

Schedule

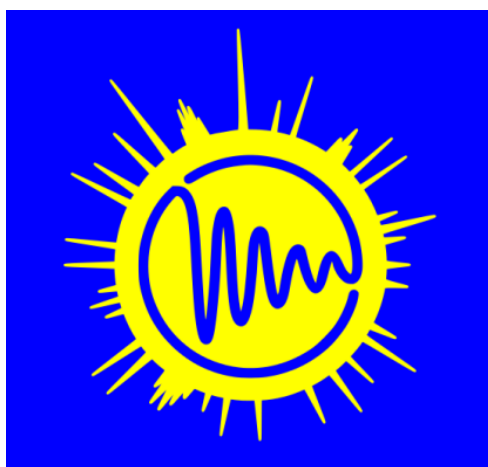
20th International School-Conference

«Magnetic Resonance and its Applications.

Spinus-2023»

March 27 - 30, 2023

St. Petersburg



| | MONDAY – 27 March 2023 |
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| Chairman | Professor Denis Markelov (Saint-Petersburg, Russia) |
| 10:00 – 10:10 | Opening |
| 10:10 – 10:40 | Vladimir Chizhik (Saint-Petersburg, Russia) Lecture: Start and passage of the School-Conference "Magnetic Resonance and its Applications" (Spinus) (to the 20 th meeting of the conference) |
| 10:40 – 11:20 | Yury Bunkov (Moscow, Russia) Lecture: Magnon-magnon interaction through phonons |
| 11:20 – 11:40 | Igor Yanilkin (Kazan, Russia) Oral report: Engineering the Exchange Spin-Waves in Graded Thin Ferromagnetic Films |
| 11:40 – 12:00 | ‘COFFEE’ BREAK |
| Chairman | Professor Marina Shelyapina (Saint-Petersburg, Russia) |
| 12:00 – 12:40 | Elena Charnaya (Saint-Petersburg, Russia) Lecture: Application of NMR to studies of nanocomposites |
| 12:40 – 13:20 | Sergey Dvinskikh (Stokholm, Sweden) Lecture: Hydrogen bonding in bulk and nanoconfined ionic liquid crystals |
| 13:20 – 13:40 | Alexey Soloninin (Ekaterinburg, Russia) Oral report: Comparison of ion dynamics in a carbon-substituted closo- |

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| | hydroborates NaCB ₉ H ₁₀ , NaCB ₁₁ H ₁₂ and solid-solution Na ₂ (CB ₉ H ₁₀)(CB ₁₁ H ₁₂): ¹ H and ²³ Na NMR studies |
| 13:40 – 14:00 | Daria Pomogailo (Moscow, Russia) Oral report: Photochemical transformations of O-containing radical-cations at low temperatures in CF ₃ CCl ₃ matrix |
| 14:00 – 14:15 | Dmitriy Fedorov (Ekaterinburg, Russia) Oral report: Sodium diffusion in scheelite-type Na ₅ M(MoO ₄) ₄ (M=Bi, La, Y) |
| 14:15 – 14:30 | Vladislav Liamin (Saint-Petersburg, Russia) Oral report: Development and characterization of new membranes based on polyphenylene oxide and its block copolymer with polydimethylsiloxane for enhanced pervaporation |
| 14:30 – 15:30 | LUNCH |
| Chairman | Professor Yury Pirogov (Moscow, Russia) |
| 15:30 – 15:50 | Enza Di Gregorio (Torino, Italy) Oral report: Targeted nanosystems for treatment of triple negative breast cancer and MRI Imaging |
| 15:50 – 16:10 | Nikolay Anisimov (Moscow, Russia) Oral report: Technological applications on a 0.5 T clinical MRI scanner |
| 16:10 – 16:30 | Mikhail Gulyaev (Moscow, Russia) Oral report: Fluorine-19 (¹⁹ F) magnetic resonance imaging in 1.5 T |
| 16:30 – 16:50 | Dmitriy Blokhin (Kazan, Russia) Oral report: Structural studies of human semen amyloid peptides by NMR spectroscopy and molecular dynamics |
| 16:50 – 17:05 | Alexander Fedotov (Saint-Petersburg, Russia) Oral report: Passively detunable wireless coil for 1.5T breast imaging |
| 17:05 – 17:20 | Zilya Badrieva (Saint-Petersburg, Russia) Oral report: Multi-Echo Spin Echo based T ₂ mapping: how can we handle the issue of variations among slices? |
| 17:20 – 17:35 | Fabian Tamayo Delgado (Santiago de Cuba, Cuba) Oral report: Plasma dynamic viscosity in Multiple Myeloma patients measured using NMR |
| 17:35 – 17:50 | Fabian Tamayo Delgado (Santiago de Cuba, Cuba) Oral report: Dalcetrapib and Reduced Glutathione effect on Hemoglobin S polymerization studied by NMR |
| | TUESDAY – 28 March 2023 |
| Chairman | Professor Yury Bunkov (Moscow, Russia) |
| 10:00 – 10:40 | Richard Shi (Vice President of Magnetic Resonance ZHONGTAI, Hefei, China) Anton Cherkasov (leading specialist of the company "ELEMENT", Ekaterinburg, Russia) Lecture: Development of ZHONGTAI W-band EPR Spectrometer |
| 10:40 – 10:55 | Pavel Zasimov (Moscow, Russia) |

