## **Schedule**

## **22<sup>nd</sup> International School-Conference**

## «Magnetic Resonance and its Applications.

Spinus-2025»

31 March - 4 April, 2025 St. Petersburg



	MONDAY –31 March, 2025		
Chairman	Prof. Denis Markelov (Saint-Petersburg, Russia)		
10:00-10:10	Opening		
10:10-10:40	Vladimir Chizhik (Saint Petersburg, Russia)		
	<b>Lecture:</b> A few little-known facts in the history of NMR in Russia and a couple of thoughts on unfortunate terminology in magnetic resonance		
10:40-11:20	Bin Xia (Beijing, China)		
	<b>Lecture:</b> DNA Binding Mechanism of the Virulence Regulator SarA of Staphylococcus aureus		
11:20-11:40	Ekaterina Boltenkova (Kazan, Russia)		
	<b>Oral report:</b> The hydrothermal treatment effect on the relaxivity of DyF <sub>3</sub> nanoparticles colloidal solution		
11:40 – 12:10	'COFFEE' BREAK		
Chairman	Prof. Cabal-Mirabal Cabal (Havana, Cuba)		
12:10-12:50	Kumaravel Kaliaperumal (Chennai, India)		
	Lecture: Antiviral metabolite isolation and characterization from		
	Acremonium sp (SIMATS2121) endophytic fungi from medicinal plant		
12:50-13:10	Galina Kupriyanova (Kaliningrad, Russia)		
	<b>Oral report:</b> Study of the influence of Au nanoparticles of various shapes on the dynamics and structure of tyrosine using <sup>1</sup> H NMR methods.		

13:10 – 13:25	Mark Smirnov (Kaliningrad, Russia)  Oral report: Influence of the shape of gold nanoparticles on the structural and dynamical properties of L-tyrosine		
13:25 – 14:05	Ilya Gridnev (Moscow, Russia)		
10.20 1.100	Lecture: Use of various NMR techniques in the study of mechanism of		
	asymmetric hydrogenation		
14:05 – 15:10	LUNCH		
Chairman	Prof. Galina Kupriyanova (Kaliningrad, Russia)		
15:10 – 15:50	Carlos Cabal-Mirabal (Havana, Cuba)		
	Lecture: Wound healing rate and treatment effectiveness determined by MRI		
15:50 – 16:10	Nikolay Anisimov (Moscow, Russia)		
	Oral report: MRI of wildlife		
16:10 – 16:25	Anna Yi (Novosibirsk, Russia)		
10.110 10.110	Oral report: Intra- and intermolecular transfer of parahydrogen-induced		
	hyperpolarization via nuclear Overhauser effect induces RASER		
16:25 – 16:40	Manuel Arsenio Lores Guevara (Santiago de Cuba, Cuba)		
	Oral report: Proton MRD profile analysis in Human Serum Albumin		
	solutions: a two site exchange model approach		
16:40 - 17:00	Leonid Grunin (Yoshkar-Ola, Russia)		
	Lecture: NMR Transverse Relaxation as the Tool for Structure and		
	Thermodynamics Analysis		
17:00-17:20	Cengiz Okay (Istanbul, Turkey)		
	<b>Oral report:</b> Investigation of Relaxation Times of Cotton Oil-Diesel Fuel Mixtures by TD-NMR		
17:20 - 17:40	Dmitry Filimonenko (Minsk, Belarus)		
	Oral report: Zero-field cross-relaxation resonances in ensembles of NV		
18-30 - 22:00	centers in diamond and fully optical magnetic field detection		
10-30 - 22.00	Welcome Party		
	TUESDAY – 1 April, 2025		
Chairman	Prof. Marina Shelyapina (Saint-Petersburg, Russia)		
10:00 - 10:40	William Price (Sydney, Australia)		
	Lecture: Accurate NMR Diffusion Measurements in Reacting Systems		
10:40 – 10:55	Bulat Mukhamadullin (Kazan, Russia)		
	Oral report: Study of fluoride nanoparticles nucleation processes by NMR		
	in the capillary system		
10:55 – 11:10	Polina Zefirova (Saint-Petersburg, Russia)		
	Oral report: <sup>1</sup> H NMR spectroscopy application for assessment catalytic		
	behavior of comb-like polyelectrolytes in Suzuki reaction		
11:10 – 11:25	Naira Gromova (Saint-Petersburg, Russia)		
	Oral report: Cell size dependence of diffusion properties of PAMAM		
	dendrimers by MD simulations		
	dentalimes by the simulations		

