Poster session Programme Advisory Committee for Condensed Matter Physics (20-21 January 2022)

Poster abstract	Remarks
1. Search for biomarkers in UV-induced NETosis	
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Neutrophil extracellular traps (NETs) are produced by neutrophilic granulocytes and consist of decondensed chromatin decorated with antimicrobial peptides. They defend the organism against intruders and are released upon various stimuli, including ultraviolet (UV) radiation. It's well known that extended exposure of the skin to UV leads to its damage and loss of protective properties. Many cells of the immune system, including neutrophils, are involved in the photoaging process [1]. In continuation of the initiated study on the activation of neutrophils by two approaches: biological (bacterial) and chemical (PMA) stimuli, we came over to examine the ability of neutrophils to realize NETs under the UVA (315-400 nm) irradiation. Human neutrophils were isolated from the whole blood obtained from healthy voluntary donor. Neutrophils unexposed to UV radiation but stimulated with PMA (50 nM). We applied sensitive Raman spectroscopy and succeeded to register citrulline Raman band evaluation during the first hour of neutrophil cells activation [2]. In the novel set of the experiments we applied UVA radiation in a dose-depended manner. Proceed to the first series of NETosis experiment on UV, we took under advisement the fact that there is a contradictory proposition in the literature on signaling pathways leading to NETosis, which suggest either NOX-independent or NOX-dependent pathway. In the case of NOX-independent signaling pathway often has to realize peptidylarginine deiminase 4 (PAD4), which citrullinates histones contributing to chromatin decondensation. Also, in accordance with literature, neutrophil cells were treated with the calcium ionophore A23187 (A23) to activate NOX-independent NETosis resulting in the citrullination of histones. Data analysis was done implementing immunofluorescence microscopy and Raman spectroscopy. It was revealed that UV-induced activation undoubtedly leads to the formation of NETotic cells in the form of cloud-like-spread in the observed immunofluorescence imaging. Nevertheless, in	
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2. Phase Composition and its Spatial Distribution in Antique and Medieval Coins <u>B. Bakirov^{1,2}, S. Kichanov¹, I. Saprikina^{1,3}, R. Khramchenkova^{2,4}</u>

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A detailed study of the chemical composition of antique and medieval numismatic materials using structurally diagnostic methods has gradually occupied its niche in the archeological natural-scientific research approaches [1-3]. Currently, coins are being intensively studied using non-destructive physical methods of metallography, electron microscopy, X-ray fluorescence and diffraction. The data obtained by these methods expand the possibilities of traditional coin research and provide knowledge about such aspects as the ratio of the nominal value of coins and the value of metal, the identification of crisis periods, trade and political ties between ancient states and cultural groups, etc. However, the data obtained by these methods on the structure, phase or chemical composition correspond only to the surface layers of the material or require the destruction of the sample, which may be critical in the study of coins. In this case, the use of non-destructive methods of neutron diffraction and tomography seems justified [1]. Neutron imaging and scattering methods are successfully used to determine and separate the components of alloys in the volume of coins. This helps to determine the bulk composition hidden by corrosion, identify coins, reconstruct minting technologies, find ore sources and describe the processes of degradation of coins, such as internal traces of corrosion and wear zones.

This work presents the results of structural studies of medieval silver coins from the territory of Volga Bulgaria and antique bronze coins from a Greek necropolis in the Krasnodar Territory. For medieval coins, the content of the silver and copper phases was established and spatial variations in composition were studied. For antique coins, the tin content, chemical composition and patina volume were determined. The neutron tomography method also restored the minting pattern of several studied coins. The results obtained shed light on the historical and economic processes of Volga Bulgaria and the Bosporan Kingdom.

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3. High pressure effect on internal structure and atomic dynamics of pharmaceutical compounds

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Due to the wide variety of phenomena realized in organic crystals at high pressure: polymorphic phase transitions, amorphization, etc., studies of pressure-induced changes in the crystal structure and atomic dynamics of complex molecular crystals is an urgent task in condensed matter physics [1,2]. In addition, structural studies of molecular crystals are important for optimization the of pharmaceutical production process, where, under additional mechanical influences (grinding or tabletting), irreversible polymorphic phase transitions or its amorphization can develop in the initial material, which entails significant changes in the physicochemical and pharmaceutical properties material. [3].