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| | Oral report: An EPR study on the radiolysis of isolated ethanol molecules in solid argon and xenon: matrix control of radiation-induced generation of radicals in cryogenic media |
| 10:55 – 11:10 | Margarita Sadovnikova (Kazan, Russia) Oral report: The Symmetry of the Hyperfine and Quadrupole Interactions of the Boron Vacancy in a Hexagonal Boron Nitride |
| 11:10 – 11:25 | Igor Veyshtort (Saint-Petersburg, Russia) Oral report: Polarization dependence of the ODMR spectrum of spin 3/2 vacancy centers in 6H and 15R silicon carbide polytypes |
| 11:25 – 11:40 | Fan Liu (Beijing, China) Oral report: The DNA binding mechanism of virulence-associated protein Ler from pathogenic Escherichia coli |
| 11:40 – 12:00 | ‘COFFEE’ BREAK |
| Chairman | Ph.D. Andrei Komolkin (Saint-Petersburg, Russia) |
| 12:00 – 12:40 | Peter Tolstoy (Saint-Petersburg, Russia) Lecture: NMR study of hydrogen and halogen bonds with P=O groups |
| 12:40 – 12:55 | Mark Kaplanskiy (Saint-Petersburg, Russia) Oral report: The factors determining ¹ H NMR chemical shift in complexes with centrally symmetric hydrogen bonds |
| 12:55 – 13:10 | Anna Titova (Saint-Petersburg, Russia) Oral report: Investigation of the mutual influence of NH-N hydrogen bonds in heterodimers of substituted diaminopyridines by means of quantum chemistry |
| 13:10 – 13:25 | Elizaveta Kononenko (Novosibirsk, Russia) Oral report: Obtaining High Resolution NMR Spectra in Inhomogeneous Magnetic Fields in Experiments with Antiphase Magnetization |
| 13:25 – 13:40 | Edem Chakalov (Saint-Petersburg, Russia) Oral report: Homoconjugated anions of phosphoric and phosphinic acids: spectral and structural peculiarities probed by low-temperature NMR spectroscopy |
| 13:40 – 13:55 | Daria Novikova (Saint-Petersburg, Russia) Oral report: Estimation of long-range interproton distances in tetrahydropyrazolo[1,5-a]pyrimidines using NOE data |
| 13:55 – 14:10 | Semyon Egorov (Saint-Petersburg, Russia) Oral report: ³¹ P NMR Spectroscopy within Investigation of Compounds Based on Hexachlorocyclotriphosphazene |
| 14:10 – 14:30 | Eugeny Pestryaev (Ufa, Russia) Oral report: What is hidden under the FID noise of entangled polymer melt? |
| 14:30 – 15:30 | LUNCH |
| Chairman | M. Sc. Alexandr Ievlev (Saint-Petersburg, Russia) |
| 15:30 – 16:30 | Oral blitz reports of young scientists (5 min × 12) |
| 16:30 – 18:30 | POSTER SESSION I |

