CONFERENCE ABSTRACTS 2017

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International Student Conference

“Science and Progress”

DAAD

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Freie Universität Berlin

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St. Petersburg – Peterhof
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A. Chemistry

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Synthesis and Catalytic Properties of Ferromagnetic Bimetallic Nanoparticles Based on Cobalt

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Monometallic cobalt nanoparticles and bimetallic nanoparticles of the "cobalt-copper" composition with a wide (20-150) nm and narrow (20-30) nm particle's size dispersion were obtained by pulsed laser ablation in liquid (PLAL).

It was used femtosecond pulsed laser with wavelength λ=800 nm and average energy $3,8*10^{-3}$ J per pulse.

Hexane and high-purity cyclopentanone were used as a liquid medium

Crystals of high-purity cobalt and layered structures with "Co-Cu" composition preparing by ion sputtering were employed like targets.

The process of magnetic field influence on the formation of final clusterization of mono- and bimetallic nanoparticles was studied. An external magnetic field makes it possible to form an ensemble of nanoparticles with a narrow dispersion in size.

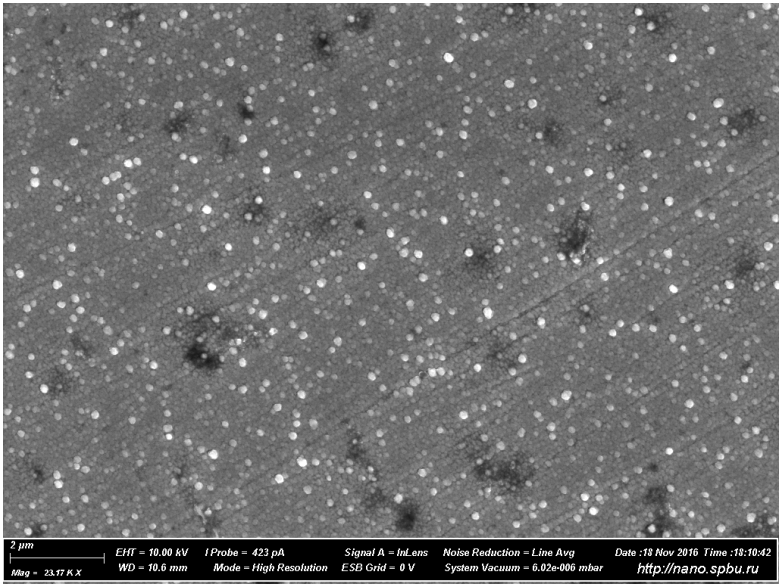

Fig.1. SEM-image of Co-Cu nanoparticles dropping on silica surface.

(3+2)- and (3+3)-Cycloaditions of 3,4-Dihydroisoquinoline-*N*-oxides to *N*-Vinylpyrroles

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The isoquinoline fragment is an important structural part of a number of alkaloids and biologically active substances [1]. Previously, the reaction of *N*-vinylpyrroles with acyclic nitrones has been studied by our research group. It was shown that the reaction can proceed as a standard 1,3-dipolar cycloaddition with high yields and stereoselectivity [2], or as formal (3+3)-cycloaddition in the presence of Lewis acids [3].

The aim of this work is to investigate an ability of proceeding the interaction of 3,4-dihydroisoquinoline-*N*-oxides with *N*-vinylpyrrole by path of (3+2)- or (3+3)-cycloaddition depending on reaction conditions and to optimize the conditions for catalytic (3+3)-cycloaddition (Fig. 1).

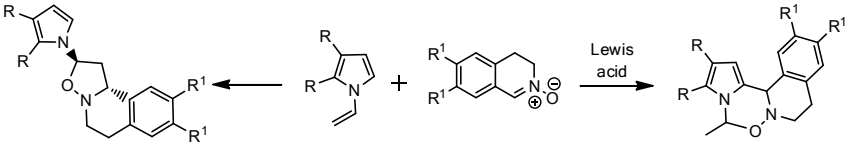

Fig. 1. The path of the reaction depending on the conditions.

It was found that 1,3-dipolar cycloaddition is carried out in the absence of a catalyst. Adding Lewis acids leads to a change of the reaction path: the products of formal (3+3)-cycloaddition are formed. To optimize the reaction conditions we used different catalysts, solvents and temperatures. All products were obtained with good yields.

The study was carried out under a financial support of the Russian Foundation for Basic Research (grant no. 16-33-00614 mol_a).

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Development and Study of Novel Green Membranes Based on PVA and Chitosan for Pervaporation Dehydration

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One of the most important fields in modern society is the development of sustainable processes to reduce the anthropic footprint of industrial development. Membrane processes may be among them due to the fact that these techniques are harmless, using compact equipment and can allow the reduction of power consumption. One of the potential membrane technologies is pervaporation, which can be used for various industrial liquid-liquid separations. The potential of this process is especially suitable for the dehydration of different mixtures. The development of a new generation of membrane treatment systems, in particular pervaporation, requires a search for new membrane materials with improved characteristics. One of the most promising ways to improve the performance of polymeric membranes is the preparation of mixed-matrix membranes to combine advantages of organic and inorganic structures. In the present research polyvinyl alcohol (PVA) and chitosan (CS) were used as polymer matrices and modified by a low-hydroxylated fullerene (fullerenol) used both as a modifier and a cross-linking agent.

This work focused on preparation and characterization of novel environmentally friendly membranes based on nanocomposites with $C_{60}(OH)_{12}$ and to study their physical-chemical and transport properties for dehydration by pervaporation. Structural and physicochemical characteristics of the membranes were studied by various physical and chemical methods of investigation (spectroscopic methods, differential scanning calorimetry, thermogravimetric analysis, scanning electron microscopy and sorption experiments). The transport properties of membranes were tested for separation of water containing binary mixtures by pervaporation. It has been shown that the addition of fullerenol particles to polymer matrix leads to the significant change and the improvement of membrane properties due to the changes in the structure and morphology.

