2013-2017: Undergraduate Student (Chemistry), Higher Chemical College of the Russian Academy of Sciences.** Courses: Organic Chemistry, Polymer Chemistry, Analytical Chemistry, Inorganic Chemistry, Physical Chemistry, Environmental Science, Quantum Chemistry, Calculus
- **2011-2013: Moscow Chemical Lyceum.** Courses: Organic Chemistry, Inorganic Chemistry, Physical Chemistry, Biology, Physics, Mathematics, English
- **2007-2011: Moscow Gymnasium №1514.** Courses: Mathematics, Computer Science, Physics, Biology, English

Scientific experience

- **2013 - present:**

Kurnakov Institute of General and Inorganic Chemistry of the Russian Academy of Sciences (IGIC RAS)

Laboratory of Applied Materials Ionics

Advisor: Prof. Dr. Yaroslavtsev A. B.

Work description: Development of low cost, environmentally friendly and simple synthetic routes of LiFePO_4 , NaFePO_4 , $\text{Na}_3\text{V}_2(\text{PO}_4)_3$ based nanocomposites for lithium and sodium ion batteries and study of their physical, chemical and electrochemical properties.

Skills: various synthetic methods of nanoscale materials (sol-gel assisted, solvothermal, solid-state, etc.); interpretation of XRD patterns, impedance spectra, SEM micrographs; assembling and testing Li-ion electrochemical cells; basic knowledge of IR and Raman spectrometry.

- **2012 - present:**

Carbohydrate Structure Database (CSDB) project (<http://csdb.glycoscience.ru>)

Advisor: Assoc. Prof. Dr. Toukach P.V.

Work description: Development of advanced NMR simulation tools tuned for carbohydrates, including those containing phosphates, amino acids, alditols, and other non-

carbohydrate constituents: ^{13}C , ^1H 1D and ^1H - ^1H COSY/COSY RCT/COSY DQF, TOCSY, ^1H - ^{13}C HSQC, HMBC, HSQC-TOCSY, HSQC-COSY 2D NMR predictors. Development of a tool for automatic unravelling of carbohydrate structures basing on experimental NMR spectra and chromatography data.

Skills: interpretation of liquid-state NMR spectra; programming in PHP/MySQL; relational and graph databases; optimization algorithms (including evolutionary programming and particle swarm optimization).

Publications

a) Materials for energy storage

1. "Conductivity and electrochemical behavior of $\text{Li}_{1-x}\text{Fe}_{1-2x}(\text{M}^{\text{II}}\text{M}^{\text{III}})_x\text{PO}_4$ with olivine structure" R. Kapaev, S. Novikova, T. Kulova, A. Skundin, A. Yaroslavtsev, *J. Solid State Electrochem.* **2015**, 9, 2793-2801.
2. "Study of the Electrochemical Behavior of Lithium Iron Phosphate Doped by Chromium and Nickel" A. Chekannikov, R. Kapaev, S. Novikova, T. Kulova, A. Skundin, A. Yaroslavtsev, *ECS Trans.* **2014**, 63 (1), 57-60.
3. "Research of Lithium Iron Phosphate as Material of Positive Electrode of Lithium-Ion Battery" A.A. Chekannikov, R.R. Kapaev, S.A. Novikova, T.L. Kulova, A.M. Skundin, A.B. Yaroslavtsev, *Int. J. Electrochem. Sci.* **2016**, 11, 2219-2229.

b) Carbohydrate NMR simulation tools

4. "Simulation of 2D NMR Spectra of Carbohydrates Using GODESS Software", R.R. Kapaev, P.V. Toukach, *J. Chem. Inf. Model.* **2016**, 56 (6), 1100-1104.
5. "Improved Carbohydrate Structure Generalization Scheme for ^1H and ^{13}C NMR simulations" R.R. Kapaev, P.V. Toukach, *Anal. Chem.* **2015**, 87 (14), 7006-7010.
6. "Carbohydrate Structure Generalization Scheme for Database-Driven Simulation of Experimental Observables, Such as NMR Chemical Shifts" R.R. Kapaev, K.S. Egorova, P.V. Toukach, *J. Chem. Inf. Model.* **2014**, 54 (9), 2594-2611.

International conferences

1. "Carbohydrate structure generalization scheme for database-driven ^{13}C NMR simulation." (oral presentation) R. Kapaev, Ph. Toukach, *6th Baltic Meeting on Microbial Carbohydrates*, Gdansk, Poland, September 7-10, 2014.
2. "Study of the Electrochemical Behavior of Lithium Iron Phosphate Doped by Chromium and Nickel" (poster) A. Chekannikov, R. Kapaev, S. Novikova, T. Kulova, A. Skundin, A.