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| | WEDNESDAY – 29 March 2023 |
| Chairman | Professor Peter Tolstoy (Saint-Petersburg, Russia) |
| 10:00 – 10:40 | Sergey Vasil'ev (Chernogolovka, Russia) Lecture: Multiple-quantum NMR dynamics in quasi-one-dimensional zigzag proton spin chains in hambergite single crystal |
| 10:40 – 10:55 | Daniil Shitov (Saint-Petersburg, Russia) Oral report: Handling of the strength of hydrogen bonds involving imidazole ring through the formation of additional non-covalent interactions |
| 10:55 – 11:10 | Julia Pronina (Saint-Petersburg, Russia) Oral report: Diastereoisomers of 3-azabicyclo[3.1.0]hexanes spiro-fused with a benzo[4,5]imidazo[1,2-a]indole fragment: structure determinations using NMR methods |
| 11:10 – 11:40 | Galina Kupriyanova (Kaliningrad, Russia) Lecture: Nuclear Quadrupole Resonance and its Applications |
| 11:40 – 12:00 | ‘COFFEE’ BREAK |
| Chairman | Professor Sergey Dvinskikh (Stokholm, Sweden) |
| 12:00 – 12:40 | Janez Stepišnik (Ljubljana, Slovenia) Lecture: Chemical exchange rate study by NMR CPMG method |
| 12:40 – 13:00 | Oleg Shushakov (Novosibirsk, Russia) Oral report: An example of the Bloch-Siegert effect in magnetic-resonance sounding |
| 13:00 – 13:20 | Aleksandra Kusova (Kazan, Russia) Oral report: Translational diffusion as a protein-protein interaction marker |
| 13:20 – 13:35 | Ksenia Panicheva (Moscow, Russia) Oral report: Translational self-diffusion of α -tocopherol in a new water-soluble form |
| 13:35 – 13:50 | Adeliya Garaeva (Kazan, Russia) Oral report: NMR relaxation of helium-3 in contact with 20-200 nm DyF ₃ particles |
| 13:50 – 14: 10 | Ayşe Maraşlı (Gebze-Kocaeli, Turkey) Oral report: Time Domain Nuclear Magnetic Resonance Investigations of Benign and Threat Liquids |
| 14:10 – 14:30 | Leonid Grunin (Yoshkar-Ola, Russia) Oral report: Solid State NMR: Validity of Relaxation Times Approach |
| 14:30 – 15:30 | LUNCH |
| Chairman | M. Sc. Alexandr Ievlev (Saint-Petersburg, Russia) |
| 15: 30 – 15:50 | Andrei Komolkin (Saint-Petersburg, Russia) Oral report: Master programs in Physics at Saint Petersburg State University (in Russian) |
| 15:50– 16: 35 | Oral blitz reports of young scientists (5 min × 9) |

