

Schedule

16-th International School-Conference, «Magnetic Resonance and its Applications. Spinus-2019»

March 31 - April 05, 2019

St. Petersburg



SUNDAY - 31 March 2019	
14:00 - 15:30	LUNCH
15:30 - 19:00	REGISTRATION OF PARTICIPANTS
19:00 -	WELCOME PARTY « <i>EVENING IN KARELIA</i> »
MONDAY - 01 April 2019	
08:45 - 10:00	BREAKFAST
10:00 - 10:30	Registration
10:30 - 10:40	Opening

10:40 – 11:10	Vladimir I. Chizhik (Saint-Petersburg, Russia) Lecture: Possibilities, Peculiarities and Areas of Applications of Quantitative Analysis by NMR in Magnetic Field of the Earth
11:10 – 11:30	GROUP PHOTO
11:30 – 12:00	COFFEE BREAK
12:00 – 12:40	Alexei Privalov (Darmstadt Germany) Lecture: Fluorine dynamics in nanosized superionic conductors as seen by NMR diffusometry
12:40 – 12:55	Sarah Schneider (Darmstadt, Germany) Oral report: Ion and Molecule Transport in Aqueous Salt Solutions in Bulk and in Nanopores - a NMR study
12:55 – 13:10	Benjamin Kresse (Darmstadt, Germany) Oral report: Spatially Resolved NMR with Micrometer Resolution in Static Field Gradients
13:10 – 13:25	Melanie Pia Reuhl (Darmstadt, Germany) Oral report: Broadband Dielectric and Nuclear Magnetic Resonance Spectroscopy Study on Dynamics of Water DMSO Mixtures, Glycerol, and Ethylene Glycol in Mesoporous Silica
13:25 – 13:40	Irina Lushpinskaya (Saint-Petersburg, Russia) Oral report: Multinuclear NMR study of hybrid organic-inorganic composites: layer perovskite-like oxides $H_2La_2Ti_3O_{10}$ with methanol, methylamine and butylamine molecules
13:40 – 14:00	Alexey Soloninin (Ekaterinburg, Russia) Oral report: Atomic Motion in the Bimetallic Borohydrides $LiLa(BH_4)_3X$ X=Cl, Br, I: NMR Study
14:00 – 15:30	LUNCH
15:30 – 16:10	Elena Charnaya (Saint-Petersburg, Russia) Lecture: NMR studies of bulk and nanostructured ferroelectrics
16:10– 16:30	Alexander Pavlov (Moscow, Russia) Oral report: NMR Spectroscopy of Paramagnetic Transition Metal Complexes: Theory and Application Examples
16:30– 16:45	Yanina Pankratova (Moscow, Russia) Oral report: Application of Paramagnetic NMR to the Magnetic Properties Investigation of Cobalt(II) Pseudotetrahedral Single-Molecule Magnet
16:45– 17:00	Erkki Lahderanta (Lappeenranta, Finland) Oral report: Masters Degree Programme in Lappeenranta
17:00 – 17:30	COFFEE BREAK
17:30 – 17:45	Manuel Becher (Darmstadt, Germany) Oral report: Dynamics of Room Temperature Ionic Liquids: Structural Relaxation Probed by 1H and ^{19}F NMR
17:45 – 18:05	Tatiana Kulagina (Chernogolovka, Russia) Oral report: Evolution of polarization of three spin groups and their contribution to line shape and solid-echo NMR
18:05 – 18:25	Rameev (Gebze, Turkey) 1H NMR relaxation times of alcohol-water mixtures