The use of high-pressure diffraction and Raman spectroscopy to study pharmacological components makes possible investigation of their structure and physical properties in the most complete way, which is necessary to understanding the nature and mechanisms of physical phenomena observed in them [4].

Therefore, the main objective of this study was detail investigation of physical properties and dynamics of the group of pharmaceutical compounds by means of different methods: X-ray diffractometry and Raman spectroscopy.

Investigation of internal structure and atomic dynamics of pharmacological components hypolipidemic agent lovastatin $C_{24}H_{36}O_5$ and antibacterial agent of loxacin $C_{18}H_{20}FN_3O_4$ were carried out.

The pressure dependence of vibrational modes of lovastatin measured at high pressures up to 9.8 GPa and room temperature were shown. The changes in a pressure behavior of the Raman lines were observed at pressures 3 and 5.2 GPa. Those changes can indicate the polymorphic phase transitions lovastatin under pressure. At pressures above 9 GPa a gradual broadening of Raman lines is followed by their disappearance up on further compression. Such a behavior corresponds to a gradual phase transition to the amorphous phase of lovastatin.

At pressure P>4.8 GPa, several changes in the X-ray diffraction data and Raman spectra of ofloxacin were observed, which indicate a pressure-induced phase transformation from initial form to HP-form of ofloxacin. Around this phase transformation, the noticeable anomalies in the pressure behaviour of different vibration frequencies of ofloxacin were found.

At P>7.3 GPa a gradual broadening of Raman modes, followed by disappearance of the most of them at about 10 GPa, were observed. Such a behavior corresponds to a gradual phase transition to the amorphous phase of the ofloxacin.

The structural mechanisms of the phase transitions in presented pharmaceutical compounds were discussed.

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4. Composite "track-etched membrane modified with metal-organic frameworks" for heavy metal adsorption

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In the last time, the problem of water purification from dangerous substances is becoming more and more acute. A large number of studies are devoted to the extraction of heavy metals from aqueous solutions [1,2,3]. In addition, the extraction and concentration of valuable heavy metals from solutions is also of interest. The creation of solid adsorbents with high capacity and stability in the aquatic medium is a very important task. One of the promising types of adsorbents is metal-organic frameworks. MOFs are crystalline materials consisting of an infinite network of metal-ions, or metal-ion clusters, bridged by organic ligands through coordination bonds into porous two- or three-dimensional extended structures. Very few MOFs are used as adsorbents from aqueous solutions because most MOFs are unstable in aqueous medium [1]. In our work, Ni-MOF {[Ni(*L*-trp)(bpe)(H₂O)]·H₂O·NO₃}_n (*L*-trp = *L*-tryptophan, bpe = 1,2-bis(4pyridyl)ethylene) and Zr-MOF MIP-202(Zr), based on *L*-aspartic acid, were synthesized. They are stable in an aquatic environment. With UV-Vis spectrometry, we investigated the properties of Ni-MOF and Zr-MOF in the process of ruthenium sorption from aqueous solutions of ruthenium chloride.

The possibility of efficient and convenient extraction of the adsorbent from the solution is significant. Most often, the sorbent is recovered by centrifugation or filtration, or using a magnet in the case of magnetic materials. Another interesting direction of the creation composite materials for adsorption is the infliction of MOFs on polymer substrates (membranes and fibers). Some researchers have proposed the use of MOFs as fillers in electrospun nanofibers [3]. Another variant is self-assembly of the adsorbent on a substrate [4]. This method was chosen in our work. A track-etched membrane, modified with chitosan, was studied as a substrate for the Ni-MOF. The membrane was received from Flerov Laboratory of Joint Institute for Nuclear Research (Dubna, Russia). The synthesis of Ni-MOF takes place under mild conditions that do not destroy either the membrane or the chitosan fibers. Only in the presence of chitosan MOF particles firmly adhere to the substrate. This is due to the structure of chitosan molecules, which can act as nucleation centers and increase hydrophilicity of the membrane. The synthesized materials were characterized by X-ray diffraction, thermal analysis, scanning electron microscopy and X-ray photoelectron spectroscopy. It was shown that the crystal structure and microstructure of pure MOF and MOF supported on the membrane are identical. In case of good adsorption properties of the obtained membranes coated with MOF particles, these composites can become a basis of filters for water purification from heavy metals.