11:25 – 11:40	Milosh Ubovich (Saint-Petersburg, Russia) Oral report: "Ionic Liquid EAN/Al(NO <sub>3</sub> ) <sub>3</sub> /H <sub>2</sub> O" System Studied by NMR and Computational Methods		
11:40 – 12:10	'COFFEE' BREAK		
Chairman	Prof. Peter Tolstoy (Saint-Petersburg, Russia)		
12:10 – 12:50	Daniil Kolokolov (Novosibirsk, Russia) Lecture: Hydrogen bonds types, strengths and dynamics in hydroxyl- and carboxyl-functionalized ionic liquids		
12:50 – 13:10	<b>Alexander Khudozhitkov (Novosibirsk, Russia) Oral report:</b> <sup>2</sup> H NMR study of [P444-D][OMs] and [N444-D][OMs] ionic liquids		
13:10 – 13:25	Daria Chetverikova (Saint Petersburg, Russia) Oral report: NMR Diffusometry for Studying Ionic Association in Plasticized Polymers		
13:25 – 13:45	Alexandr Ievlev (Saint Petersburg, Russia)  Oral report: Study of complex ionic liquids according to NMR relaxation and diffusion measurements		
13:45 – 14:05	Nikita Slesarenko (Chernogolovka, Russia)  Oral report: Competitive ion transport in polymer gel electrolytes studied by NMR		
14:05 – 15:10	LUNCH		
Chairman	Prof. Denis Markelov (Saint Petersburg, Russia)		
15:10- 16:20	Oral blitz reports of young scientists		
16:20-16:30	CONFERENCE PHOTO		
16:30-18:30	Oral blitz reports of young scientists		
	POSTER SESSION I		
	WEDNESDAY – 2 April, 2025		
11:00 – 14:00	Excursion to the Grand Menshikov Palace		
14:00 – 15:00	LUNCH		
15:00– 17:00	Excursion to Magnetic Resonance Research Centre of St. Petersburg State University		

	THURSDAY – 3 April, 2025		
Chairman	Dr. Andrei Egorov (Saint-Petersburg, Russia)		
10:00 - 10:40	Elena Charnaya (Saint Petersburg, Russia)		
	Lecture: Metals under nanoconfinement: NMR studies		
10:40 - 11:00	Ilya Yakovlev (Novosibirsk, Russia)		
	<b>Oral report:</b> Silicon-enhanced incorporation of boron into AlPO-11 framework according to <sup>11</sup> B solid-state NMR		
11:00- 11:15	Danil Markelov (Novosibirsk, Russia)		
	<b>Oral report:</b> Hyperpolarization of <sup>77</sup> Se nuclei using signal amplification by reversible exchange (SABRE) at microtesla fields		
11:15– 11:30	Allisher Vasilev (Saint Petersburg, Russia)		
	<b>Oral report:</b> Directional solidification in gallium under strong magnetic field: NMR studies		
11:30–11:45	Aliya Galimova (Kazan, Russia) / Bulat Rameev (Gebze, Turkey)		
	Oral report: Theory of two-stage quantum transduction based on use of magnetic material coupled to erbium-doped crystal		
11:45 – 12:10	'COFFEE' BREAK		
Chairman	Prof. Elena Charnaya (Saint Petersburg, Russia)		
12:10 – 12:40	Kev Salikhov (Kazan, Russia)		
	<b>Oral report:</b> Further development of the theory of spin exchange in dilute solutions of paramagnetic particles		
12:40 – 13:00	Kocharyan Gaspar (Yerevan, Armenia)		
	<b>Oral report:</b> Determination of anti-peroxyl radical capacity of flavonoids (quercetin, morin and rutin) by the kinetic EPR method with pulse reactant injection.		
13:00– 13:15	Daria Pomogailo (Moscow, Russia)		
	<b>Oral report:</b> Electron Spin Resonance of Fe-doped TiO <sub>2</sub> nanoparticles		
13:15 – 13:30	Anastasia Batueva (Saint Petersburg, Russia)		
	<b>Oral report:</b> Registration of nickel and nitrogen spin centers signals by their interactions with negative NV centers in diamond by		
	photoluminescence		
13:30 - 14:10	Alexandr Trifonov (CIQTEK, Moscow, Russia)		
	Lecture: The development and results of magnetic resonance technology		
	and instruments		
	EPR Round Table and connected demonstration		
14:10 – 15:10	LUNCH		
Chairman	Prof. Denis Markelov (Saint Petersburg, Russia)		
15:10– 16:30	Oral blitz reports of young scientists		
16:30-18:30	POSTER SESSION II		
19:00- 23:00	Conference Dinner		