Acknowledgements. This work was supported by Russian Science Foundation [grant No. 17-73-20060]. The experimental work was facilitated by equipment from Resource Centers: for Nano technology, X-ray Diffraction Methods, Thermal Analysis and Calorimetry, Chemical Analysis and Materials Research Centre and GEOMODEL at St. Petersburg State University.

Exploration of 1,2,4-Thiadiazole-Containing Scaffolds in the Design of Free Fatty Acid Receptor 1 (GPR40) Agonists

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The deorphanization of GPR40 as free fatty acid receptor 1 (FFA1) in 2003 and the demonstration of its involvement in the regulation of insulin secretion [1] offered much hope for the development of novel therapeutic approach to the treatment of type II diabetes mellitus. Last year, we reported 1,2,4-thiadiazole derivative as a moderately potent FFA1 agonist [2]. More recently, we have continued the exploration of 1,2,4-thiadiazole core as a basis for FFA1 agonist design.

A series of 1,2,4-thiadiazole FFA1 (GPR40) agonist compounds was synthesized, which consists of two structurally different series of compounds (Fig. 1). One of the series (structurally related to known FFA1 agonist GW9508) displayed low micromolar potency while the other (representing a truncated version of the earlier reported potent FFA1 agonists) was, surprisingly, found to be devoid of agonist potency. In silico docking of representative compounds into the crystal structure of FFA1 revealed possible structural grounds for the observed SAR.

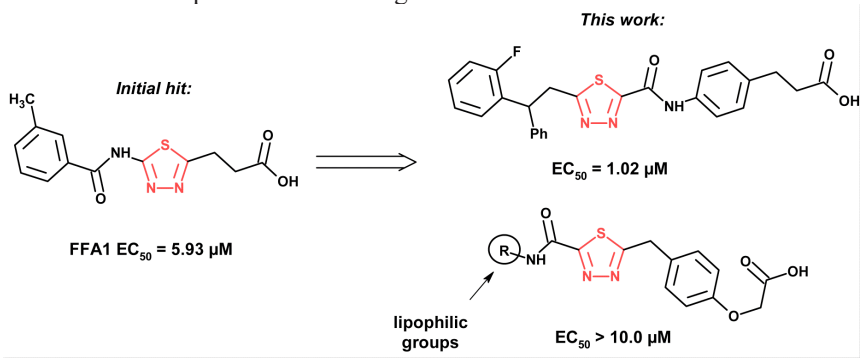

Fig. 1. 1,2,4-Thiadiazole-containing.

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Laser-Induced Deposition of Catalytically Active Metal Nanoparticles and Highly Porous Nanostructured Films from Salt Solutions for Catalysis of Organic Reactions

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The method of laser-induced chemical deposition of metal from solution was applied in the continuous in situ laser generation of metal copper catalysts for model organic synthesis reactions. The gas phase products producing during laser-induced copper deposition were analyzed by gas mass spectroscopy whereas solutions used for the copper deposition were investigated before and after laser irradiation using chromato-mass and NMR spectroscopy. It was found out that the catalysis of the studied organic reactions by metal catalysts generated during laser deposition process occurs only upon laser irradiation of the reaction mixture (Fig. 1), in turn, the copper structures deposited under laser light exhibit no catalytic activity.

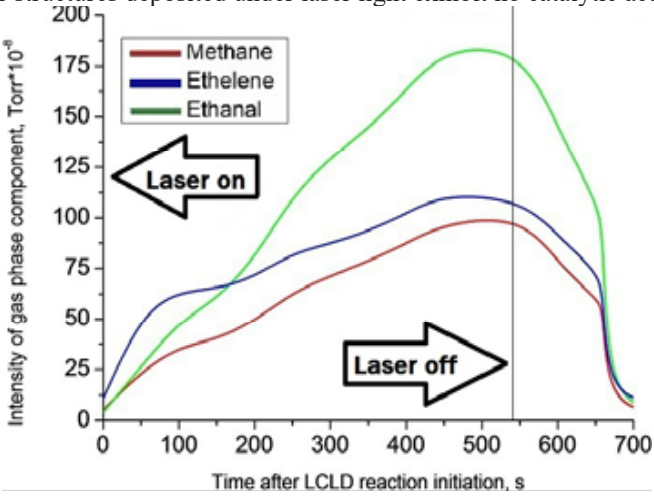

Fig. 1. The changes in time of the intensities of gas phase products generated from solution containing $CuCl_2$ (0.02 mol L^{-1}) and ethanol.

Acknowledgements. Authors wish to acknowledge Russian Fund for Basic Research (grants 16-33-00645 and 16-03-00436). The authors also express their gratitude to the Centre for Optical and Laser Materials Research, Magnetic Resonance Research Centre and Chemistry Educational Centre of Research Park at St. Petersburg University.

Direct Determination of Fluorine in KTP Single Crystals by Pulsed Glow Discharge Time-of-Flight Mass Spectrometry

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Fluorine plays an important role in many fields [1]. For example, introduction of KF into KTP ($KTiOPO_4$) crystals substantially increases their radiation strength thanks to reducing the formation rate of coloring centers. Electrical properties of KTP crystals doped fluorine ($KTiOPO_4$:KF), which is promising nonlinear materials for different applications, was studied in previous research for the first time[2], but researchers were faced with the problem of quantitative determination of fluorine. The current state of analytical chemistry of fluorine does not correspond in full measure to the existing requirements now. For example, the $KTiOPO_4$:KF crystals are water insoluble, whereas the chemical properties of fluorine, present in low concentrations in the crystal, does not allow to apply the majority of conventional methods, such as electrochemical ones, ICP AES and ICP MS, molecular absorption spectrometry, XRF, etc., for its accurate quantification. Problems related to formation of the analyzed signal, technical difficulties of the applied instruments and the necessity of qualified operators for their maintenance restrict the field of application of direct analytical methods of determination of fluorine in solid materials [1].

