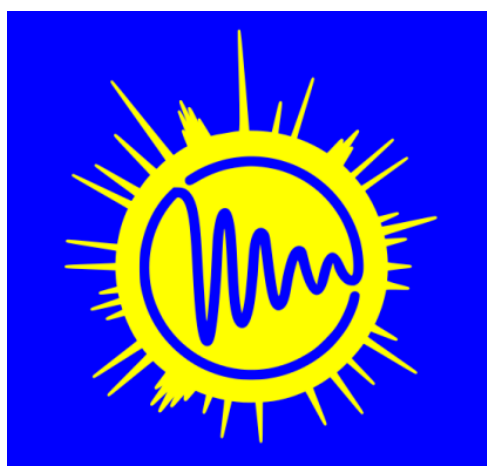


# Schedule

## 15-th International School-Conference, «Magnetic Resonance and its Applications. Spinus-2018»

01 - 06 April, 2018

St. Petersburg



SUNDAY - 01 April 2018	
14:00 - 15:30	LUNCH
15:30 - 19:00	REGISTRATION OF PARTICIPANTS
19:00 -	WELCOME PARTY «EVENING IN KARELIA»
MONDAY - 02 April 2018	
08:45 - 10:00	BREAKFAST
10:00 - 10:30	Registration

<b>10:30 - 10:40</b>	<b>Opening</b>
<b>10:40 - 11:10</b>	<b>Vladimir I. Chizhik (St. Petersburg, Russia)</b> <b>Lecture:</b> Some Problems of Quantitative Analysis by NMR Method
<b>11:10 - 11:30</b>	<b>GROUP PHOTO</b>
<b>11:30 - 12:00</b>	<b>COFFEE BREAK</b>
<b>12:00 - 12:40</b>	<b>Georgios Papavassiliou (Athens, Greece)</b> <b>Lecture:</b> Freezing Polarons and the Quantum Liquid-Crystal Phase in Ferromagnetic Metallic Manganites. A combined NMR and HRTEM study in the temperature range 3.2K to 1000K
<b>12:40 - 13:20</b>	<b>Luis Miguel Varela (Santiago de Compostela, Spain)</b> Lecture: Computer simulation of ionic liquids
<b>13:20 - 14:00</b>	<b>Sergey V. Dvinskikh (Stockholm, Sweden)</b> <b>Lecture:</b> Strategies for measuring <sup>13</sup> C- <sup>15</sup> N dipole-dipole couplings in liquid crystalline samples with natural isotropic abundance
<b>14:00 - 15:30</b>	<b>LUNCH</b>
<b>15:30 - 15:45</b>	<b>Sergei S. Bystrov (St. Petersburg, Russia)</b> Influence of residual water on NMR-relaxation in ionic liquids on basis of [bmim] <sup>+</sup> cation
<b>15:45- 16:00</b>	<b>Valeriia E. Barauskaite (St. Petersburg, Russia)</b> NMR studies of the 'water-in-salt' ternary LiCl-CsCl-D <sub>2</sub> O system
<b>16:00- 16:15</b>	<b>Ekaterina I. Shuvarakova (Novosibirsk, Russia)</b> EPR study of electron-acceptor sites during dehydrochlorination of 1-chlorobutane over metal oxides
<b>16:15- 16:30</b>	<b>Gleb Dolgorukov (Kazan, Russia)</b> Atomic-scale probing of paramagnetic centers in nanodiamonds by <sup>3</sup> He NMR at low temperature
<b>16:30- 16:45</b>	<b>Sultonazar Mamadazizov (Kaliningrad, Russia)</b> Multiexponential distribution of <sup>14</sup> N NQR relaxation times in tetrazole derivatives
<b>16:45- 17:05</b>	<b>Vadim Zorin (Santiago de Compostela, Spain)</b> Global Spectrum Deconvolution and its applications in NMR spectroscopy
<b>17:05 - 17:30</b>	<b>COFFEE BREAK</b>
<b>17:30 - 17:45</b>	<b>Sergei A. Izmailov (St. Petersburg, Russia)</b> EPR spectra simulation from MD data using Redfield theory and direct propagation method
<b>17:45 - 18:00</b>	<b>Sevastyan O. Rabdano (St. Petersburg, Russia)</b> Dynamic modes in spin-labeled protein revealed by MD simulations: experimental and computed EPR spectra

