Poster session
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Poster abstract	Remarks

1. Study on the Impact of Nickel Substitution on the Structural and Magnetic Characteristics of $SrFe_{12}O_{19}$

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$SrFe_{12}O_{19}$ is a magnetically hard material with high coercivity, high magneto-crystalline anisotropy, and an easy magnetization axis along the ***c*** axis. This material can be used in magnetic recording media, in magnetic hyperthermia, in microwave devices, and in components of high-frequency and magneto-optical devices [1].

Ceramic samples of solid solution of $SrFe_{12-x}Ni_xO_{19}$ (***x= 0-0.3***) hexaferrites prepared by the sol-gel technique were studied at room temperature on an HRFD neutron diffractometer, which made it possible to study the properties of the crystal and the magnetic structure of this ferrimagnetic material depending on the degree of substitution of magnetoactive ions. The refinement of neutron diffraction patterns was carried out by the Rietveld method in the FullProf software package.

Partial substitution of magnetoactive Fe ions by Ni ions leads to a monotonic decrease in the unit cell volume from 692.97 (2) $Å^3$ (***x = 0.0***) to 692.07 (2) $Å^3$ (***x = 0.3***). The decrease in the magnetic moment calculated from the neutron spectra is confirmed by a decrease in the Curie temperature from 659 *K* (***x = 0.1***) to 655 *K* (***x = 0.3***) with increasing ***x***. The values of magnetic saturation (M_s) coercivity (H_c), remanent magnetization (M_r), and anisotropy field (H_a) were determined for the each concentration of Ni. The obtained data shows minimal changes in the main magnetic parameters for the different concentration. Such behavior of the material in terms of magnetic properties can be caused by the disruption of super-exchange interactions between Fe-O-Fe ions, similar to [2]. Morphological changes in the sample were observed according to the concentration of Ni.

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2. Polymer Brushes Synthesized by the "Grafting-through" Approach: Characterization and Scaling Analysis

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Polymer brushes are a class of surface coatings consisting of macromolecules attached to a surface and they have been widely studied in recent years due to their broad range of applications: effective lubricants, smart coatings, protective coatings, passivated surfaces for laboratory studies and etc. There are many approaches to synthesize the polymer brush, but from the variety of methods the "grafting-through" can be distinguished for its simplicity and purity of the synthesis. Despite the fact that "grafting-through" is a promising technique for comparatively simple surface modification, its main problem is related to self-limiting nature (the possibility of controlled growth of final polymer brushes) and lack of understanding of final structure of such brush.

In order to analyze the "grafting-through" technique as an approach to synthesize the dense polymer brushes, here, we propose the combined morphological and scaling analysis of the brushes synthesized by the "grafting-through" method, demonstrate the possibility of regulation of the thickness of brushes and represent the scalability for industrial application. The chemical composition of the surface in the proposed three-step approach was analyzed and proved by photoelectron and infrared spectroscopy. The growth of the brush was verified and controlled with X-ray reflectometry and atomic-force microscopy. It was shown that the thickness of the dried brush can be tuned in a controlled manner by varying the polymerization temperature. The scaling dependence of the thickness of the dried brushes d on the length of the polymer $d \sim L^{\nu}$ was obtained by comparing reflectometry and dynamic light scattering data. The value of the exponent $\nu = 0.82$ corresponds to a rather high grafting density, exceeding the density of mushroom-like ($\nu \sim 1/3$) brushes and approaching the value for stretched polymer brushes ($\nu \sim 1$). A 10-fold increase in the polymer molecular weight leads to a slight decrease in grafting density by a factor of 2, which suggests that the "grafting-through" approach allows obtaining brushes with a high grafting density independently of attached polymer chain length. Herein, the possibility of attachment of uniform polymer brush on large substrates with this approach was demonstrated, which means the scalability of the "grafting-through" technique. The considered approach opens up a simple way for surface modification with polymer nanolayers of controlled thickness.

3. The influence of phospholipid composition on membrane interaction with amyloid beta peptides within molecular dynamics simulations

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At the present time there is a hypothesis about the key role of amyloid beta peptide in the onset of Alzheimer's disease. It is considered that its interaction with cell membranes causes a disruption of their permeability and integrity, which may trigger further neurodegenerative processes [1]. The experimental study showed that the peptide takes part in the morphological changes of the phospholipid membrane during its transition through the main lipid phase transition temperature [2]. However, this research did not allow us to look into the processes and resulting structures at the atomic level. The latter results are better achieved in theoretical studies that we have carried out recently.