- Yaroslavtsev, *The 15th International Conference on Advanced Batteries, Accumulators and Fuel Cells*, Brno, Czech Republic, August 27-24, 2014.
3. “Conductivity of materials based on LiFePO_4 with olivine structure” (poster), Svetlana Novikova, Roman Kapaev, Vladimir Skopetc, Andrey Svitanko, Andrey Yaroslavtsev, *XII Meeting “Fundamental Problems of Solid State Ionics”*, Chernogolovka, Russia, July 3-5, 2014.
 4. a) “GODESS software: simulation of the ^{13}C , ^1H and 2D NMR spectra of carbohydrates” (oral presentation), R. Kapaev, Philip Toukach; b) “Carbohydrate Structure Database” (poster), K. S. Egorova, Roman R. Kapaev, Y. A. Knirel, Ph. V. Toukach, *18th European Carbohydrate Symposium (Eurocarb18)*, Moscow, Russia, August 2-6, 2015.
 5. a) “Lithium iron phosphate doped by vanadium or manganese as cathodes for rechargeable Li-ion batteries” (poster), R. Kapaev, S. Novikova, A. Chekannikov, T. Kulova, A. Skundin, A. Yaroslavtsev; b) “Maricite NaFePO_4 synthesized via the Pechini process for sodium-ion batteries” (poster), R. Kapaev, S. Novikova, A. Chekannikov, T. Kulova, A. Skundin, A. Yaroslavtsev, *4th International Symposium on Surface Imaging/Spectroscopy at the Solid/Liquid Interface (ISSIS 2015)*, September 2-4, 2015.
 6. a) “Low temperature synthesis of maricite sodium iron phosphate for sodium-ion batteries” (poster), Kapaev R.R., Novikova S.A., Chekannikov A.A., Kulova T.L., Skundin A.M., Yaroslavtsev A.B.; b) “Vanadium doped LiFePO_4 as a cathode material for lithium-ion battery” (poster), Kapaev R., Novikova S., Yaroslavtsev A., Kulova T., Skundin A., Chekannikov A., *10th International Frumkin Symposium on Electrochemistry*, October 20-23, 2015.
 7. a) “Conducting and electrochemical properties of LiFePO_4 -based cathode materials” (oral presentation), Novikova S.A., Kapaev R.R., Chekannikov A.A., Gryzlov D.Y., Kulova T.L., Skundin A.M., Yaroslavtsev A.B.; b) “Activated maricite NaFePO_4 for cathode materials of sodium-ion batteries” (poster), Kapaev R.R., Novikova S.A., Chekannikov A.A., Gryzlov D.Y., Kulova T.L., Skundin A.M., Yaroslavtsev A.B.; c) “Sodium iron phosphate as a positive electrode material for sodium-ion batteries” (poster), Chekannikov A.A., Kapaev R.R., Novikova S.A., Gryzlov D.Y., Kulova T.L., Skundin A.M., Yaroslavtsev A.B., *XIII Meeting “Fundamental Problems of Solid State Ionics”*, Chernogolovka, Russia, June 27- July 1, 2016.

Grant list

1. Russian Foundation for Basic Research (RFBR) grant N15-04-01065, 2015-2017 (executor)
2. Russian Science Foundation (RSF), grant 14-13-01388, 2014-2016 (executor)
3. Russian Science Foundation (RSF), grant 16-13-00024, 2016 (executor)

Olympiads and challenges

1. Diplomas (II, III degrees) for successful participation in Moscow Chemical Olympiad for high school students (2010, 2011, 2012, 2013)
2. Diploma (II degree) for successful participation in All-Russian Olympiad “*Pokory Vorobyevy Gory!*” organized by Moscow State University, Chemical Section (2013)
3. Commendation award of the "3rd Singapore International Mathematics Challenge" (2012)

Other experience

a) IT experience

- Experience in web programming: PHP/MySQL/HTML5/CSS3 (Bootstrap)/JavaScript (jQuery). My personal website is <http://rkapaev.ru>
- Basic knowledge of C/C++; graph databases (Neo4j); programming under Linux environment; Pascal/Delphi.
- I am familiar to Microsoft Word, Excel and Powerpoint, CorelDRAW, Adobe Illustrator, Adobe Photoshop and ChemDraw/Chem3D programs.

b) Volunteering

- International Student Science Fair 2014 in Moscow, Russia (coordinating international students)