In this reason, the study is devoted to the development of a new approach to the quantitative determination of fluorine in dielectric crystals in the framework of the pulsed glow discharge time-of-flight mass spectrometry (PGD TOF MS) in Combined Hollow Cathode (CHC) for the example of $KTiOPO_4$: KF. It is shown that the fluorine intensity largely depends on the delay time, the discharge duration, the pressure in the discharge cell and the voltage. The delay time was 3 mks. Approaches have been developed to take into account the interests of $^{19}F^+$ with $^{38}Ar^{2+}$ and $1H_3{}^{16}O^+$. The detection limit of fluorine was 0.05 mass. %. Also, for comparison, XRF analysis was carried out, which used to analyze fluoride in various materials, however, did not show satisfactory results.

The research was carried out at the expense of the Russian Science Foundation grant (project No. 17-73-20089).

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Low-Temperature Equilibrium in Solutions of (Isocyanide)(Phosphine)Palladium (Ii) Complexes

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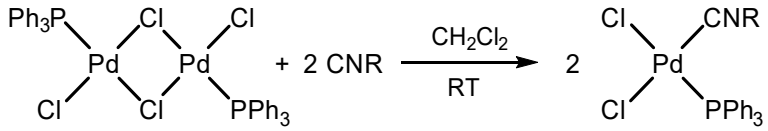
Metal-bound isocyanides, in particular ligated to the late transition metals, e.g. platinum or palladium, attract attention as plausible precursors for generation of complexes with both N-heterocyclic carbenes (M-NHCs) and acyclic diaminocarbenes (M-ADCs) [1]. M-NHCs and M-ADCs represent powerful alternatives to phosphine catalysts in a wide range of organic processes, because they exhibit lower sensitivity to air and moisture and thermal stability as compared to metallophosphines [2]. This causes an interest in the structure of the isocyanide complexes of palladium(II) and their behavior in solution.

The complexes *cis*-[$PdCl_2(CNR)(PPh_3)$] (**5**–**7**) were synthesized by the interaction of [$Pd_2Cl_4(PPh_3)_2$] (**1**) with isocyanides **2**–**4** in CH_2Cl_2 at RT (90–98%)



1 R = Cy **2**, *t*-Bu **3**, $C(Me)_2CH_2(Me)_3$ **4** R = Cy **5**, *t*-Bu **6**, $C(Me)_2CH_2(Me)_3$ **7**

The complexes **5**–**7** were characterized by HR ESI^+-MS, IR, ^1H $^{13}C\{^1H, ^{31}P\}$ and $^{31}P\{^1H\}$ spectroscopies. All complexes are isomerically pure in solid state and in $CHCl_3$ and CH_2Cl_2 solutions. For compound **5** in the solution of CH_2Cl_2 was detected an equilibrium between equatorial and axial isomers (2:1 at 95 °C).

Acknowledgements. The work was supported by the Russian Foundation for Basic Research (grant 14-03-31204 mol_a_dk) and Grant of Russian Federation President (MK-7425.2016.3). The authors are grateful to the Center for Magnetic Resonance, Center for X-ray Diffraction Studies, Center for Chemical Analysis and Materials Research, Computing Center and Chemistry Educational Centre (all belong to St. Petersburg State University).

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A Cloud Point Microextraction Approach Using Octylamine for the Separation a3nd Preconcentration of Tetracyclines in Urine

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In the present research a cloud point microextraction procedure based on a flow system has been developed and coupled with a HPLC-UV system for the determination of tetracyclines in urine. In this microextraction procedure octylamine was used to extract and preconcentrate tetracyclines. The procedure involves the aspiration of octylamine and sample solution into a mixing chamber followed by their air babbling mixing resulting to isotropic solution formation. To provide phase separation a salting out agent solution was added into the mixing chamber. After phase separation, the micellar phase containing the analytes was mixed with methanol and transported to the HPLC-UV system. Under the optimal conditions, the detector response of the analytes was linear in the concentration ranges of 0.03-3 μmol L^{-1}. The limit of detection (LOD), calculated from a blank test based on 3σ, was 0.01 μmol L^{-1}. The results demonstrated that the developed approach is highly cost-effective, simple and rapid.

Lewis Acid/Base Stabilized Phosphanylalanes $IPrAlH_2PH_2$ and $IPrAlH_2PH_2W(CO)_5$: Synthesis and Characterization

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Polymers, which are based on main-group elements except carbon, appear to be attractive materials owing to their uses in optoelectronics, as elastomers, biomaterials, polyelectrolytes and lithographic resists [1]. Recently, the main research focus has been directed on the hydrogen-containing compounds [$H_2E{-}E'H_2$] (E = B, Al, Ga; E' = P, As) as the precursors for semiconductor materials. These monomers are unstable due to oligomerization and polymerization. Compounds of the type $H_2E{-}E'H_2$ could be stabilized by Lewis acids (LA) or Lewis bases (LB) [2, 3].

In present work, by applying donor-acceptor stabilization concept, two novel monomeric phosphanylalanes were synthesized and characterized by NMR spectroscopy. The molecular structures were determined by single crystal X-ray diffraction.

Compound $IPrAlH_2PH_2$ (**1**) (IPr – 1,3-bis-(2,6-diisopropylphenyl)imidazol-2-ylidene), stabilized only by LB, was obtained via a salt metathesis route (Fig.1, a). Compound $IPrAlH_2PH_2W(CO)_5$ (**2**), stabilized by LA and LB, was synthesized using H_2 elimination reaction (Fig.1, b).

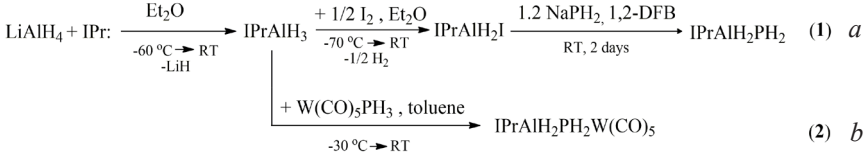

Fig. 1. Synthetic routes towards **1** *(a) and* **2** *(b).*

Financial support from SPSU-DFG grant 12.65.44.2017 and SPSU grant 12.42.719.2017 is gratefully acknowledged. We are grateful to Michael Seidl (University of Regensburg) for help with the X-ray structure determination of **2**.