It has been suggested that different phase states within one membrane may play a key role in the process of phospholipid membrane destruction in the presence of amyloid beta peptides. In order to shed some light on this, the interaction of Aβ(25-35) with DPPC and DOPC phospholipids, which have different tail lengths and might form rafts, at different temperatures was simulated using the coarse-grained and all-atom molecular dynamics method in the GROMACS 2019.3 software package. Using the coarse-grained approach, we have obtained the type of structures that are formed from a box of randomly distributed components at different temperatures below and above the main transition. Whereas all-atom consideration has allowed us to determine the influence of rafts on the internal location of peptides in the membrane.

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4. Methods of high-performance numerical study of physical characteristics of superconducting Josephson structures in dependence of parameters of the models

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Methods and software packages for parallel implementation of studying two models of superconducting structures are presented. The first model describes a system of coupled long Josephson junctions taking into account the inductive and capacitive coupling between neighboring junctions and electromagnetic radiation at their boundaries. The second model describes the structure of a point φ_0 junction with spin-orbit coupling in a ferromagnetic layer and a pulsed current source acting on it.

The developed parallel computing methods made it possible to successfully study the physical characteristics in these models in a wide range of parameters. The parallel software packages have been deposited to the JINR program library and are freely available. The calculations were performed on the HybriLIT computing resources of the JINR Multifunctional Information and Computing Complex.

5. The analysis of PhTNS and nanoarbidol structure

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Modernization and improvement of existing methods of drug delivery is one of the most important tasks in pharmaceuticals. [1]. A phospholipid transport nanosystem (PhTNS) was developed at the Orekhovich Institute of Biomedical Chemistry. This system has small dimensions compared to conventional liposomal systems, which leads to an increase in the effectiveness of drugs [2].

One of the most informative ways to study the structure of such aggregates is the small-angle scattering method. This report will present an analysis of neutron small-angle data from PhTNS and a vesicular nanodrug: nanoarbidol. During the data analysis, the main structural characteristics (the radius of the system and the thickness of the lipid bilayer) were obtained.

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6. Wide aperture Back-Scattering detector (BSD-A) for the High-resolution Fourier diffractometer

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The high-resolution Fourier diffractometer (HRFD) has been in routine operation since 1994 at the long-pulse neutron source, the IBR-2 reactor, in Dubna. Its fast Fourier chopper provides probably the best compromise between very high resolution in reciprocal space ($\Delta d/d \approx 0.001$) and the intensity. For further improving intensity of TOF-diffraction pattern, a wide-aperture ring backscattering detector (BSD) has been developed on the basis of ZnS(Ag)/^{6}LiF scintillator. BSD is designed in the form of 6 concentric rings, each of which is subdivided into 12 identical parts. The main parameters of the detector are the following: range of scattering angles is 2θ = (133 - 175) degrees, covered solid angle is $\Omega d \approx 2.0$ sr, average percentage absorption efficiency gets closer to 85%, geometrical contribution to resolution function does not exceed $\Delta d/d = 0.0005$. In the report the concept of the detector is described and its data acquisition system is presented. The start of operation of the detector at the HRFD is scheduled for 2025.

7. Effects of Non-Isovalent Substitution on the Structural and Magnetic Properties of $SrFe_{12-x}(CoSn)_xO_{19}$ Solid Solutions (x = 0–0.5)

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Such unique properties of strontium hexaferrites as high magnetic anisotropy and coercivity have enabled these materials to find widespread practical applications in permanent magnets, microwave devices, and magnetic information storage media [1-3].

The features of the crystalline and magnetic structure of the ferrimagnetic material, depending on the degree of substitution by Co and Sn ions, were studied using neutron diffraction on the HRFD neutron diffractometer at room temperature. Refinement of the spectra was performed using the Rietveld method in the FullProf software package.

The substitution of magnetoactive Fe ions with Co and Sn ions in the solid solution $SrFe_{12-x}(CoSn)_xO_{19}$ results in a non-monotonic change in the unit cell volume, increasing from 691.088 Å³ (x = 0) to 693.213 Å³ (x = 0.3) and then decreasing to 692.005 Å³ (x = 0.5).This is attributed to the larger ionic radii of Co and Sn ions (r = 0.885 Å and r = 0.83 Å, respectively) compared to Fe ions (r = 0.785 Å).

The observed decrease in the Curie temperature from 674 K (x = 0.1) to 660 K (x = 0.6) with increasing x indicates a disruption of superexchange interactions between Fe-O-Fe ions forming the crystal lattice. A comparison of the neutron diffraction results shows that the concentration dependence of the total magnetic moment is influenced by the types of crystallographic positions in which Co and Sn ions substitute Fe ions, due to varying distortions of individual structural fragments. A reduction in the total magnetic moment, determined using neutron diffraction, is observed when Co and Sn ions occupy the crystallographic positions $4f_{II}$ and *2b* (as x increases from 0.1 to 0.2) and the $4f_{II}$ positions (as x increases from 0.3 to 0.5).