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5. Radiation genomic research in the Laboratory of Nuclear Problems <u>N.E. Kharchenko</u>, K.P. Afanasyeva, M.V. Alexandrova, I.D. Alexandrov

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Through our Radiogen project in the Laboratory of Nuclear Problems research on the different quality radiation effects on the genes and genome of *Drosophila melanogaster* is conducting. In 2021, a pilot experiment to sequence the entire genome of individual offspring of intact and irradiated males was carried out. The radiation was produced by 60Co γ -rays at a dose of 40 Gy.

A special isogenic *Drosophila melanogaster* line was constructed for the experiment. A technique of genomic DNA extraction from one fly was developed and improved. The primary data obtained after the bioinformatics processing of this experiment will be present and discussed.

6. Neutron and X-Ray reflectometry studies of planar interfaces for power sources <u>Ye.N. Kosiachkin^{1,2,3}</u>, M.V. Avdeev^{1,5}, I.V. Gapon^{1,4}, V.I. Petrenko^{6,7}, L.A. Bulavin²

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Nowadays, rapid development of technologies leads to abundance of the most diverse electronic devices. As well, green energy development and popularization is not less important, while we have drastically high level of Earth pollution. Both of these trends leads to the need of reliable and safe accumulators with high capacities. Now, the highest specific capacity in industrial batteries is achieved for intercalating type lithium-ion accumulators. The prospects are foreseen for the batteries with metal electrodes, especially lithium anodes. However, the processes on electrochemical interfaces with liquid electrolytes are not fully understood, which slows the progress in this area. This concerns the controllable formation of solid electrolyte interphase (SEI), as well as the inhomogeneous lithium deposition on metal electrodes, which both affect performances and safety operation of such kind of batteries.

The given work reports about the applications of X-ray (XRR) and neutron (NR) reflectometry to study planar interfaces related to the lithium power sources. Firstly, XRR is applied for controlling and optimizing substrates for neutron experiments. It is well suited for determining the initial comparatively simple structures with thin (thickness ~50 nm) metal electrodes deposited (magnetron spattering) on crystalline silicon. More complicated heterostructures including multilayers with regulated mean scattering length density in quasihomogeneous approximation are also tested in the frame of the general task of optimizing NR experiment [1,2]. This problem appears, since the changes of the working electrochemical interfaces are small, and certain steps are to be done to enhance relative reflectivity changes during interface evolution. The application of NR makes it possible to investigate the influence on the interface evolution of the environmental parameters, anode initial characteristics, electrolyte composition, current density, overvoltage and so on. For this purpose, electrochemical cells for simultaneous monitoring of voltage/current at the interface under study is designed [3]. The results of the adaptation of the NR experiment to study the structure of electrochemical interfaces are summarized.

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7. Crystal and magnetic structure properties of van der Waals material CrBr₃ at extreme conditions

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Among layered transition-metal compounds, chromium tribromide, which crystal structure is comprising two-dimensional sheets of composition $CrBr_3$ van der Waals bonded to one another, is of particular interest due to its extraordinary electronic and magnetic properties. $CrBr_3$ is a layered material with ferromagnetic ordering between layers. The Curie temperature for $CrBr_3$ is reported to be about 37K [1]. The recent discoveries of magnetism in the monolayer limit have opened up new possibilities for the study of two-dimensional materials. Therefore, these compounds, especially $CrBr_3$, are perfect model systems to search for possible spin-lattice coupling phenomena in CrX_3 family due to absence of structural phase transitions at low temperatures and similarity of magnetic order in bulk and few-layer forms.

The present work focuses on the investigations of crystal structure of chromium tribromide. Detailed studies of the crystal structure of CrBr₃ were carried out using neutron diffraction on a DN-6 diffractometer of a pulsed high-flux IBR-2 reactor (FLNP, JINR, Dubna, Russia) in temperature range of 6-300 K and at pressure up to 5 GPa. Neutron diffraction investigations of CrBr₃ revealed to observe the formation of the long-range ferromagnetic order which leads to the negative thermal volume expansion and anomalous thermal variation of interatomic distances and angles, caused by the spin-lattice coupling. Related effects were found in vibrational spectra of this compound. We also obtained the evolution of the unit cell parameters, bond lengths, and magnetic moments under high pressure.