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Isostructural Cl/Br Exchange in Adducts of Dimethylcyanamide Platinum(II) Complexes with Tetrabromomethane

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Halogen bonding is one of the most intensively investigated non-covalent systems in modern science. It has been recently recognized as a useful method for crystal engineering, design of supramolecular systems, organic catalysis, etc. [1] Use of metal complexes is promising for the creation and ordering of supramolecular systems by means of halogen bonds. In our previous work, the adducts of dialkylcyanamide platinum(II) complexes with iodoform were studied. [2] Tetrabromomethane—another halomethane—can also be halogen bonding donor toward various halide metal complexes.

In current study isostructural Cl/Br exchange were found in the 1:1 adducts of *trans*-$[PtX_2(NCNMe_2)_2]$ (X = Cl, Br) with CBr_4, taken as a halogen bond donor. Besides the $Br_3C–Br•••X–Pt$ (X = Cl, Br) halogen bonding, the $C_{cyano}•••Br–CBr_3$ contacts were identified (Fig. 1). All types of weak interactions were confirmed theoretically by DFT calculations on the experimentally determined atomic coordinates, followed by Bader's topological electron density distribution.

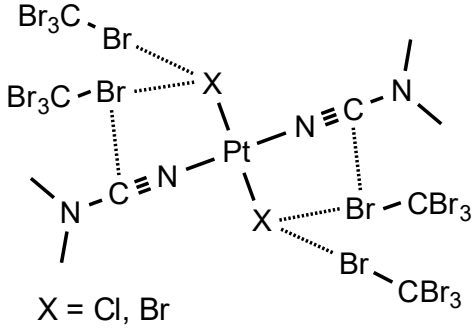

Fig. 1. The environment of complex molecules in the trans-$[PtX_2(NCNMe_2)_2]$•CBr_4 adducts.

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Critical Phenomena for the Quaternary System Propionic Acid – Ethanol – Ethyl Propionic – Water at 313.15 K

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Scrutiny of critical phenomena appeals for different lines of industry beginning from pharmacy and ending off manufacture of perfumery products. They are used for the fractionation of polymers, biodiesel fuel's generation, the supercritical fluid chromatography and also for formation of above-critical reactional media. The research of corresponding systems gives new thermodynamic information and allows to install advanced physicochemical regularities. At the same time investigation is of concern to practical interest, in particular, for elaboration of methods to separate and purify substances, as well, for simulation of chemical-technological process in complex system, in critical phases and in the near-critical area.

The study of critical phenomena and solubility in the propionic acid – ethyl alcohol – ethyl propionate - water system at 313.15 K was carried out by isothermal titration method.

The survey was conducted for two ternary systems (propionic acid - ethyl propionate - water and ethyl alcohol - ethyl propionate – water) and five quaternary systems with diverse concentrations of propionic acid and ethanol. As a result of research there were afforded 7 compositions of critical phenomena. In terms of obtained experimental data there were constructed critical states at triangles of Gibbs-Rosebaum and "critical curve"(Fig. 1) at concentration tetrahedron of compounds.

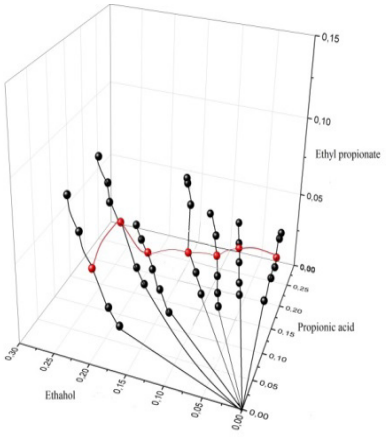

Fig. 1. Critical curve at concentration tetrahedron of compounds.

Synthesis and Reactivity of New Indolyl and Pyrrolyl Substituted Izoxazolidines

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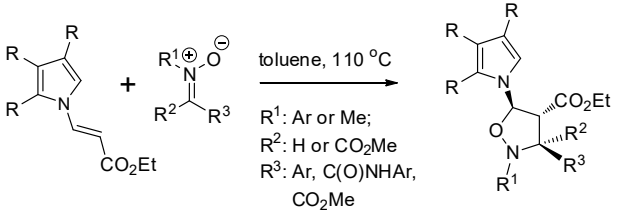
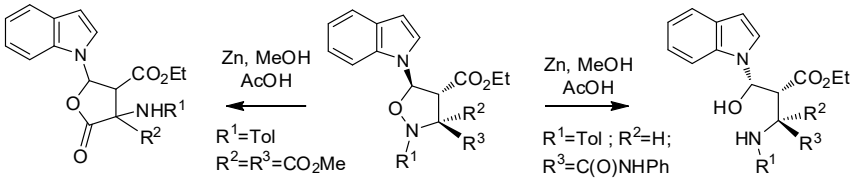
Isoxazolidines are very interesting objects for bioorganic and medical chemistry. Thus, substituted isoxazolidines are able to exhibit antitumor, antiviral and antibacterial activity [1]. The efficiency of using of *N*-vinylpyrroles for obtaining pyrrolyl substituted izoxazolidines via (3+2)-cycloaddition was shown earlier [2]. Furthermore, depending on conditions and substrate's structure, reaction can proceed as formal (3+3)-cycloaddition. In this case adducts are pyrrolo[2,1-*d*][1,2,5]oxadiazine [3].

First part of our study is devoted to interaction of 3-pyrrolyl- and 3-indolylacrylates with nitrones, regio- and stereo selectivity of this process.



Next part of this work describes reactivity of the products. It was found aminoalcohols and lactones can be obtained.



As a result high level of the regio- and stereo selectivity was shown for all reactions.

The study was carried out under a financial support of the Russian Foundation for Basic Research (grant no. 16-33-00614 mol_a).