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8. Quantum fluctuations in triangular lattice Kitaev-Heisenberg magnets

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Order-by-disorder, whereby fluctuations lift an accidental classical ground state degeneracy to stabilize a subset of ordered states, is a recurrent and prominent theme in the field of frustrated magnetism where magnetic moments are subject to competing interactions. The Kitaev-Heisenberg model [1] is one such Hamiltonian, which does not have the required symmetry but the ground state is largely degenerate [2,3]. It implies that quantum fluctuations are necessarily stabilize the ordered ground phase.

Motivated by this, the magnetic phase diagram and magnon spectra of the anisotropic Kitaev-Heisenberg model with nearest neighbor ferromagnetic coupling are investigated using linear and non-linear spin wave theory. We find that interplay of several bond-dependent interactions of Kitaev-Heisenberg model stabilize several ferromagnetic states through quantum fluctuations. Moreover, quantum effects are also prominently pronounced in the magnetic spectrum. The results are corroborated by the numerical density matrix renormalization group (DMRG) calculations.

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9. Simulation of a controllable magnetization reversal in a chain of Phi-0 junctions by an ac voltage pulse

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In Phi-0 Josephson junctions, the spin-orbit interaction in a ferromagnet layer provides a mechanism for direct coupling between the magnetization and the superconducting current, which makes it possible to control the magnetic properties by means of the Josephson current, as well as the effect of magnetization on the Josephson current. Recently, the possibility of developing cryogenic memory based on the magnetization reversal in the Phi-0 junction has been studied [1, 2]. However, when using several Phi-0 junctions in a single chip, it becomes necessary to realize the magnetization reversal in a selected Phi-0 junction. We propose a solution to this problem based on mathematical modeling of the dynamics of a system consisting of three Phi-0 junctions connected via LCR-circuits, which is reduced to solving the Cauchy problem. It is shown that by applying an AC external voltage pulse with a frequency coinciding with the eigenfrequency of the LCR-circuit, it is possible to realize the magnetization reversal in a selected Phi-0 junction, i.e., the possibility of controlled reversal of magnetization is demonstrated. The influence of system parameters on the dynamics of magnetization in each of the Phi-0 junction is studied in detail. We have developed a software module for the performed calculations. The developed materials are publicly available on the ML/DL/HPC ecosystem of the HybriLIT platform (LIT JINR) [3] in the form of electronic books Jupyter Book [4, 5].

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10. Structural and vibrational properties of the $Cu_3Bi(SeO_3)_2O_2Cl$ francisite at high-pressure

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In the last few decades, low-dimensional magnetic materials have attracted considerable attention in experimental and theoretical studies. They have been found to exhibit physical phenomena such as ferroelectricity, spin liquid, spin ice, and properties inherent to multiferroics. This makes them promising for practical applications in spintronics and quantum computing. Such compounds include materials based on $Cu_3R(SeO_3)_2O_2X$ (R is a rare earth element, and X is Cl, Br), which are called francisites [1,2]. The application of external pressure allows controlled changes in interatomic distances and valence angles in such compounds, which can significantly change their physical properties [3].

In our work we present the results of the study of the compound $Cu_3Bi(SeO_3)_2O_2Cl$ by X-ray diffraction and Raman spectroscopy in a wide pressure range up to ~18 GPa at room temperature. By means of the X-ray diffraction under high pressure it has found the crystal structural transition from the original orthorhombic crystal structure with the *Pmmn* space group to the *Pcmn* space at pressure is 5.5. GPa. The lattice parameters, bond lengths and bulk modulus have been determined for this crystal structure phase. The results of the Raman spectroscopy indicate to the same crystal structural transitional under high pressure. Also, the Raman vibrational mode spectra show significant anomalies around 5 and 10 GPa. These pressure-induced effects can also lead to changes in the magnetic properties of this geometrically frustrated magnetic material.

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11. Beam diagnostic tools for the LINAC-200 linear accelerator

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The Dzhelepov Laboratory of Nuclear Problems (DLNP) is currently working on the commissioning of the LINAC-200 linear electron accelerator. This accelerator will allow to conduct methodological studies of elementary particle detectors developed in the DLNP and other JINR laboratories using test electron beams with energy from 20 to 200 MeV in a wide range of beam intensity.

The beam diagnostic system of the LINAC-200 facility provides continuous monitoring of beam parameters (current, position, profile) along the accelerator and measurement of its output parameters.

The accelerator uses high-frequency traveling-wave monitors, TV beam position monitors, compton scattering electron detectors, and magnetic induction sensors. Bending magnets are used to measure the beam electron energy.