	FRIDAY – 4 April, 2025		
Chairman	Prof. Yury Bunkov (Moscow, Russia)		
10:10 - 10:30	Sergey Dvinskikh (Stockholm, Sweden)		
	Oral report: Ion dynamics in liquid crystal-electrolyte mixtures		
10:30 - 10:50	Sergei Bystrov (Saint Petersburg, Russia)		
	<b>Oral report:</b> Unified NMR: towards universally accessible NMR workflow with TQT "Nuclei"		
10:50 – 11:10	Pavel Kupriyanov (Gebze, Turkey)		
	<b>Oral report:</b> RFI suppression system for NQR detection in unshielded conditions		
11:10- 11:25	Alexander Snadin (Novosibirsk, Russia)		
	<b>Oral report:</b> Development of a new class of adiabatic inverting MCA pulses combining constant and offset-independent adiabaticity		
11:25 – 11:40	Gleb Dolgorukov (Kazan, Russia)		
	<b>Oral report:</b> Low field setup for DNP studies in stray field of superconducting magnet		
11:40 – 12:10	'COFFEE' BREAK		
Chairman	Dr. Andrei Komolkin (Saint-Petersburg, Russia)		
12:10 – 12:30	Pavel Yushmanov (Stockholm, Sweden)		
	<b>Oral report:</b> Electrophoretic NMR and its application in studying the electrokinetic transport of water and methanol in Nafion membranes		
	electronimetre transport of water and mentanion in realization		
12:30 – 12:50	Natalia Yevlampieva (Saint-Petersburg, Russia)		
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12:30 - 12:50 12:50 - 13:10	Natalia Yevlampieva (Saint-Petersburg, Russia) Oral report: Magnetic relaxation properties of metal-carbon		
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	POSTER SESSION I (TUESDAY, 16:30-18:30)			
1	Omar	Alkhuder	Exploring the Ability of the P=O Group to Form Multiple Hydrogen Bonds	
2	Anastasiia	Antonenko	125 Te NMR spectra in Td-phase WTe <sub>2</sub>	
3	Ekaterina	Batueva	Multifunctional Heptanuclear Iron Complexes: Magnetic Properties and Potential Applications in MRI	
4	Aleksandra	Sashina	Phase structure and molecular mobility of drug delivery systems based on liposomes with Pluronics by nuclear magnetic resonance method	
5	Vyacheslav	Gonyalin	NMR assignment of eucaryotic initiation translation factor 5A of Candida albicans	
6	Anastasia	Dmitrieva	Potential of NMR spectroscopy for assessing the hydrophobicity of microsphere cellulose carriers for spiking cancer cells	
7	Ekaterina	Dmitrieva	Analysis of hyperfine and quadrupole interactions in the first coordination sphere of <sup>14</sup> N in hexagonal boron nitride	
8	Albina	Gafarova	Study of conformation of mechanically activated calcium gluconate irradiated with gamma quanta	
9	Ekaterina	Zaitseva	NMR Study of the fibrile-forming peptide SEM1(86-107)	
10	Kristina	Gorkovaia	NMR control of the synthesis of pharmaceutical intermediates	
11	Ilya	Grishanovich	The optimization of the conditions of 2D NMR spectra registration for the analysis of thermoplastic organic compounds in molten state	
12	Roman	Haponchyk	Investigation of the magnonic nonlinear phase shifter based on forward volume spin waves	
13	Artem	Igonin	Effect of palladium(II) on NMR spectra of coordinated semicarbazones	
14	Dmitry	Ivanov	Features of the study of the pore space of the core by the method of nuclear magnetic resonance	
15	Natalya	Karmanova	Modelling localization of various statins within a POPC bilayer by molecular dynamics and metadynames	
16	Daniil	Khroshin	Modeling of spin-wave spectrum for YIG films at sub-THz frequencies	
17	Savelii	Levit	NMR analysis of surfactants characteristics based on methacrylic acid.	
18	Daria	Malakhova	Study of intramolecular mobility in ionic liquid [BMIM] <sub>2</sub> Cd(SCN) <sub>4</sub> using NMR relaxation data.	
19	Daria	Melnikova	Effect of the disulfide reducing agent TCEP on the translational mobility of $\alpha$ - and $\kappa$ -casein and their ability to form supramolecular structures	
20	Daria	Melnikova	NMR diffusometry and micellar solubilization using biological surfactants	
21	Artem	Alexandrov	Generator of arbitrary sequences of commands/pulses	
22	Sergey	Andronenko	The FMR/EPR studies of magnetite/maghemite nanoparticles, synthesized by different methods	

