Schedule

18-th International School-Conference

«Magnetic Resonance and its Applications. Spinus-2021»

March 29 - April 02, 2021

St. Petersburg

	MONDAY – 29 March 2021
Moscow time!	
10:00 – 10:20	**Opening**
10:20 – 11:00	**Malcolm Levitt (Southampton, UK)** **Lecture:** Navigating the space of spin operators
11:00 – 11:40	**Kev Salikhov (Kazan, Russia)** **Lecture:** On the importance of the paradigm in the development of science
11:40 – 12:00	**COFFEE BREAK**
12:00 – 12:40	**Kazunobu Sato (Osaka, Japan)** **Lecture:** Spin manipulation of organic radicals by advanced pulsed ESR spectroscopy
12:40 – 13:20	**Georgios Papavassiliou (Athens, Greece)** **Lecture:** Tracing the "invisible" Polarons in Ferromagnetic Manganites. A combined NMR and HRTEM study in the temperature range 3.2 - 1000K

13:20 – 13:40	**Andrey Gavrilenko (Kazan, Russia)** **Oral report:** Study of Doped Chalcopyrite Cu1-XPdXFeS2 Compounds by 63,65Cu NMR and EPR Methods
13:40 – 14:00	**Egor Alakshin (Kazan, Russia)** **Oral report:** Nanostructures research using nuclear magnetic resonance of helium-3
14:00– 14:15	**Georgii Andreev (Kazan, Russia)** **Oral report:** Deviant behaviour of magnetization of microsized powder of Ising dipolar antiferromagnet LiDyF4 at temperatures T > TN
14:15– 14:30	**Alina Rakhimova (Surgut, Russian)** **Oral report:** Electron spin resonance method data for core samples from the Tomsk region deposits
14:30 – 15:30	**LUNCH**
15:30 – 16:10	**Olga Lapina (Novosibirsk, Russia)** **Lecture:** Modern SSNMR for studing structure of functional materials
16:10– 16:25	**Larisa Tsyro (Surgut, Russian)** **Oral report:** Spin properties of the water-Portland cement system
16:25– 16:40	**Junko Ikeda (Chiba, Japan)** **Oral report:** The simple method of estimation of a retarder influence on the cement hardening process
16:40– 16:55	**Anastasiia Nagmutdinova (Bologna, Italy)** **Oral report:** Time domain NMR Pake-Doublet analysis of sorption cycles experiments of cement materials
16:55– 17:10	**Arina Parfishina (Kazan, Russia)** **Oral report:** The first observation of NMR in 169Tm in magnetically diluted Van Vleck paramagnet LiTm0.02Y0.98F4
17:10 – 17:30	**COFFEE BREAK**
17:30 – 18:10	**Stefan Jurga (Poznań, Poland)** **Lecture:** Copolymer systems studied by NMR and other complementary techniques
18:10– 18:50	**Elena Charnaya (Saint-Petersburg, Russia)** **Lecture:** NMR studies of phase transitions in confined metals and alloys
	TUESDAY – 30 March 2021
Moscow time!	
10:00 – 10:40	**Sergey Vasiliev (Turku, Finland)** **Lecture:** Atomic hydrogen in solid molecular crystals. Magnetic Resonance and Quantum Diffusion
10:40 – 11:20	**Yury Bunkov (Moscow, Russia)** **Lecture:** Spin Superfluid Quantum Computing
11:20 – 11:40	**Oksana Koplak (Chernogolovka, Russia)** **Oral report:** Ferromagnetic resonance of magnetic multilayered structures

11:40 – 12:00	**COFFEE BREAK**
12:00 – 12:40	**Jacques Friassard (Paris, France)** **Lecture:** NMR Studies of metals and supported metal particles
12:40 – 13:20	**Jozef Kowalewski (Stockholm, Sweden)** **Lecture:** Paramagnetic relaxation in solution: an overview
13:20 – 13:40	**Giuseppe Ferrauto (Torino, Italy)** **Oral report:** Supramolecular interaction between macrocyclic Gd (III) complexes and polyaromatic systems as innovative way to enhance relaxivity
13:40 – 13:55	**Wassilios Papawassiliou (Stockholm, Sweden)** **Oral report:** Broadband High Resolution NMR Studies of Topological Matter
13:55 – 14:10	**Edem Chakalov (Saint-Petersburg, Russia)** **Oral report:** Using electronic criterion towards to the halogen bond for prediction 31P NMR chemical shift of phosphine oxides as probe acceptors
14:10 – 14:30	**Rustem Khusnutdinov (Kazan, Russia)** **Oral report:** Two-frequency flat gradiometer for searching explosives hidden under clothing – modeling and experiment
14:30 – 15:30	**LUNCH**
15:30 – 16:10	**Bernhard Bluemich (Aachen, Germany)** **Lecture:** Advances and Adventures with Compact Magnetic Resonance
16:10–17:10	Oral blitz reports of young scientists (5min × 10); see speakers below in the list of **POSTER SESSION I**
17:00 – 17:30	**COFFEE BREAK**
17:30 – 18:50	**POSTER SESSION I**
	WEDNESDAY – 31 March 2021
Moscow time!	
10:00 – 10:40	**Igor Koptyug (Novosibirsk, Russia)** **Lecture:** Parahydrogen-induced polarization: bridging the gap between homogeneous and heterogeneous catalysis
10:40– 10:55	**Anna Mastova (Novosibirsk, Russia)** **Oral report:** The 1H NMR and CIDNP study of the interaction of nonsteroidal anti-inflammatory drug ketoprofen with L- and D-tryptophan
10:55– 11:10	**Polina Kononova (Novosibirsk, Russia)** **Oral report:** The 1H NMR and MD study of the interaction of the antiviral agent glycyrrhizin with lipid membranes: an effect on lipid mobility and membrane fusion