<b>18:00 - 18:20</b>	<b>Anna S. Semisalova (Dresden, Germany)</b> Ferromagnetic resonance study of FeRh thin films near the antiferromagnetic-ferromagnetic phase transition
<b>18:20 - 18:40</b>	<b>Leonid Y. Grunin (Yoshkar-Ola, Russia)</b> Fast Technique for Crystallinity Estimation of Solids by the Transverse Magnetization and Double Quantum Relaxation
<b>18:40- 19:00</b>	<b>Vadim V. Kachala (Moscow, Russia)</b> How to optimize NMR approach for structure elucidation of small molecules on Bruker spectrometers
<b>19:00 - 20:00</b>	<b>DINNER</b>
<b>20:00 -</b>	<b>CULTURAL AND SPORTING ACTIVITIES</b>
	<b>TUESDAY - 03 April 2018</b>
<b>08:45 - 09:45</b>	<b>BREAKFAST</b>
<b>10:00 - 10:40</b>	<b>Franz Fujara (Darmstadt, Germany)</b> Lecture: 1H NMR at Larmor frequencies down to 3 Hz by means of Field-Cycling
<b>10:40 - 11:00</b>	<b>Alexei F. Privalov (Darmstadt, Germany)</b> Fast Field cycling as a tool for studying molecular dynamics in solids
<b>11:00 - 11:15</b>	<b>Vyacheslav A. Chertkov (Moscow, Russia)</b> Vibration effects in NMR spectroscopy for studies of ultra fast conformational dynamics
<b>11:15 - 11:30</b>	<b>Vyacheslav A. Ryzhov (St. Petersburg, Russia)</b> Magnetic phase separation and its temperature evolution in porous carbon-based nanomaterials doped by Au and Co
<b>11:30 - 12:00</b>	<b>COFFEE BREAK</b>
<b>12:00 - 12:40</b>	<b>Jacques Fraissard (Paris, France)</b> <b>Lecture:</b> NMR studies of metal particles
<b>12:40 - 13:20</b>	<b>Dieter Michel (Leipzig, Germany)</b> <b>Lecture:</b> Solid State NMR in nanosized systems: MAS NMR studies in combination with pulsed field gradient techniques
<b>13:20 - 14:00</b>	<b>Bulat Rameev (Gebze, Turkey)</b> <b>Lecture:</b> Combination of Microwave & NMR Techniques for Effective Detection of Dangerous Materials
<b>14:00 - 15:30</b>	<b>LUNCH</b>
<b>15:30 - 16:40</b>	Oral blitz reports of young scientists (5min x 14); see speakers below in the list of <b>POSTER SESSION I</b>

<b>16:40-17:00</b>	<b>Erkki Lahderanta (Lappeenranta, Finland)</b> Masters Degree Programme in Lappeenranta
<b>17:00 - 17:30</b>	<b>COFFEE BREAK</b>
<b>17:30 - 19:00</b>	<b>POSTER SESSION I</b>
<b>19:00 - 20:00</b>	<b>DINNER</b>
<b>20:00 -</b>	<b>CULTURAL AND SPORTING ACTIVITIES</b>
	<b>WEDNESDAY - 04 April 2018</b>
<b>08:45 - 09:45</b>	<b>BREAKFAST</b>
	<b>EXCURSION DAY</b>
<b>19:00 - 20:00</b>	<b>DINNER</b>
<b>20:00 -</b>	<b>Round table: "PROBLEM BOOKS ON NMR SPECTROSCOPY"</b> <b>Chairman: Nickolai M. Sergeev (Moscow, Russia)</b>
	<b>THURSDAY - 05 April 2018</b>
<b>08:45 - 09:45</b>	<b>BREAKFAST</b>
<b>10:00 - 10:40</b>	<b>C. Cabal Mirabal (Havana, Cuba)</b> <b>Lecture:</b> MRI basics and application
<b>10:40 - 10:55</b>	<b>Alexandra Svyatova (Novosibirsk, Russia)</b> In situ NMR/MRI of Hyperpolarized Molecules
<b>10:55 - 11:10</b>	<b>Anna Mikhailovskaya (St. Petersburg, Russia)</b> An inductively-coupled volumetric resonator based on wire metamaterials for local sensitivity enhancement on a 3 T MRI system
<b>11:10 - 11:30</b>	<b>Andrey A. Drozdov (St. Petersburg, Russia)</b> Evaluation the delayed contrast enhancement as a tool for the differential diagnostics between brain metastases and neurotoxoplasmosis
<b>11:30 - 12:00</b>	<b>COFFEE BREAK</b>
<b>12:00 - 12:20</b>	<b>Corentin Schepkens (Mons, Belgium)</b> In vitro and in vivo applications of <sup>1</sup> H-NMR spectroscopy in the biological field
<b>12:20 - 12:40</b>	<b>Matthieu Dallons (Mons, Belgium)</b> Study of the metabolic doxorubicine-induced alterations in H9C2 cells and the effect of preincubation with dexrazoxane, a cardioprotective agent
<b>12:40 - 13:00</b>	<b>Kaliaperumal Kumaravel (Guangzhou, China)</b> Isolation and Characterization of Bioactive Secondary Metabolites from the Deep Sea Derived Fungi <i>Penicillium</i> sp.