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| 16:35– 18:30 | POSTER SESSION II |
| | THURSDAY – 30 March 2023 |
| Chairman | Professor Elena Charnaya (Saint-Petersburg, Russia) |
| 10:00 – 10:40 | Marina Shelyapina (Saint-Petersburg, Russia) Lecture: Recent advances in NMR of hierarchically organized zeolites |
| 10:40 – 10:55 | Milosh Ubovich (Saint-Petersburg, Russia) Oral report: The state of concomitant water in system "ionic liquid - aluminum salt" |
| 10:55 – 11:10 | Nadezhda Pokhvishcheva (Saint-Petersburg, Russia) Oral report: Diffusion studies in polymeric membranes plasticized by ionic liquids |
| 11:10 – 11:25 | Kirill Mukhin (Saint-Petersburg, Russia) Oral report: Local structure and dynamics in concentrated “water-in-salt” mixed LiOAc and KOAc solutions according to data of NMR |
| 11:25 – 11:45 | Nikita Slesarenko (Chernogolovka, Russia) Oral report: Local motion of water molecules and Li ⁺ , Na ⁺ , Cs ⁺ cations in sulfonic cation-exchange membranes studied by spin relaxation of ¹ H, ⁷ Li, ²³ Na, ¹³³ Cs nuclei. |
| 11:45 – 12:00 | ‘COFFEE’ BREAK |
| Chairman | Ph.D. Leonid Grunin (Yoshkar-Ola, Russia) |
| 12:00 – 12:20 | Georgy Mozzhukhin (Gebze-Kocaeli, Turkey) Oral report: The detection of NQR signals with use of the single-turn toroid |
| 12:20 – 12:40 | Cengiz Okay (Istanbul, Turkey) Oral report: Microwave (MW) Dielectric Spectroscopy investigations of benign and threat liquids |
| 12:40 – 13:00 | Ilya Yakovlev (Novosibirsk, Russia) Oral report: Hydrogen pulverization of metallic cobalt observed by ⁵⁹ Co Internal Field NMR of Co-Zr cermet precursor |
| 13:00 – 13:15 | Anton Kashnikov (Surgut, Russia) Oral report: On the spin properties of cement and its components |
| 13:15 – 13:30 | Sergei Bystrov (Saint-Petersburg, Russia) Oral report: NMR to Industry: developing the portable NMR solution |
| 13:30 – 13:50 | Pavel Kupriyanov (Gebze-Kocaeli, Turkey) Oral report: Detection of organophosphorus liquids by NMR in the Earth’s magnetic field |
| 13:50 – 14:30 | Pavel Yushmanov (Stockholm, Sweden) Lecture: Electrophoretic NMR and applications |
| 14:30 – 15:30 | MEETING OF AWARDING COMMISSION |
| 15:30 – 16:00 | AWARDING and CLOSING |

POSTER SESSION I (TUESDAY, 15:30 – 18:30)

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| 1 | Ivan | Adyukov | Homo- and heteronuclear NMR spectroscopy experiments in studying structure of 3-bromo-3-nitro-1-phenylprop-2-en-1-one |
| 2 | Dmitry | Aleshin | Analysis of thermodynamics properties of Fe(II) spin-crossover complexes by the ^1H chemical shifts analysis |
| 3 | Andrey | Bagautdinov | Induced nonlinear frequency shift of an active ring resonator on a magnonic crystal |
| 4 | Marcel | Bakirov | Increasing the effective relaxation time in Carr-Purcell-Meiboom-Gill sequence |
| 5 | Valerii | Bezrodnyi | Molecular dynamics simulation of lysine based peptide dendrimers with neutral and protonized histidine |
| 6 | Viktor | Demidov | ESR spectroscopy of temperature accessible lowest electronic triplet biradical states of d-elements biologically active 1,10-phenanthrocyanines (bi-1,10-phenanthrolylenes), soft colloidal glasses |
| 7 | Nina | Djapic | Eugenol and piperine proton spectra |
| 8 | Mariia | Dmitrenko | Development and characterization of novel pervaporation mixed matrix membranes based on carboxymethyl cellulose modified with Zn-based MOF for hybrid process |
| 9 | Maria | Egorova | Water molecules mobility in microporous mordenite by molecular dynamics simulation |
| 10 | Albina | Gafarova | EPR study of mechanically activated calcium gluconate monohydrate irradiated with gamma quanta |
| 11 | Kirill | Gomonov | Study of the structure of reaction products of acetyl-containing furancarboxylates with hydrazine hydrate by 1D and 2D NMR spectroscopy |
| 12 | Timur | Islamov | Pravastatin with transition metal ion studied by NMR |
| 13 | Alexander | Khudozhitkov | Deuterium Isotope Effects in Protic Ionic Liquids |
| 14 | Aleksandr | Koltsov | Nuclear magnetic resonance in eutectic Cs-Li-OAc-H ₂ O “water-in-salt” solution |
| 15 | Alexandr | Kondrashov | Ways of optimization of the magnonic reservoir computer performances |
| 16 | Vladilina | Koryakina | Solid-State ^{13}C NMR of Annealing Nanodiamonds |
| 17 | Andrei | Zolotarev | Development and characterization of novel ultrafiltration membranes based on cellulose acetate modified with Zn-based MOFs |
| 18 | Anastasia | Nikitina | Investigation of NMR relaxation properties of contrast agents based on magnetic nanoparticles |
| 19 | Denis | Lyzov | Homo- and heteronuclear NMR methods for signal assignments in ^1H and ^{13}C spectra of 1-aminoacyloxygermatran |
| 20 | Darya | Melkova | Tautomeric transformations N- and C-acyl derivatives of tetrahydro-1,4-diazepines |
| 21 | Ivan | Mershiev | Cogwheel phase cycling for T ₂ -T ₂ exchange NMR |
| 22 | Igor | Neelov | Investigation of complex formation by Lys-2Leu dendrimer with oligopeptides of different degree of hydrophobicity |
| 23 | Kenan | Mamedgasanov | Molecular Dynamics Study of the Process of Extraction Purification of Model Fuel |