11:10– 11:25	**Polina Skvortsova (Kazan, Russia)** **Oral report:** Pillar[5]arene complexes with palindromic DNA decamer and plasmid DNA
11:25– 11:40	**Alina Pichugina (Surgut, Russia)** **Oral report:** The role of radicals in the formation of pathogenic organomineral formations in the body
11:40 – 12:00	**COFFEE BREAK**
12:00 – 12:40	**Yuri Pirogov (Moscow, Russia)** **Lecture:** Multinuclear MRI investigations
12:40 – 13:20	**Uwe Eichhoff (Gaggenau, Germany)** **Lecture:** Advanced MRI-methods for evaluation of Parkinson`s disease
13:20– 14:00	**David Lurie (Aberdeen, United Kingdom)** **Lecture:** Fast Field-Cycling Magnetic Resonance Imaging
14:00 – 14:15	**Elizaveta Kononenko (Novosibirsk, Russia)** **Oral report:** Operando 3D MRI visualization of complex heterogeneous catalytic system using parahydrogen
14:15 – 14:30	**Vladimir Koshman (Novosibirsk, Russia)** **Oral report:** The 1H NMR study of lipid peroxidation processes involving chelate complexes of thiosemicarbazone Dp44mT
14:30 – 15:30	**LUNCH**
15:30 – 16:10	**Thomas Meersmann (Nottingham, United Kingdom)** **Lecture:** Monoatomic spin systems as magnetic resonance probes for biomedical and engineering applications
16:10 – 16:30	**Daniela Lalli (Alessandria, Italy)** **Oral report:** Mn-Based Silica Nanoparticles as Potential MRI Probes
16:30– 16:45	**Aleksandra Kusova (Kazan, Russia)** **Oral report:** Protein intermolecular interactions according to the translational diffusion by PFG NMR and DLS
16:45– 17:00	**Carlos Cabal Mirabal (La Habana, Cuba)** **Oral report:** The sense of the development of MRI.
17:00 – 17:30	**COFFEE BREAK**
17:30– 17:50	**Carlos Cabal Mirabal (La Habana, Cuba)** **Oral report:** Curie Spin relaxation contribution during the aggregation process of HbS Hemoglobin
17:50– 18:05	**Fabian Tamayo Delgado (Santiago de Cuba, Cuba)** **Oral report:** Correlation times and water fractions distribution in HbA and HbS intracellular solutions
18:05– 18:20	**Mariia Dmitrenko (Saint-Petersburg, Russia)** **Oral report:** Development and investigation of pervaporation green high-performance hydroxyethyl cellulose/sodium alginate membranes for dehydration