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1,3,4-Thiadiazole-2-Carboxamide Scaffold as a Precursor for the Synthesis of Free Fatty Acid Receptor 1 (FFA1) Agonists

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Free fatty acid receptor 1 (FFA1), for a long time known as GPR40 is a G protein-coupled receptor and a new purpose for treatment of type 2 diabetes. 1,3,4-Thiadiazole derivative is a moderately potent FFA1 agonist.

Previously, FFA1 agonists based on 1,3,4-thiadiazole core were obtained in our laboratory, but they did not possess such a good potency and selectivity level as a series of substances that were synthesized recently (Fig. 1).

We have obtained two chemical series as FFA1 receptor agonists: (**1**) 1,3,4-thiadiazole-2-carboxamide plays the role of the core scaffold and (**2**) 1,3,4-thiadiazole-2-carboxamide moiety is as a periphery group reformative the 3-phenylpropanoic acid core [1]. These chemical series show excellent selectivity.

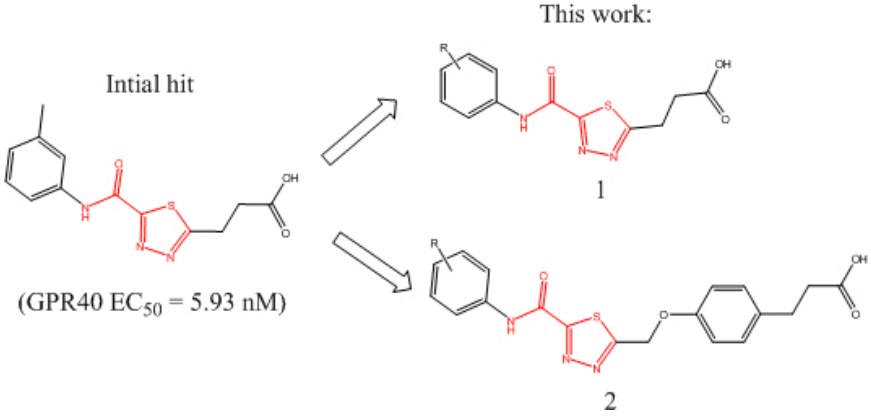

Fig. 1. 1,3,4-Thiadiazole-containing.

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Molecularly Imprinted Macroporous Polymeric Layers: Preparation and Properties Exploration

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A method of molecular imprinting consists in the copolymerization of functional and cross-linking monomers in presence of a specially introduced target template molecule. The resulting product represents a polymer matrix containing three-dimensional imprints that are capable to specific complementary interactions with the target molecule. This method has become an attractive synthetic possibility of obtaining the novel functional polymers with pre-designed molecular target selectivity. Molecularly imprinted polymers (MIP) are of value due to their inherent robustness, reusability and reproducibility. MIPs have a significant application in various areas such as chemical and biological sensors, solid phase extraction, HPLC, drug assays, etc.

Nowadays, more and more studies are devoted to macroporous monolithic materials as the modern design of sorbents intended to the separation processes based on biorecognition. Their positive distinctive features are the simplicity of synthesis, variation of surface chemistries, high reproducibility, as well as fast mass transport predominantly controlled by convection. The series of macroporous molecularly imprinted monolithic platforms, obtained in the frame of this work, were differed in pore size and amount of template used for imprinting. Their properties were studied.

As monomers in the copolymerization process methacrylate monomers, such as 2-(2-methoxyethoxy)ethyl methacrylate, 2-hydroxyethyl methacrylate, 2-aminoethyl methacrylate were used. Dodecanol and toluene were applied as the porogenic solvents and 2-hydroxy-2-methylpropiophenone as initiator. The porogenic system was optimized to reach similar macroporous structure for both molecularly imprinted and control non-imprinted polymer materials. The amino acid phenylalanine was chosen as a model small template compound. The scanning electron microscopy and etalon porosimetry were applied for the surface morphology analysis and the determination of an average pore size of materials, respectively. The recognition efficiency of a series of obtained molecularly imprinted macroporous monolithic platforms was evaluated in binding studies in comparison with non-imprinted ones.

Acknowledgements. Thermogravimetric and Calorimetric Research Centre and Centre for Geo-Environmental Research and Modeling (Geomodel) of Saint-Petersburg State University are acknowledged for porosimetry analysis and SEM, respectively.

Laser-Induced Migration of Alkali Ions in Phosphate Glasses

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It is known that laser modification is used to improve and/or change the properties of materials. Modification of multicomponent phosphate glasses allows to change their properties in a micro level. Such modified materials can be used as a calibration elements, diffraction gratings and elements of integral optics. The effect of laser radiation causes the migration of ions in the glass and a change in the structure as a consequence. Therefor phosphate glasses modification attracts the increasing interest not only because of their practical application but also for investigation laser-induced diffusion of alkali ions which is not completely clear yet.

Glasses Li_2O-Na_2O-P_2O_5-Nb_2O_3 were synthesized, modified with laser radiation and exposed to a temperature gradient. The elemental composition along the cross-section of samples was investigated. It revealed that the direction of diffusion of alkali metal ions with respect to the most heated part did not coincide in laser modified samples and in the samples subjected to a temperature gradient. Consequently diffusion of alkali metal ions could not be induced by the heat of laser beam. In this work a new mechanism for laser-induced diffusion was suggested.

Acknowledgements. The authors highly appreciate the contribution of Prof. Dr. Sokolov I.A.