POSTER SESSION II (WEDNESDAY, 15:50 – 18:30)

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| 1 | Igor | Neelov | The SCF study of micelle formation of the amphiphilic hybrid molecules consisting of a polylysine dendron with several hydrophobic tails |
| 2 | Igor | Neelov | Molecular dynamics study of complex formation of the dendrigraft DG2 with charged oligopeptides AED, GED and ED |
| 3 | Andrey | Nikitin | Modeling of nonlinear spin-wave transient processes in magnonic active-ring oscillators |
| 4 | Anna | Kuzminova | Novel pervaporation membranes based on poly(ester-block-amide) modified with MOFs. |
| 5 | Anastasia | Nikitina | New methods of magnetic resonance theranostics |
| 6 | Boris | Nikolaev | Low-field Bench-top NMR analysis of pharmaceutical, food products in chemical laboratory |
| 7 | Vasilii | Pelipko | Configuration Determination of Regioisomeric Spirocyclopropanes Using NMR Spectroscopy Methods |
| 8 | Alina | Petrova | Investigation of biosilification mechanisms by experimental EPR methods and calculated DFT method on the example of orthosilicic acid oligomers |
| 9 | Andrey | Rochev | Slowdown of spin-lattice relaxation of quadrupole nuclei in crystals by additional magnetic excitation |
| 10 | Alexey | Salin | Synthesis and NMR structure of Michael adducts derived from phosphine-catalyzed reaction of sesquiterpene lactone arglabin with nucleobases |
| 11 | Leila | Sharipova | The environment effect on the intramolecular mobility of pillar[5]arene |
| 12 | Anzhelika | Sheremeta | Identification of diosmin in Hyssopus officinalis L by ^1H NMR spectroscopy. |
| 13 | Semen | Shestakov | Optimization of the duration of ^{31}P -NMR analysis of lignin functional composition |
| 14 | Nadezhda | Sheveleva | Mechanical Relaxation of PPI and PAMAM Dendrimers of Low Generations |
| 15 | Mark | Smirnov | Application of ^1H and ^{13}C NMR spectroscopy for the determination of the key parameters of vegetable oils |
| 16 | Vladislav | Stanishevskiy | Topical problems of ^{15}N NMR spectroscopy. |
| 17 | Milosh | Ubovich | Effect of addition of lithium and aluminum salts on molecular mobility in ethylammonium nitrate. A molecular dynamics simulation study |
| 18 | Andrey | Uskov | Atomic mobility in metallic sodium confined to porous glass |
| 19 | Allisher | Vasilev | Freezing and melting transitions and atomic mobility in the nanoconfined Ga-Sn eutectic alloy |
| 20 | Vitalii | Vitko | Investigation of transmission characteristics of active ring resonator on nonlinear ferrite-ferroelectric delay line |
| 21 | Vladimir | Voronov | On the possibility of using nuclear magnetic resonance to create a quantum computer based on a top-down approach |
| 22 | Timophey | Zhivotikov | Applied possibilities of using the ^{35}Cl NQR line in KClO_3 |
| 23 | Anna | Kuzminova | Development and characterization of novel membranes based on sodium alginate modified with Zr-MOFs. |