18:20– 18:35	**Anna Kuzminova (Saint-Petersburg, Russia)** **Oral report:** The correlation of structure with transport properties of novel pervaporation sodium alginate membranes modified by Zr-MOFs
18:35– 18:50	**Vladislav Liamin (Saint-Petersburg, Russia)** **Oral report:** Investigation of novel pervaporation membranes based on sodium alginate – fullerene derivative composites
	THURSDAY – 01 April 2021
Moscow time!	
10:00 – 10:40	**William Price (Sydney, Australia)** **Lecture:** NMR Diffusion Measurements and Time-Dependent Samples
10:40 – 11:20	**Janez Stepišnik (Ljubljana, Slovenia)** **Lecture:** Frequency selection of molecular translation dynamics with different NMR MGSE sequences
11:20 – 11:40	**Georgy Mozzhukhin (Gebze-Kocaeli, Turkey)** **Oral report:** Quadrupole coupling constants in compounds with aminogroups in liquids
11:40 – 12:00	**COFFEE BREAK**
12:00 – 12:40	**Leonid Grunin (Kirchheim/Teck, Germany)** **Lecture:** Review of Pulse Sequences Applicable in Time-Domain NMR.
12:40– 13:00	**Tatiana Kulagina (Chtunogolovka, Russia)** **Oral report:** Structure and Mobility of Elastomers Studied by the signals of primary and stimulated echoes
13:00– 13:20	**Sergey Vasil'ev (Chtunogolovka, Russia)** **Oral report:** Hambergite (Be2BO3OH) as a model of one-dimensional dipolar coupled 1H zig-zag spin chain.
13:20– 13:35	**Maria Ivanova (Yoshkar-Ola, Russia)** **Oral report:** TD-NMR in study of fat melting
13: 35– 13: 50	**Sirvan Sultan Uguz (Ankara, Turkey)** **Oral report:** Use of TD NMR Approaches for Characterisation of Bovine and Porcine Gelatin Based Soft Candies
13: 50– 14:05	**Lydia Gkoura (Athens, Greece)** **Oral report:** 2D NMR diffusion-relaxation (DT2) studies of water in hydrophobic carbon nanotubes
14:05– 14:20	**Naira Khusnutdinova (Saint-Petersburg, Russia)** **Oral report:** Modeling the system of the melt of carbosilane dendrimers
14:20 – 15:30	**LUNCH**
15:30 – 16:50	Oral blitz reports of young scientists (5min × 14); see speakers below in the list of **POSTER SESSION II**

16:50 – 17:10	**Andrei Komolkin (Saint-Petersburg, Russia)** **Oral report:** Master programs in Physics at Saint Petersburg State University
17:10 – 17:30	**COFFEE BREAK**
17:30 – 19:00	**POSTER SESSION II**
	FRIDAY – 02April 2021
Moscow time!	
10:00 – 10:40	**Vladimir Chizhik (Saint-Petersburg, Russia)** **Lecture:** A new model of the microstructure of mixtures of ionic liquids with water: an alternative to " water pockets"
10:40– 11: 10	**Sergey Dvinskikh (Stokholm, Sweden)** **Oral report:** Ionic liquid crystals studied by solid-state NMR spectroscopy
11: 10– 11: 25	**Milosh Ubovich (Saint-Petersburg, Russia)** **Oral report:** Rotational motion of ions in alkylammonium nitrate ionic liquids by molecular dynamics simulation method
11: 25– 11: 40	**Elisaveta Fedotova (Saint-Petersburg, Russia)** **Oral report:** Computer simulation of atactic polymers
11:40 – 12:00	**COFFEE BREAK**
12:00 – 12:40	**Peter Tolstoy (Saint-Petersburg, Russia)** **Lecture:** Self-assembly of small molecules by H-bonds: how to distinguish dimers, trimers, tetramers by NMR
12:40– 12:55	**Valerii Karpov (Saint-Petersburg, Russia)** **Oral report:** Sensitivity of 77Se chemical shift to the selenium atom surroundings in water media
12:55– 13:10	**Aleksandr Koronatov (Saint-Petersburg, Russia)** **Oral report:** 2D NMR Structure Determination of 3,4-Dihydro-1,2,4-triazine Intermediate in Novel Rh(II)-catalyzed Transannulation Reaction
13:10– 13:25	**Nadezhda Antonova (Saint-Petersburg, Russia)** **Oral report:** Micelle formation in magnesium hexanoate solution in the presence of a peptide 1B03
13:25– 13:40	**Andrey Stanislavovas (Kazan, Russia)** **Oral report:** Spin kinetics of gaseous 3He in oriented aerogels
13:40– 13:55	**Konstantin Belov (Ivanovo, Russia)** **Oral report:** Comparison of the spatial structure of the mefenamic acid molecule in solution at normal and supercritical state

13:55– 14:10	**Elizaveta Andronova (Saint-Petersburg, Russia)** **Oral report:** Proton mobility in Dion-Jacobson phase HCa2Nb3O10 studied by 1H NMR
14:10– 14:25	**Anna Tyurtyaeva (Saint-Petersburg, Russia)** **Oral report:** Nanoconfined water in pillared zeolites probed by 1H NMR
14:25– 16:00	**MEETING OF AWARDING COMMISSION**
16:00 – 17:00	**AWARDING and CLOSING**

POSTER SESSION I (Tuesday, 17:30 – 18:50)