Acyclic Diaminocarbene Complexes of Iridium(III): Synthesis, Structure and Properties

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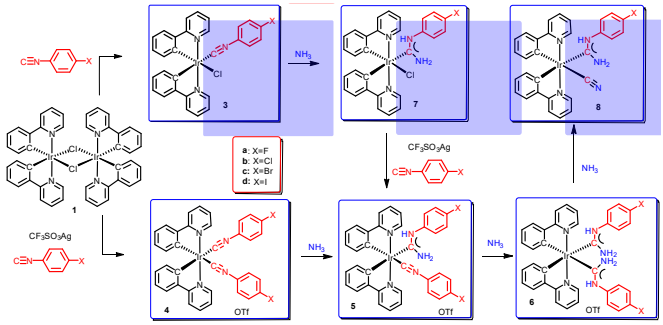
Cyclometalated iridium(III) complexes continue to draw attention because of their superior optoelectronic properties such as long excited-state lifetimes and high phosphorescence quantum yields. Heteroleptic cyclometalated iridium complexes such as $[Ir(C\hat{}N)_2(LL')]^{0/+}$, where C^N = cyclometalating ligand and LL′ = ancillary ligand, are of particular interest because the structures of the C^N and LL′ ligands control the emission energy and tunes the excited-state character [1,2]. Acyclic diaminocarbenes are strong σ-donor ligands and have a significant effect on the electronic structure of the complexes. In the work by interaction of new isocyanide complexes of iridium(III) (**3**–**4**) with ammonia were synthesed four series acyclic diaminocarbene complexes of iridium(III) (**5**–**8**).



Compounds **3**–**8** were obtained in 75–87% yields and were fully characterized by ESI^+-MS, IR and ^1H, and $^{13}C\{^1H\}$ NMR spectroscopies, the structures of 8 complexes were also confirmed by the X-ray diffraction method.

Acknowledgements. The work was supported by Russian Foundation for Basic Research (grant 14-03-31204 mol_a_dk) and Grant of Russian Federation President (MK-7425.2016.3). The authors are grateful to the Center for Magnetic Resonance, Center for X-ray Diffraction Studies, Center for Chemical Analysis and Materials Research and Chemistry Educational Centre (all belong to Saint Petersburg State University).

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Molecular Dynamics Simulation of Methane Hydrate Nanocluster Melting in Water and Nitrogen Environment

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Gas hydrates are clathrates made from the various gases and water, which exist at low temperatures and high pressures. Methane hydrates are widely spread in nature and can be used as a source of fuel. Replacement of methane in hydrates by carbon, nitrogen and sulfur oxides is important process for industrial and ecological purposes.

The aim of the work is to investigate spherical methane hydrate nanocluster (Fig. 1) stability in nitrogen atmosphere and in liquid water in the temperature range from 180 to 280 K using molecular dynamics method in NVT-ensemble. Energies of systems, radial distribution functions (RDF) and diffusion coefficients of the components were obtained. All calculations were carried out using Gromacs v.5.0.4 software package.

It was shown, that the melting of hydrate in nitrogen atmosphere occurs in temperature range from 220 to 230 K and from 250 to 260 K in liquid water. During the hydrate melting methane molecules mix with environment in the both systems, while water molecules form the drop than surrounded by nitrogen. It can be concluded, that methane hydrate nanocluster is more stable in the liquid water.

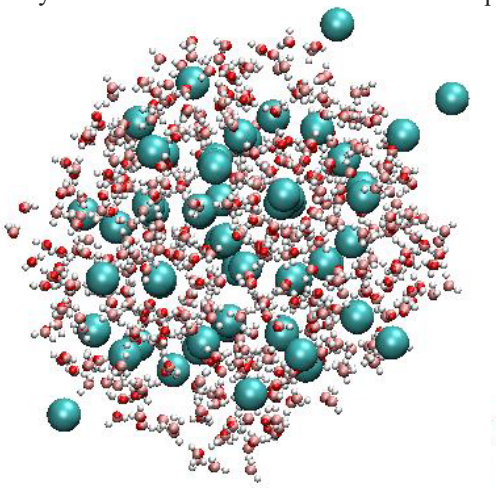

Fig. 1. Methane hydrate nanocluster at 180 K.

Water-Insoluble Complexes of Polyacrylic Acid with Low Molecular Weight Counterions Having Different Number of Amino Groups

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The polyelectrolytes due to having a large number of ionogenic groups are able to form complexes with multicharged ions. Such complexes are the special class of compounds, which find application as physiologically active substances, carriers for targeted drug delivery and stabilizers of colloidal systems. Currently, complexes of polyacids with inorganic ions are widespread in the literature; however, there is almost no information about multifunctional organic compounds as counterions.

In this work, we studied the complex formation between polyacrylic acids (PAA) of various molecular weights (2000 and 450000) with multifunctional amines (hexamethylenediamine and oligoethyleneamines with 3, 4 or 5 amino groups). Turbidimetry was used to study the possibility of the water-insoluble complex formation and to determine the NH_2/COOH ratios corresponding to the different steps of the process. It was found that water-insoluble compounds are obtained in all systems under investigation except for the systems with the diamine. In all these cases complexes are formed already after the addition of very small amount of the amine (NH_2/COOH < 0,1) and dissolve when NH_2/COOH > 0,6 (for PAA(2000)) and NH_2/COOH > 1,5 (for PAA(450000)). Moreover, the influence of the components ratio in the solution, their concentration and the number of amino groups in low molecular weight counterion on the formation of the complex was investigated. Characteristics of the obtained compounds, such as composition, structure, and particle size, were determined by dynamic light scattering, nuclear magnetic resonance spectroscopy, atomic force microscopy, small-angle x-ray scattering.

This work was supported by RFBR (grant № 15-03-08690a and 16-03-00803a) and the resource centers of St. Petersburg State University: Centre for X-ray Diffraction Studies, Magnetic Resonance Research Centre, Centre for Optical and Laser Materials Research.

Novel «Prolongated» Ir(III) Complexes as d-Blocks for Multiple Emissive Materials: Synthesis and Photophysical Properties

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In recent years, multiple emissive compounds have received substantial attention due to intensive applications in optoelectronics, photonics, ratiometric measurements, biological imaging, etc. The popular trend is obtaining of molecules where two independent metal centers with different luminescent properties are connected by ditopic ligand. Usually, such compounds are synthesized from appropriate «blocks».

We report herein synthesis of a series of novel Ir(III) complexes **$[(CN)_2Ir(NN{-}NN)]PF_6$ (1,2)** as building «d-blocks» for multiple emissive materials (Fig. 1).