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8. The study of metal artifacts of slavic populations in the territory of the Moscow region by neutron tomography and diffraction methods

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Recently, in archaeological research, there has been a significant increase in interest in the study of archaeological finds by methods of non-destructive structural diagnostics [1]. For such a study, two encolpion crosses, two underwear pectoral crosses and a pommel of a dagger or wand, in the shape of a bear's head and skin were referred to FLNP JINR.

To study the phase composition, the neutron diffraction method was used, which was carried out on a specialized DN-12 diffractometer at the IBR-2 reactor [2]. The spatial distribution of phases and components within the volume of the product was restored using the method of neutron radiography and tomography at a specialized experimental station on the 14th channel of the IBR-2 pulsed reactor [3].

Neutron tomography shows uneven phase distribution in the samples. In encolpion crosses, such unevenness is associated with the spread of corrosion in the connecting parts of the sample. It can also be seen that corrosion penetrates deep enough into the thickness of the bear-shaped figurine. Unfortunately, the contents of the encolpion crosses have not survived. The technology of making all the samples is casting. All samples are composed of tin bronze with a tin content of 1.9% to 6.8%, which indicates the artificial addition of tin to the alloy. In pectoral crosses, lead is also present as an additive at a concentration of 7.4 - 7.8%. Corrosion on all samples consists of Cu2O. One sample contains quartzite.

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9. Isolation of new methylotrophic species *Bacillus baksanea* from deep underground hot spring of Baksan Neutrino Observatory

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Life in farthermost corners of the Earth with extreme conditions poses many interesting questions concerning principles of evolution and possibility of existing live organisms on other planets (astrobiology). Investigation of extremophilic organisms provide insights on driving forces of nature and can be of great use for biotechnology due to existence of unique pathways and enzymes, far-divergent from what we observe in surface organisms. Thus, we present the isolation, whole genome sequencing, phylogeny analysis and metabolic characterisation of new species *Bacillus baksanea* from hot highly-mineralized spring of deep underground tunnel of Baksan Neutrino Observatory, North Caucasus.

10. A facile synthesis of carbon coated amorphous SiO₂ from rice husk as anode material for Li-ion batteries

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The rapid pace of economic development requires progressive improvements in modern energy storage devices such as lithium-ion batteries. One of the methods is the use of silicon, which in comparison with commercial carbon, has a higher efficiency in using silicon. Despite this, SiO2 has a number of disadvantages that limit its widespread use as an anode material for lithium-ionic materials associated with changes in volume during the movement of the first lithium, low electrical conductivity and short service life. To solve these disadvantages, an inexpensive and simple method is proposed for obtaining a hybrid SiO2 / C composite in a graphene shell. SiO2, carbon and graphene were obtained from biologically waste material - rice husk. The proposed inexpensive and scalable method for producing a hybrid SiO2 / C @ Graphene composite is a possible solution for creating the next generation of lithium-ion batteries.

Today, lithium-ion batteries (LIB) are widely used and are an integral part of everyday human life due to their superior properties such as high energy density, long service life, high power density and low self-discharge rate . Nevertheless, the graphite used for the commercial production of LIBs, the theoretical capacity of which is 372 mAh / g, imposes significant restrictions on the manufacture of highly efficient LIBs. The development of new and / or improvement of existing technologies for the production of efficient anode materials with high specific capacity is a priority task for many research groups.

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11. Biological effects of reduced natural background radiation: transcriptome profiling of model organism developed in the deep underground laboratory DULB-4900 BNO INR RAS

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Natural background radiation is a permanent multicomponent factor of terrestrial and cosmic origin influencing all living organisms, but effects of its deprivation still remain uncertain. Biophysical studies, rapidly evolving in the end of 2010s at physical research centers with low background laboratories (LNGS Gran Sasso, CNRS Modane, SNOLAB Sudbary etc.), attempt to reveal mechanisms of responses to chronic background doses of radiation with implementation of new methods including omics techniques. Deep underground low background laboratory DULB-4900 of Baksan Neutrino Observatory INR RAS encouraged Dzhelepov Laboratory of Nuclear Problems JINR initiative of collaboration in Life Science studies and hosted experiments concerning determination of low radiation background impact on model organisms. Our goal was to determine for the first time a response of D. melanogaster Oregon-R line to the reduced natural background radiation at the whole transcriptome level after complete developmental cycle (14 days of exposure) in low and natural radiation background laboratories by comparison RNA-seq gene expression profiles and by comparative transcriptome analysis with data deposited at NCBI GEO and NASA GeneLab databases. We hypothesize that obtained D. melanogaster responses to DULB-4900 conditions were not specific to radiation-related stress and may be a result of chronic lack of external natural stimuli.