1	Dmitry Aleshin	Double step spin transition in binuclear Fe-Fe helicates with incapsulated anion by NMR spectroscopy
2	Aleksandra Andrzejowska	Molecular dynamic of bound water in Antarctic lichenized fungus Umbilicaria antarctica Frey & I.M. observed by sorption isotherm and 1H-NMR
3	Valerii Bezrodnyi	Computer simulation and NMR study of the temperature dependencies of the structural and dynamic characteristics of Lys2Arg peptide dendrimers
4	Dmitriy Blokhin	The spatial structure of SEM1(86-107) peptide in “protein–micelle of dodecylphosphocholine” complex by NMR spectroscopy
5	Agata Bogdał	The classification of residual bound water fractions in rehydrated phospholipid lyophilizates
6	Anna Butyugina	Computer simulation of ionic liquid [C12-Im-C12]+[BF4]– in smectic-A phase
7	Mariia Dmitrenko	The application of bulk and surface modifications for sodium alginate membranes for enhanced pervaporation dehydration
8	Emil Fatullaev	The Brownian dynamics and numerical self-consistent field simulations of the dendrigraft nanocontainers
9	Albina Gafarova	EPR Study and DFT-Assisted Identification of Radicals in γ-Irradiated Calcium Gluconate
10	Irina Golubeva	Primary echo signals in flexible polymers with isolated three-spin groups
11	Sofia Mikhtaniuk	The structural and dynamic characteristics of Lys2Gly and Lys2Lys peptide dendrimers. The molecular dynamics simulation and NMR relaxation at different temperatures
12	Alexander Selivanov	Optimization of parameters for molecular dynamics modeling of ionic liquid [BMIM][SCN].
13	Nina Djapic	Chiral carbon bearing the hydrogen: a porphyrin and the tetrapyrroles

14	Grigorii Karnaukh	Direct exchange of identical quantum objects with a finite number of eigenstates
15	Pavel Kupriyanov	Peculiarities of processing and analysis of NMR spectra of liquids with a low abundance of studied nuclei in the Earth magnetic field
16	Yury Neronov	Determination of the magnetic moments of the 6Li and 7Li nuclei using a spectrometer that registers simultaneous signals from two types of nuclei
17	Mikhail Rudavets	Mellin-Barnes Integral Approach for Exact Evaluation of Spin Echo Signals from Fluids with Magnetizible Grains.
18	Arseniy Slobodyuk	NMR spectra, structure and ionic motions in the new potassium fluoridooxalate zirconates
19	Murat Tagirov	Magnon quantisation in the magnetic field gradient

POSTER SESSION II (Thursday, 17:30 – 18:50)

1	Olga Kokh	Investigation of the molecular mobility of the ionic liquid BmpyrrNTF2 by NMR methods
2	Mikhail Kostin	The study of non-covalent interactions in complexes of CH3Br by quantum-chemical calculations
3	Karol Kubat	Hydration properties of tadalafil preparations in the matrix of the soluplus polymer.
4	Anna Kuzminova	Development and characterization of novel pervaporation membranes based on sodium alginate modified by FeBTC
5	Anna Lavrova	The basic physics of ASL perfusion and its applications in neuroimaging: a review
6	Sultonazar Mamadazizov	14N Quadrupole Coupling Constants calculation in some compounds with amino groups
7	Yulianela Mengana	Evaluation of the dynamic viscosity in protein solutions applying Nuclear Magnetic Relaxation.
8	Anastasia Nikitina	Research and development of an information system for optimizing the contrast of a magnetic resonance image
9	Vasilii Pelipko	Nuclear Overhauser effect in determination the geometric configuration of the N'-substituted hydrazone methylpyruvate
10	Julia Popova	The Application of Nuclear Magnetic Resonance Spectroscopy to the Calculation of Lignin Structure Formulas
11	Mark Smirnov	1H High-resolution NMR spectrometry and relaxometry for soybean oil research
12	Viktoria Vasinovich	Peculiarities of microstructure in mixtures SLAS-DTAB-D2O according to NMR data
13	Irina Yefimova	Molecular Dynamics simulation of ethylenediamine-Cu2+

		complex and copper-II chloride in aqueous solutions
14	Valerii Bezrodnyi	Novel lysine-based peptide dendrimers modeled by the self-consistent field approach
15	Sofia Mikhtaniuk	The self-assembly of the amphiphilc molecules consisting of polylysine dendrons with the single and double hydrophobic tails
16	Dmitriy Kitanin	The distribution of electron density in orpiment. Crystalline and amorphous phases.
17	Daniel Jakubiec	1H-NMR spectroscopy and relaxometry studies of hydration from gaseous phase of foliose lichenized fungi: Roccellina nigricans from Atacama Desert region Chañaral.
18	Arseniy Slobodyuk	NMR study of structure and inner motion types of $ZnZrF_6 \cdot 6H_2O$ and its dehydration products
19	Alexandr Ievlev	Modern capabilities of NMR magnetometry.
20	Yury Neronov	NMR spectra of potassium-39 nuclei in aqueous solutions and determination of the magnetic moment of the 39K nucleus.