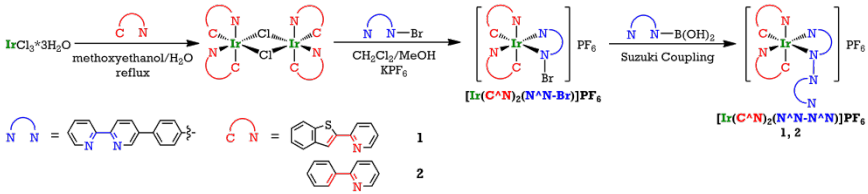

*Fig. 1. Synthesis of complexes **1** and **2**.*

Suzuki coupling between **$NN{-}B(OH)_2$** and **$[(CN)_2Ir(NN{-}Br)]PF_6$** results in prolongation of **NN** ligand with **NN−NN** ditopic ligand formation in good (up to 90%) yields. All of starting materials and compounds obtained has been fully characterized by spectroscopic methods.

The photophysical properties of the compounds obtained were studied. Absorption, excitation, emission spectra and excited state lifetimes have been measured.

The authors greatly appreciate financial support from the Russian Science Foundation, grant 16-13-10064. The work was carried out using equipment of St. Petersburg State University Research Park: Centers of Magnetic Resonance, Optical and Laser Materials Research, Chemical Analysis and Materials Research; and the X-ray Diffraction Centre.

On the Using of Equations AGA8 and PC-SAFT for the Calculation of Thermodynamic Properties of Natural Gas

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The main goal of the study is to adapt the thermodynamic methods for solving such problems of chemical technology as an express analysis of the properties of multicomponent systems formed by natural gas components. The task of the research is to minimize the number of experimentally measured parameters of gas of various compositions (including model gas mixtures). For the calculation of density, compressibility and other properties of natural gas, the use of equation of state AGA8 (American Gas Association) and PC-SAFT model (Perturbed-Chain Statistical Association Fluid Theory) is assumed. In this case initial data are the temperature, pressure and composition of natural gas, and the result of calculations – the remaining properties. It should be noted that calculation methods [1] have many advantages over experimental. A number of equipment is commonly used to measure the gas properties such as ultrasonic pulse-time flow-meters, turbine meters, etc. Unfortunately such devices are sensitive to the effects of the environment (e.g. vibration) and, therefore, require frequent calibrations [2]. In our study we considered some aspects of model and empirical calculations of properties of natural gas and collected the main approaches for the solving of the problem of express methods of these calculations. We also discussed some thermodynamic relationships which could be useful for indirect calculation of gas properties (e.g. with the use of the data on sound speed). The result of the work will serve as a prepared database on the properties of different natural gases, as well as a detailed analysis of the possibility of the using AGA8 equation of state and the PC-SAFT complex to calculate the density and compressibility of natural gases.

Acknowledgements. Authors are grateful to the Russian Foundation for Basic Research (grant 17-58-560018) for the support of this study.

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Molecular Simulation of CO_2/CH_4 Mixed Hydrates

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Due to depletion of traditional hydrocarbon resources, it is necessary to find the alternative sources of energy. One of the promising sources of fossil fuels is natural gas hydrates reservoirs, which contains a great amount of methane. Injection of carbon dioxide allows to intensify the methane recovering and to sequestrate CO_2 in the form of hydrate.

In this work, grand canonical Monte Carlo (GCMC) simulations were applied to calculate gas hydrates occupancy at various pressures and CO_2/CH_4 mixtures compositions (Fig. 1). Selectivity of the clathrate framework to the carbon dioxide was also obtained (Fig. 2). All calculations were carried out at 270 K.

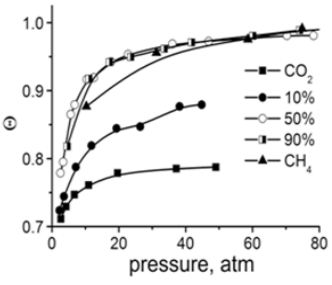

Fig. 1. Total cage occupancies Θ in CO_2/CH_4 mixed hydrates.

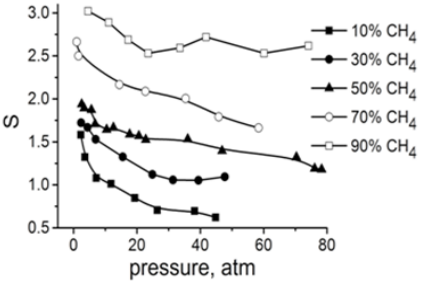

Fig. 2. Selectivity of clathrate framework S to the carbon dioxide.

From the results of the study, it can be concluded that two factors, selectivity to carbon dioxide and total cage occupancies, should be combined properly to improve the efficiency of methane replacement from the hydrates by carbon dioxide.

Complexes of AlX_3 (X=Cl, Br) with Bifunctional N-donors: From Molecular Complexes to 1D, 2D Coordination Polymers

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Metal–organic frameworks (MOFs) are prospective materials for chemistry and technology [1]. Despite the fact that the chemistry of MOFs has attracted much attention in the recent years, there are only a few MOFs based on group 13 halide complexes. N-donors have a variety of lengths and functionalities therefore they can control the channel dimensions and surface properties of MOFs [1]. Thus synthesis and characterization of new complexes of AlX_3 (X=Cl, Br) with bifunctional N-donors are important tasks.