12. Neutron tomography studies of Ancient ceramic utensils from the Akterek burial ground, Republic of Kazakhstan

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The paper presents the results of neutron diagnostics of seven ceramic vessels from excavations near the village of Akterek, Zhambyl district, Almaty region. The experiment was carried out at the specialized experimental station TITAN, located on the 1st horizontal channel of the research reactor WWR-K [1].

Three-dimensional models of ceramic vessels were obtained, from which data on the volume distribution of inhomogeneities in the samples, in particular the internal pore space, were extracted. The average pore volume and porosity of the samples varies from a minimum of 0.08% and a maximum of 0.39%. Some samples contain additional inclusions characterized by a high neutron attenuation coefficient, with a volume of 0.36% and 0.14%, respectively. Based on previous studies, these may be calcite phases. After the procedure of pore segmentation from the volume of the studied ceramic objects, the average sizes of the internal pores of the ceramic vessels were studied, their morphological parameters were obtained. To systematize the structural data of neutron tomography, contour diagrams of the ratio of pore sizes to their elongation parameter were constructed. The generalized contour plot shows that most pores have a size in the range of 1.2-1.5 mm, and the elongation varies from 0.0 to 0.8 regardless of the particle size. However, in the zone of large pore sizes from 3 to 5 mm, contours of low-symmetry formations with an elongation of 0.2 are observed. This indicates the existence of a small number of large shapeless voids in a number of the studied ceramic samples.

Raman spectroscopy was used to identify the phases that make up the material of ceramic products. Raman scattering spectra at room temperature were obtained using a Solver Spectrum spectrometer with an excitation wavelength of 473 nm. The dominant phase of quartz was detected, as well as phases of hematite, orthoclase and anatase, which are common clay-forming components. In almost all the ceramic vessels studied, an amorphous carbon phase was found inside the volume, according to the relative height of the Raman doublet of which the annealing temperature of the ceramic products was estimated [2].

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13. Investigation the impact of Biowaste Composition and Activated Carbon structure on the Electrochemical Performance of Supercapacitors

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The increasing demand for sustainable and efficient energy storage materials has led to significant research into utilizing waste biomass for producing activated carbons. This study investigates the impact of the structural properties of activated carbons derived from various lignocellulosic biomasses—barley straw, wheat straw, and wheat bran—on the electrochemical performance of supercapacitors. The Fourier Transform Infrared (FTIR) spectroscopy analysis reveals the presence of key functional groups and their transformations during carbonization and activation processes. The Raman spectra provide detailed insights into the structural features and defects in the carbon materials. Electrochemical tests indicate that the activated carbon specific capacitance and energy density are influenced by the biomass source. It is shown that the wheat bran-based electrodes exhibit the highest performance. This research demonstrates the potential of waste biomass-derived activated carbons as high-performance materials for energy storage applications, contributing to sustainable and efficient supercapacitor development. The increasing demand for sustainable and efficient materials has driven significant research into the utilization of waste biomass as a renewable source for producing activated carbons for high power energy storage systems such as supercapacitors and li-ion capacitors. Waste biomass, a byproduct of various agricultural and industrial processes, offers an abundant and low-cost precursor for activated carbon production. This approach not only addresses waste management challenges but also provides a sustainable pathway for creating high-value materials with diverse applications. Activated carbons are renowned for their high surface area, porosity, and adsorption capacitance, making them ideal candidates for environmental and energy storage applications, particularly in the development of electric double-layer capacitors (i.e. supercapacitors). These energy storage devices require materials with high electrical conductivity, electrochemical stability, and large surface area to achieve high energy and power densities. Activated carbons derived from waste biomass possess these characteristics, making them promising materials for supercapacitor electrodes. This study not only enhances the fundamental knowledge of biomass-derived activated carbons but also offers practical insights for developing high-performance supercapacitor electrodes from sustainable resources. These findings underscore the importance of selecting appropriate biomass sources and optimizing activation processes to enhance the electrochemical performance of supercapacitors. This study provides valuable insights into the sustainable production of advanced materials for energy storage, promoting the development of efficient and eco friendly supercapacitors.

14. Research of the RF photogun and the accelerating structure of the linear electron accelerator LINAC-200

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This work is devoted to the study of the resonant structure of the accelerating sections of the LINAC-200 accelerator [1] and the RF photogun of the photoinjector test bench [2]. For this purpose, models were created in the CST Studio software package. Simulations were carried out for different operating conditions of the structures: at room temperature (T = 20 °C) and with the thermal stabilization system in operation (T = 45 °C). Obtained results will be used for tuning of the temperature regime for the accelerator sections and the RF gun cells.

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