18:25 – 18:40	Maria Ivanova (Yoshkar-Ola, Russia) Oral report: Development of a technique for determination of total fat content in food products by NMR-relaxation
18:40 – 19:00	Leonid Grunin (Yoshkar-Ola, Russia) Oral report: Up-to-Date Industrial Applications of Time-Domain NMR
19:05 – 20:00	DINNER
20:00 –	CULTURAL AND SPORTING ACTIVITIES
	TUESDAY – 02 April 2019
08:45 – 09:45	BREAKFAST
10:00 – 10:40	Petr Tolstoy (Saint-Petersburg, Russia) Lecture: How to estimate hydrogen bond energies from NMR spectra
10:40 – 11:00	Vadim Zorin (Santiago de Compostela, Spain) Oral report: StereoFitter and 3D Computer-Assisted Structure Elucidation
11:00 – 11:15	Jarno Järvinen (Turku, Finland) Oral report: Dynamic Nuclear Polarization of Doped Silicon at High Fields and Low Temperatures
11:15 – 11:30	Valeriia Baranauskaite (Saint-Petersburg, Russia) Oral report: Dynamical Characteristics of the Ternary Systems (Chlorides of Li, Mg, and Cs) in Wide Temperature and Concentration Ranges by NMR Method.
11:30 – 12:00	COFFEE BREAK
12:00 – 12:40	Jacques Friassard (Paris, France) Lecture: Xe NMR Technique: Various Applications
12:40 – 13:20	Thomas Meersmann (Nottingham, United Kingdom) Lecture: Hyperpolarized (hp) ^{83}Kr and hp ^{129}Xe as MRI Contrast Agents
13:20 – 13:40	Ago Samoson (Tallinn, Estonia) Oral report: H-MAS
13:40 – 14:00	Sergey Dvinskikh (Stockholm, Sweden) Oral report: Multinuclear Dipolar NMR Spectroscopy in Ionic Liquid Crystals
14:00 – 15:30	LUNCH
15:30 – 15:45	Ramadan Atta (Damietta, Egypt) Oral report: Preparation and Pervaporation Performance of Polyphenylene Isophthalamide Membranes Modified by Fullerene Derivatives
15:45–17:00	Oral blitz reports of young scientists (5min × 15); see speakers below in the list of POSTER SESSION I
17:00 – 17:30	COFFEE BREAK

17:30 – 19:00	POSTER SESSION I
19:00 – 20:00	DINNER
20:00 –	CULTURAL AND SPORTING ACTIVITIES
	WEDNESDAY – 03 April 2019
08:45 – 09:45	BREAKFAST
	EXCURSION DAY
19:00 – 20:00	DINNER
20:00 –	
	THURSDAY – 04 April 2019
08:45 – 09:45	BREAKFAST
10:00 – 10:40	C. Cabal Mirabal (Havana, Cuba) Lecture: MRI Synopsis of the Physical and Hardware bases.
10:40 – 11:00	Guzel Musabirova (Kazan, Russia) Oral report: Interaction of Statins with Cell Membrane by NMR Spectroscopy
11:00 – 11:15	Manuel Arsenio Lores Guevara (Santiago de Cuba, Cuba) Oral report: Evaluation of Protein Viscosity in Sickle Cell Disease
11:15 – 11:30	Manuel Arsenio Lores Guevara (Santiago de Cuba, Cuba) Oral report: NMRD study of the Bound water rotational correlation time in protein solutions
11:30 – 12:00	COFFEE BREAK
12:00 – 12:40	Uwe Eichhoff (Rheinstetten, Germany) Lecture: The human brain: development and aging explored by MRI.
12:40 – 12:55	Sergey Efimov (Kazan, Russia) Oral report: Various NMR Approaches in Studies of Polypeptides: Application to Insulins and Cyclosporins
12:55 – 13:35	Nikolai R. Skrynnikov (West Lafayette, USA) Lecture: When Molecular Dynamics met NMR (and various other experimental methods)
13:35 – 14:00	Andrei Komolkin (Saint-Petersburg, Russia) Oral report: Visualization of the DNA Environment from the Molecular Dynamics Simulation
14:00 – 15:30	LUNCH
15:30 – 15:50	Lidia Konopleva (Kazan, Russia) Oral report: Optimization of based on DW MRI fiber tracking results. Simulated phantom results

15:50 – 17:00	Oral blitz reports of young scientists (5min × 14); see speakers below in the list of POSTER SESSION II
17:00 – 17:30	COFFEE BREAK
17:30 – 19:00	POSTER SESSION II
20:00 –	CONFERENCE DINNER
	FRIDAY – 05 April 2019
09:10 – 10:30	BREAKFAST
10:30 – 11:00	Vladimir Matveev (Saint-Petersburg, Russia) Lecture: Comparison of Ionic Liquids and Highly Concentrated Electrolyte Solutions: Similarity and Differences in Structure and in Dynamics
11:00 – 11:15	Sergei Bystrov (Saint-Petersburg, Russia) Oral report: Molecular Mobility in a Set of Imidazolium-based Ionic Liquids
11:15– 11:30	Alexandr Khrapichev (Oxford, United Kingdom) Oral report: LiverMultiScan – a diagnostic aid for liver disease
11:30 – 12:00	COFFEE BREAK
12:00 – 12:40	Dieter Michel (Leipzig, Germany) Lecture: EPR and NMR Study of Nitric Oxide - an Interesting Molecule for Bio-Medical Applications
12:40 – 13:20	Anna Semisalova (Dresden, Germany) Lecture: From ESR to FMR – a Powerful Tool to Investigate Novel Ferromagnets, Illustrated with the Study of Tunable Magnetic Properties of Thin Metallic FeRh Films
13:20 – 13:35	Daria Shurtakova (Kazan, Russia) Oral report: Study of Calcium Phosphate by EPR Methods
13:35– 13:50	Dahiana Avila (Jena, Germany) Oral report: Mechanism of Hydrolysis of Cobalt Oxide-Doped Bioactive Phosphate Glasses: P-31 MAS NMR, P-31 NMR and ESR
13:50– 14:05	Yuriy Neronov (Saint-Petersburg, Russia) Registration of NMR Signals in Magnetic Fields of 0.13 and 2.1 T for Estimation of the Age-Related Changes in Living Tissues
14:05– 15:30	LUNCH
15:30 – 16:10	Yury Bunkov (Kazan, Russia) Lecture: Spin Superfluidity at room temperature
16:10– 16:30	Galina Kupriyanova (Kaliningrad, Russia) Oral report: ¹⁴ N NQR relaxation in 5 Aminotetrazole