12. Investigation of superconductivity and magnetism in layered nanostructures by polarized neutron reflectometry with secondary radiation registration

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Nowadays studying of proximity effects at the interface between two media are in focus of view [1-5]. In particular it relates to the interface between superconductor and ferromagnet. Due to the mutual influence of ferromagnetism and superconductivity, because of the finite values of the coherence lengths, a significant modification of the magnetic and superconducting properties occurs. It appears, in particular, as changing of magnetization's spatial distribution. It is important to establish the correspondence of the magnetic spatial profile (spatial dependence of magnetization) to the nuclear spatial profiles of the elements of the contacting media. To determine the spatial magnetic profile, the standard method of reflectometry of polarized neutrons is used, which makes it possible to determine the energy of the potential interaction of a neutron with a medium. At the interface between two media, the interaction potential is the sum of the interaction potentials of elements penetrating each other. Standard neutron reflectometry does not make it possible to establish which elements are associated with changes in the interaction potential and, in particular, in the magnetic profile. To determine the profile of the interaction potential of a neutron with individual elements, it is necessary to register the secondary radiation of the elements. At the moment, channels for recording charged particles [6], gamma quanta and spin-flip neutrons [7] have been implemented at the REMUR spectrometer of the IBR-2 reactor in Dubna. Several tens of isotopes and magnetic elements are available for measurements.

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13. Results of studying ceramic and metal samples-objects of Kazakhstan's cultural heritage by neutron scattering methods

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Modern methods of non-destructive research make it possible to obtain unique scientific information about the elementary, chemical and phase composition of the object under study, to restore the spatial distribution of components, and to visualize hidden elements of decor or fasteners. Special mention should be made of such methods of structural non-destructive diagnostics as neutron diffraction and tomography. The nature of the interaction of neutrons with matter determines the high penetrating ability of these methods and the sensitivity to hydrogen-containing phases or components of the investigated object.

The territory of East Kazakhstan, including Tarbagatay, has been an important ethnocultural center of various tribes and peoples since ancient times. The emergence of ceramics and all changes in it are determined by economic prerequisites, cultural development of ancient communities, the level of development of the technical base of pottery. The report presents the results of studies of several fragments of ceramic objects found in the ancient cities of modern Kazakhstan.

To determine the mineral phase composition of the studied ceramics, we used the neutron diffraction method using a DN-6 neutron diffractometer [1] of the IBR-2 pulsed reactor (JINR, Dubna, Russia). The features and spatial distribution of phases were studied by neutron radiography and tomography [2] at a specialized experimental station NRT on the 14th channel of the IBR-2 high-flux pulsed reactor. The obtained data on the mineral composition of the studied ceramic materials indicate the production of dishes, mainly from clay with a natural admixture of feldspars, quartz and mica. In addition, diffraction peaks associated with the presence of graphite, anatase and calcite phases were detected. Some fragments contain inclusions of organic impurities, presumably vegetation and manure or bird droppings. The data on neutron tomography made it possible to put forward an assumption about the firing times of the studied ceramics, about the uniformity of the heat treatment of earthenware. Neutron tomography showed that the outer layer of ceramics is exposed to higher temperatures. The obtained experimental data allow us to make an assumption about the recipes of molding masses for ancient pottery crafts of different eras of ancient Kazakhstan, to reveal the level of development of this craft in a specific chronological period.

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14. PCR-analysis of direct radiation-induced mutations of *white* gene in *Drosophila melanogaster*

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As part of DLNP Radiogen project radiation induced white mutations of D. melanogaster were researched using PCR method. Study is in work-in-progress status so current results are representing intermediate progress. Characteristic features of gamma- and neutron-induced mutations are shown.