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<b>13:00 - 13:40</b>	<b>Nikolai R. Skrynnikov (West Lafayette, USA)</b> <b>Lecture:</b> Many faces of disulfide bond
<b>13:40 - 14:00</b>	<b>Boris Kharkov (St. Petersburg, Russia)</b> Skin-Effect Compensated Optimal Control Pulses for Excitation in a Conductive Medium
<b>14:00 - 15:30</b>	<b>LUNCH</b>
<b>15:30 - 17:00</b>	Oral blitz reports of young scientists (5min x 18); see speakers below in the list of <b>POSTER SESSION II</b>
<b>17:00 - 17:30</b>	<b>COFFEE BREAK</b>
<b>17:30 - 19:00</b>	<b>POSTER SESSION II</b>
<b>20:00 -</b>	<b>CONFERENCE DINNER</b>
	<b>FRIDAY - 06 April 2018</b>
<b>09:10 - 10:30</b>	<b>BREAKFAST</b>
<b>10:30 - 11:10</b>	<b>Sergey A. Vasiliev (Turku, Finland)</b> <b>Lecture:</b> DNP of shallow donors in silicon at ultra-low temperatures
<b>11:10 - 11:30</b>	<b>Georgy V. Mozzhukhin (Gebze, Turkey)</b> Low Field <sup>14</sup> N Nuclear Magnetic Resonance Detection of Liquid Substances
<b>11:30 - 12:00</b>	<b>COFFEE BREAK</b>
<b>12:00 - 12:20</b>	<b>Ramadan Atta (Damietta, Egypt)</b> Physical and transport properties of the novel dense membranes based on Polysulfone/Pluronic F127 composite
<b>12:20- 12:35</b>	<b>Ekaterina Krylova (St. Petersburg, Russia)</b> Dehydration/rehydration processes in sodium- and copper-exchanged mordenites studied by TGA and NMR
<b>12:35 - 12:50</b>	<b>Ekaterina V. Pokochueva (Novosibirsk, Russia)</b> NMR signal enhancement in hydrogenation reactions with parahydrogen
<b>12:50 - 13:05</b>	<b>Sergei A. Marchenko (St. Petersburg, Russia)</b> Complete assignment in <sup>1</sup> H NMR spectra and conformational analysis of some modified triterpenoids in solution.
<b>13:05 - 13:20</b>	<b>Alexandr V. Ievlev (St. Petersburg, Russia)</b> Analysis of NMR spectra of ionic liquid EAN with the addition of inorganic salts
<b>13:20 - 13:40</b>	<b>Olga A. Babanova (Ekaterinburg, Russia)</b>