16:30- 17:10	Georgy Mozzhukhin (Gebze, Turkey) Lecture: Low field ^{14}N NMR as a tool for estimation of quadrupole coupling constants and correlation times in liquids
17:10 - 17:30	COFFEE BREAK
17:30 - 18:00	AWARDING CLOSING
19:00 - 20:00	DINNER
	SATURDAY - 06 April 2019
08:45 - 09:45	BREAKFAST
	DEPARTURE

POSTER SESSION I (Tuesday, 17:30 - 19:00)

1	Vladimir Petrov	Isotopic shift of Xe nuclei precession frequencies caused by spatial inhomogeneity of optically oriented alkali atoms.
2	Milosh Ubovich	Conformational dynamics of the two-domain Pax5 protein in aqueous solution. A molecular dynamics simulation study.
3	Alina Pichugina	Electron spin resonance in the study of association processes of gallstones
4	Viacheslav Frolov	Zonal harmonics calculation to compensate a magnetic field heterogeneity in a magnet gap
5	Dmitrii Bogdanov	EPR study of copper complexes in mordenite channels
6	Polina Kobchikova	Studying of Cyclosporin D by High Resolution NMR: Obtaining Information on the Spatial Structure
7	Irina Avilova	Interaction of fullerene derivative with biomembranes - studied by pulsed field gradient NMR technique
8	Mariia Dmitrenko	Development and study of novel pervaporation membranes based on polyphenylene isophthalamide, modified by Pluronic F127
9	Thai Ly	Single Pulse NQR for Broad Resonance Lines
10	Ksenia Kass	The study of ionic liquids using NMR.
11	Elena Razina	EPR of Calixarenes Doped by Lu, La, Tb, Gd, Yb, Er, Dy Ions
12	Markus Rosenstihl	DAMARIS - An open source NMR instrumentation software
13	Verena Fella	Crystallisation and Dynamics of Water Confined to Mesoporous Silica
14	Edda Klotz	NMR studies on ion dynamics in solid electrolytes for Li-ion batteries
15	Siqi Wang	Synthesis and NMR study of adducts of ninhydrin-derived azomethine ylide with cyclopropenes.
16	Armando Consiglio	Computer Simulations of PEDOT:PSS/solid interface
17	Anton Ryzhkov	Analyzing the parameters of atom-atom interactions for Molecular dynamics simulations of micelle formation.
18	Alexander Selivanov	NMR Relaxation in ionic liquid Bmim-AC, comparison

		on different frequency
19	Alexandra Slivka	NMR characterization of structure of cyclosporin B
20	Shaza Darwish	Behavior of cyclosporine C in solvents of different polarity
21	Irina Golubeva	Solid-echo signal in a three-spin system with arbitrary dipole-dipole interaction constants
22	Natalya Uskova	NMR studies of nanocomposite based on the organic ferroelectric DIPAB
23	Anna Kuzminova	Development and investigation of mixed-matrix membranes based on PVA modified by various organic nanoparticles
24	Elena Galitskaya	NMR STUDIES OF VARIOUS PERFLUOROSULFONATED MEMBRANES IN WIDE TEMPERATURE RANGE
25	Elena Uskova	NMR method for assessing the inhibitory properties of drilling fluids
26	Nadezhda Antonova	Computer simulation of micelle formation in magnesium hexanoate solution
27	Roman Haponchik	Investigation of the nonlinear frequency shift of a ferromagnetic film resonator
28	Nikolay Kuznetsov	Investigation of a nonlinear phase shifter based on spin waves
29	Magomed Khasanov	Temperature dependences of NMR spectra of ionic liquid EAN with addition of inorganic nitrates
30	Julia Popova Anna Faleva	Application of solid-state NMR to the study of water sorption with hydrolysis lignin
31	Ozgul Karatas	Textured growth of magnetic nanoparticles in implanted TiO ₂ and ZnO single crystals as revealed by FMR
32	Ilgiz Abdullin	Progressive saturation technique in ultralow field