23	Nikolay	Anisimov	Simultaneous detection of nuclei <sup>13</sup> C, <sup>23</sup> Na, <sup>27</sup> Al and <sup>55</sup> Mn at 0.5 Tesla
24	Nikolay	Anisimov	Construction of sensitivity maps for wireless coils using <sup>19</sup> F MRI
25	Konstantin	Bozhenko	Quantum-Chemical study of Interactions of Fe <sub>2</sub> O <sub>n</sub> (n=7, 9) Clusters with H <sub>2</sub> and O <sub>2</sub> Molecules
26	Nina	Djapic	Proton attached to nitrogen in porphyrins and tetrapyrroles
27	Alexey	Kiryutin	Determination of Rotational Correlation Time of and Iridium Dihydride Complex in Aqueous Medium by Means of NMR Relaxometry with High-resolution

	POSTER SESSION II (THURSDAY, 16:30-18:30)			
1	Olga	Mikhailovskaya	Modification approaches to the development of pervaporation sodium alginate-based membranes with enhanced properties	
2	Marina	Mikhalap	Determination of the spirocyclopropanoxindole fine structure using NMR spectroscopy	
3	Anna	Mikulan	Novel blend cellulose nitrate/cellulose acetate ultrafiltration membranes for enhanced water treatment	
4	Veronika	Minaeva	Determination of the structure of regioisomeric furan- containing naphthofuranes based on 1D and 2D NMR spectroscopy experiments	
5	Guzel	Minnullina	Conformational behavior of cyclic peptides cyclosporin C and alisporivir in acetonitrile and their interaction with Dy <sup>3+</sup> ions	
6	Dmitriy	Mizyulin	Hydrogen/deuterium isotope effects on the microstructure and molecular mobility in the aqueous solution of europium nitrate. A molecular dynamics simulation study	
7	Ilya	Pilipenko	Application of <sup>1</sup> H- <sup>13</sup> C HMBC NMR spectroscopy for identification of regioisomeric polycyclic dihydrofurans	
8	Julia	Pronina	The spiro[1-azabicyclo[3.2.0]heptane] frameworks: structures determination using NMR methods	
9	Julia	Pronina	The spiro[1-azabicyclo[3.3.0]octane] frameworks: structures determination using NMR methods	
10	Andrej	Rochev	Different mechanisms of spin-lattice relaxation of gallium in semi-insulator GaAs	
11	Margarita	Sadovnikova	Effect of rare earth impurities on structural properties of calcium phosphate-based materials by EPR spectroscopy	
12	Azamat	Samadov	Effect of alkaline treatment on structure, morphology, CO2 sorption of mesoporous ZSM-5 zeolites	
13	Stepan	Galiakhmetov	Influence of substitutes and chalcogen atom nature on the alkylation of phosphine chalcogenides	
14	Georgiy	Shonin	Synthesis of 4,5-diethynyl-1,2,3-triazoles and structure analysis by NMR spectroscopy	
15	Artyom	Tarasov	Spectral characteristics of cyclosporin G and L in deuterated acetonitrile with water solution determined by NMR spectroscopy	
16	Anastasia	Troshkina	The structural features of the fibril-forming peptide SEM2(49-107) by NMR spectroscopy and its role in enhancing HIV activity	
17	Sergey	Cheremensky	Microstructure and molecular mobility in the ternary LiCl-Cs-Cl-H <sub>2</sub> O system. A molecular dynamics simulation study	
18	Valentina	Yakovleva	Study of NV- centers in natural diamonds (carbonado) by micron scale scanning spectroscopy	
19	Andrei	Komolkin	NMR <sup>1</sup> H/ <sup>13</sup> C study of biocompatible copolymer of divinyl ether and maleic anhydride	
20	Yulianela	Mengana	Evaluation of plasma viscosity in patients with hyperviscosity syndrome using Proton Magnetic Relaxation.	
21	Valerii	Bezrodnyi	Molecular dynamics simulation of C <sub>60</sub> /C <sub>70</sub> fullerene complexes with peptide dendrimer containing histidine	

			spacers
22	Igor	Neelov	Computer simulation of interaction of fullerenes C <sub>60</sub> with short amyloid peptides
23	Igor	Neelov	Investigation of interaction of cyclic peptide with short amyloid peptides by computer simulation
24	Anastasia	Nikitina	Investigation of magnetic characteristics of magnetite nanoparticles in various organic shells
25	Konstantin	Tyutyukin	Study of slow molecular motions by NMR relaxation
26	Yamirka	Alonso	Physicochemical characterization of carbon-coated magnetic cobalt nanoparticles