	Dynamical properties of novel imidazolate borohydrides: NMR studies
<b>13:40 - 14:00</b>	<b>Boris M. Okrugin (St. Petersburg, Russia)</b> Influence of the charged peptide dendrigrafts topology on the large-scale properties and their internal structure
<b>14:00 - 15:30</b>	<b>LUNCH</b>
<b>15:30 - 15:50</b>	<b>Maxim Dolgushev (Paris, France)</b> NMR relaxation of fractal macromolecules
<b>15:50 - 16:10</b>	<b>Valeriya A. Shpotya (Moscow, Russia)</b> Determination of the structure of hyperbranched polyester boltorn and its derivatives with l-lactide and methyl ether of polyethylene glycol using NMR-spectroscopy methods
<b>16:10 - 16:30</b>	<b>Tatiana Zinkevich (Karlsruhe, Germany)</b> 7Li diffusion in solid electrolytes as studied by NMR spectroscopy
<b>16:30 - 16:45</b>	<b>Denis D. Kosenkov (St. Petersburg, Russia)</b> NMR relaxometer for the estimation of the spin-spin proton relaxation time of the living tissue
<b>16:45 - 17:00</b>	<b>Yuriy I. Neronov (St. Petersburg, Russia)</b> An estimate of the change in the spin-spin relaxation time of protons of living tissue upon its cooling
<b>17:00 - 17:30</b>	<b>COFFEE BREAK</b>
<b>17:30 - 17:50</b>	<b>Tatiana P. Kulagina (Chernogolovka, Russia)</b> Topological Structure and Mobility of Polymer Chains in Branched Poly(meth)acrylates Studied by NMR
<b>17:50 - 18:30</b>	<b>Ago Samoson (Tallinn, Estonia)</b> <b>Lecture:</b> New MAS Technologies
<b>18:30 - 19:00</b>	<b>AWARDING CLOSING</b>
<b>19:00 - 20:00</b>	<b>DINNER</b>
	<b>SATURDAY - 07 April 2018</b>
<b>08:45 - 09:45</b>	<b>BREAKFAST</b>
	<b>DEPARTURE</b>

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

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| 1* | Ganina Tatyana        | Dynamic Structure of Noradrenalin According to NMR Data and Quantum Mechanical Calculations |
| 2* | Avila Salazar Dahiana | Structure-dissolution relationships in Co(II)-  |
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	Andrea	containing phosphate glasses
3*	Khusnutdinova Naira	Analysis of correlation functions by method of molecular dynamics
4*	Bogdanov Dmitrii	Fe/Ag bimetallic system supported on mordenites: EPR, NMR and Mössbauer study
5*	Filippova Anna	Synthesis of sulfonated phthalocyanine complexes having triazole and naphthyl fragments
6*	Beshanov Vsevolod	Molecular dynamics simulations of alkylammonium nitrate ionic liquids. The effect of nitrate-anion model parameters
7*	Matsidon Maria	Hydrogen/deuterium isotope effects on water molecule mobility. A molecular dynamics simulation study
8*	Agureeva Angelina	Influence of polysaccharide shell on magnetic resonance relaxation and colloidal stability of SPIONs nanosuspension
9*	Kostin Mikhail	Quantum-mechanical calculations of hydrogen-bonded complexes of phosphine oxide H <sub>3</sub> PO with various proton donors
10*	Efimova Aleksandra	MRI study of the influence of superparamagnetic iron oxide nanoparticles (SPIONs) entrapped in cellulose microbeads on the relaxation properties of water in agarose matrix
11*	Kerner Anastasiya	Synthesis of phthalodinitriles having bifunctionally-substituted fragments
12*	Edinach Elena	Aluminum and gallium nuclei as microscopic probes for pulsed ENDOR diagnostics in garnet ceramics doped with paramagnetic ions
13*	Dmitriev Alexander	Ultra-narrow low-field nuclear spin resonance in NV centers in bulk diamond crystal

14*	Likerov Rodion	Investigation of neodymium doped YVO <sub>4</sub> with EPR method
15*	Ovcherenko Sergey	The Dynamics of Lactaptin in solution by NMR
16*	Vladislav Stanishevsky	High Resolution NMR Spectra and Dynamic Structure of Vinylcyclopropane
17*	Knapkiewicz Magdalena	Collective dynamics in various antiferroelectric liquid crystal mesophases probed by NMR relaxometry
18	Kupriyanova Galina	<sup>71</sup> Ga, <sup>77</sup> Se, <sup>115</sup> In MAS NMR study of TlGaSe <sub>2</sub> and TlInSe <sub>2</sub> powder
19	Pavchenko Maxim	Determination of the fine structure of the spiro-carboheterocycle using NMR spectroscopy and X-ray diffraction analysis
20	Khusnutdinov Rustem	The possibility of nuclear quadrupole resonance for distinguishing paracetamol different manufacturers and different forms (parties) from the same manufacturer of the spectral characteristics
21	Kukin Nikolay	Definition of the NV-centers orientations relatively to the crystal plane
22	Deriglazov Vladimir	Characterization of complex superparamagnetic colloids by electron magnetic resonance (EMR) and second-harmonic magnetic response (M <sub>2</sub> )
23	De Luca Deborah, Tagliatti Vanessa, and Delsinne Virginie	The application of the metabonomic approach to predict drug-induced liver injury: the case of acetaminophen and its non-toxic isomer
24	Soloninin Alexey Viktorovich	NMR study of reorientational motion in borohydrides of Mg(BH <sub>4</sub> ) <sub>2</sub>
25	Tertyshnaya Yulia	Molecular mobility of polylactide investigated by electronic paramagnetic resonance