POSTER SESSION II (Thursday, 17:30 - 19:00)

1	Veronika Mamontova	Micelle formation of azobenzene-containing surfactant: investigation by molecular dynamics method
2	Pavel Kupriyanov	Influence of fast fluctuation of Earth magnetic field on NMR-spectra
3	Nina Djapic	Free colours tetrapyrroles: yellow
4	Igor Kiselev	Magnetic resonance study of the peculiarities of the paramagnetic-ferromagnetic transition in manganites on the example of $\text{La}_{0.78}\text{Ca}_{0.22}\text{MnO}_3$
5	Anastasia Kozlenko	Study of a new salt spiropyran structure containing carbomethoxy group in the 6'-position of 2H-chromene moiety
6	Konstantin Smolyarov	Investigation of Re-Pt vinylidene complex $\text{Cp}(\text{CO})_2\text{RePt}(\mu\text{-C=CHPh})(\text{PPh}_3)_2$ by solid-state NMR
7	Anastasia Nikitina	Simulation and optimization of pulse RF sequences for contrast enhancement of MR images in the presence of magnetic nanoparticles
8	Olga Bavrina	Hydrogen solubility and diffusion in V-Pd substitution alloys studied by DFT
9	Dmitry Aleshin	Spin state of 2,6-di(pyrazol-3-yl)pyridine complexes of iron(II) and cobalt(II) in solution by paramagnetic NMR method
10	Aleksandra Efimova	MRI study of magnetic field distortions generated by cellulose microbeads labelled with iron oxide nanoparticles in phantom samples
11	Oleg Shavykin	Computer simulation of orientational dynamics in alpha- and epsilon-lysine peptides
12	Alina Pichugina	Analysis of the kernels of the Yuzhno-Cheremshansky field by the method of electron spin resonance
13	Ekaterina Krylova	Multinuclear NMR for structural study of lamellar mordenite and ZSM-5 zeolites
14	Alexander Dmitriev	Two-quantum optically detected resonances in NV centers in diamond in zero magnetic field.
15	Roman Lozov	On the realization of the extremely small value of a TFC at the frequency 6.834 GHz of atomic magnetic resonance in quantum frequency standards on ^{87}Rb -absorption cells containing two anti-relaxation components (coating + inert gas)
16	Oleg Shavykin	Molecular dynamics simulation of global and local dynamics in dendrigraft of second generation
17	Emil Fatullaev	Interaction of dendrigraft of second generation with molecules of LVFFAE peptide. Molecular dynamics simulation
18	Sofia Mikhtaniuk	Investigation of complex of lysine dendrimer of 2nd generation with 8 molecules of therapeutic vezugen peptide by computer simulation
19	Alexey Ostras	Phosphine Oxides as Probes In Study of Halogen Bonds: Quantum Chemistry Approach

20	Maria Egorova	Fluctuations of local electric fields at Li ⁺ , Cl ⁻ , and NO ₃ ⁻ ions in aqueous solution studied by Car-Parrinello molecular dynamics simulations
21	Anastasia Nam	Partitioning of solutes between micelles and water studied by diffusion NMR and micellar liquid chromatography
22	Radik Zaynullin	NMR and EPR in mechanochemically synthesized chalcopyrite nanocrystals
23	Vladislav Konovalov	Microstructure and dynamics of ions in mixtures of imidazolium-based ionic liquids with water. A molecular dynamics simulation study.
24	Stanislav Garkavyi	Nuclear spin-lattice relaxation ⁶³ Cu in semiconductor compound CuAlO ₂
25	Pavel Simeshchenko	Multiparameter MRI protocol for evaluating the results of surgical treatment of brain gliomas
26	Rustem Khusnutdinov	Spin-Lattice Relaxation of nuclear spins in magnetic semiconductor CuFeS ₂
27	Viacheslav Ivanov	Adjustable tuning range RF-coil for heteronuclear MRI
28	Naira Khusnutdinova	Modeling of dynamics and calculation of relaxation parameters for monomer of bovine insulin
29	Vladislav Salikov	Protein unfolding (denaturation) as monitored by PFG NMR measurements of translational diffusion
30	Sergey Shubin	Experimental results of an impact of the spin echo pulse sequence on a J-coupled two-spin system
31	Vladislav Panov	MRI projection technique in low magnetic field
32	Anastasia Sklyarova	Influence of morphology on the magnetic behavior in nano-EuFeO ₃ : NMR study