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26	Kupriyanov Pavel	Neutralization of fluctuations in resonance conditions during registration of NMR spectra in the Earth's magnetic field
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\* Oral blitz reports of young scientists before POSTER SESSION I

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

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1*	Mulloyarova Valeriya	Cyclic trimers of phosphinic acids: symmetry, chirality, proton transfer and H/D isotope effects on NMR chemical shifts
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2*	Salikov Vladislav	Optimization of bacterial expression of MdmX N-terminal domain for NMR studies
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3*	Kuzminova Anna	Novel mixed -matrix membrane based on composite PVA - carboxyfullerene: preparation and characterization
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4*	Vasin Semen	Preparation and Characterization of Polysulfone/Pluronic F127 ultrafiltration membranes
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5*	Garkavyi Stanislav	Inhomogeneous magnetic state in mechanochemically synthesized nanopowder sample of CuFeS <sub>2</sub> according to <sup>63,65</sup> Cu NMR spectrum in the local field
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6*	Bogdan Andrey	Comparison of MRS and PET data in neurodegenerative disorders.
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7*	Dorian Maroil	Exploration of the hypothyroidic effect of Sunitinib, a tyrosine kinase receptor inhibitor, by metabolomic approach, in the rat
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8*	Muradova Anna	Definition of the NV-centers orientations relatively to the crystal plane
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9*	Korchevaya Irina	Definition of the NV-centers orientations relatively to the crystal plane
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10*	Dmitrenko Mariia	Investigation and characterization of mixed-matrix membranes based on composite PVA -
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		fullerenol
11*	Ovcherenko Sergey	The determination of the relaxation properties of the emulsion consisted of proxyl type nitroxide radicals proposed as MRI contrast agent
12*	Nikitina Anastasia	Investigation of MRI contrast efficiency and aggregation stability of magnetic nanoparticles by NMR-relaxometry
13*	Pichugina Alina	<sup>1</sup> H NMR and ESR studies of the mechanism of gallstones formation
14*	Popova Elena	Effect of dendrimer generation on the kinetics of peptide complex formation
15*	Mershiev Ivan	<sup>14</sup> N NQR with Frank sequence excitation
16*	Belyakov Denis	Development of a standard base for the "medium" and "strong" constant field's magnetic induction measurement
17*	Pelipko Vasilii	<sup>1</sup> H, <sup>13</sup> C, <sup>15</sup> N NMR spectroscopy in the study of the structure of alkyl 3-nitropropanoates containing one asymmetric carbon atom in the structure
18*	Lushpinskaya Irina	Calculation of the magnetic shielding tensor on <sup>125</sup> Te and <sup>207</sup> Pb nuclei in PbTe
19*	Sheveleva Nadezhda	Study of Local Orientation Mobility in Lysine Dendrimers by NMR method
20*	Ubovich Milosh	Small-angle x-ray scattering profile of the two-domain Pax-5 protein in aqueous solution by molecular dynamics simulations
21*	Ievleva Svetlana	DWI/PWI Techniques of MRI
22*	Shavykin Oleg	Influence of the asymmetry of branching on the structural properties of dendrimers. Brownian

		dynamics simulation
23	Tsyro Larisa	Research of kern of an electronic spin resonance method
24	Demidov Viktor	Investigation of the electron-rich binuclear Pt(II) 1,10-phenanthrocyanine [(py) <sub>2</sub> Pt(μ-phencyanine-)Pt(py) <sub>2</sub> ]Cl <sub>3</sub> by the ESR method. Localization of PSC in temperature accessible electron-excited radical states
25	Bogachev Yury	55 Years of EPR laboratory at St.-Petersburg Electrotechnical University "LETI"
26	Drozdovskii Andrey	Investigation of spin-wave oscillators

\* Oral blitz reports of young scientists before POSTER SESSION II