Solid state structures of five new complexes of aluminum trihalides with 1,2-bis(4-pyridyl)ethylene (bpe) have been established by single crystal X-ray analysis. Isostructural complexes $AlCl_3 \cdot bpe \cdot AlCl_3$ ***(1)*** and $AlBr_3 \cdot bpe \cdot AlBr_3$ ***(2)*** are analogous to the complexes of group 13 halides with pyrazine [2] and 4,4'-bipyridine [3]. In case of initial 1:1 stoichiometric ratio ionic $[Al_2Cl_4(bpe)_5]^{2+}[Al_2Cl_4(bpe)_6]^{2+}[AlCl_4]_4^{-}$*3bpe ***(3)*** and $[Al_3Br_8(bpe)_3]^{+}[AlBr_4]^{-}$ ***(4)*** complexes have been formed. Note that ***3*** is mixed 1D-2D coordination polymer, where 1D $[Al_2Cl_4(bpe)_6]^{2+}$ chains are located between 2D $[Al_2Cl_4(bpe)_5]^{2+}$ sheets. In contrast to ***3*** complex ***4*** forms a 1D ionic structure in which Al atoms in the $[Al_3Br_8(bpe)_3]^{+}$ cation achieve both octahedral and tetrahedral environments. The presence of large excess of bpe provides isolation of $[Al_2Br_4(bpe)_5]^{2+}[AlBr_4]_2^{-}$*bpe ***(5)*** coordination polymer. Complex ***5*** contains 2D $[Al_2Cl_4(bpe)_5]^{2+}$ cations which are isostructural to the $[Al_2Cl_4(bpe)_5]^{2+}$ sheets in ***3***. Ionic complexes ***3***, ***4***, ***5*** belong to new structural types of group 13 metal halides complexes with bifunctional N-donors.

Acknowledgements. We are grateful to M. Bodensteiner, A.V. Virovets and E.V. Peresypkina (University of Regensburg) for the X-ray structure determination.

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Influence of Calixarene Polymorphic Modification on its Receptor Properties for Guest Vapors

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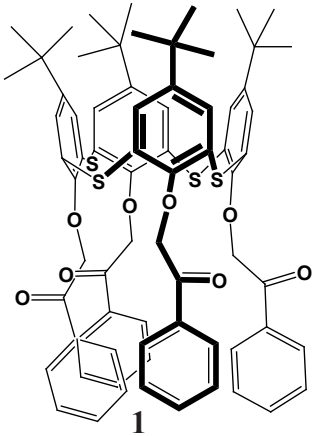
Calixarenes are good model compounds to study polymorphism. This phenomenon is a key problem for pharmaceutical chemistry, where all possible polymorphs should be identified and reproducible ways of their preparation must be developed. Suitable polymorphs of calixarenes are used in sensory systems and to separate gases. In present work, selectivity of calixarene **1** for guest vapors was studied as a function of its preparation history. Besides, the possibility of changing the direction of polymorphic transitions was investigated.



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Two polymorphic modifications of calixarene **1** and its clathrates with different guests were characterized by simultaneous TG/DSC/MS method and by X-ray powder diffractometry. A method of polymorph preparation using solid-phase guest exchange was developed. The possibility to control the receptor properties of calixarene **1** by its treatment with guest vapors was studied. This property can be used to prepare the host polymorph with a desired receptor capacity and selectivity of clathrate formation.

The work was supported by RFBR (grant no. 17-03-01311) and by Ministry of Education and Science of Russian Federation (grant №14.Y26.31.0019).

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Molecular Dynamics Simulations of Double-Stranded RNA Oligomer with G-quadruplex DNA Ligands

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G-quadruplex deoxyribonucleic acid (G4 DNA) is a specific four-stranded nucleic acid, which is formed by self-assembly of guanine-rich DNA. The formation of G4 DNA in human telomeric sequence interferes with telomere maintenance and elongation in cancer cells, thus G4 DNA is considered as an attractive target for drug design.

H_2TMPyP_4 and $ZnTMPyP_4$ porphyrins are well-known G4 DNA ligands because of their high binding affinity towards G4 DNA. Another important property of an effective G4 ligand is its higher selectivity to the quadruplex over a duplex nucleic acid [1].

To address the selectivity issue, we study interactions between double-stranded 12-mer Poly(A)-Poly(U) and both $TMPyP_4$ porphyrins by means of molecular dynamics simulations. The research found that H_2TMPyP_4 and $ZnTMPyP_4$ form stable complexes with Poly(A)-Poly(U), which are more resistant to heat-induced denaturation than pure RNA.

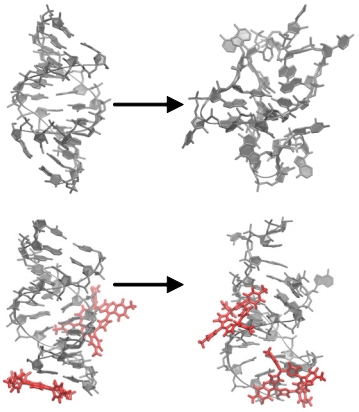

Fig. 1. RNA oligomer (top) and its complex with H_2TMPyP_4 (bottom) before and after heating.

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Separation of N_2/CO_2 Mixture by Adsorption in Modified CMK-5: Molecular Simulation Study

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Adsorptive separation of gaseous mixtures has been steadily gaining popularity over the last two decades. The use of porous solids for separation and purification of gases is a particularly promising approach for important industrial mixtures such as flue gas. To improve the existing separation technics the detailed knowledge of thermodynamic and transport properties of adsorbate is necessary.

In this work, the adsorption and diffusion of CO_2/N_2 (1:5) gas mixture in the mesoporous carbonaceous CMK-5 material modified by acetonitrile and water was investigated. The simulations were performed using Monte Carlo and molecular dynamics methods in grand canonical and canonical ensembles, respectively, at temperature of 298 K and various pressures. The amount of preadsorbed additives in the pores was for 0%, 6% and 20 mass.%.

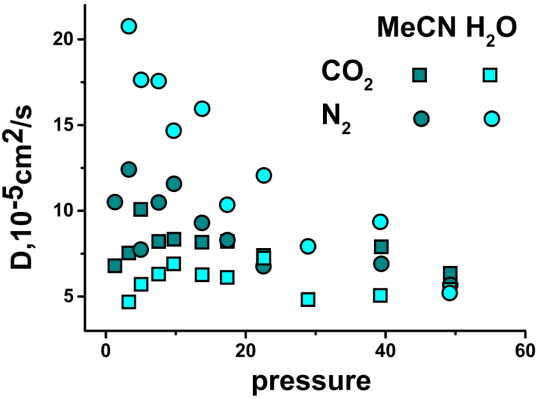

Fig. 1. Diffusion coefficients of CO_2 and N_2 in CMK-5 with 20% of additives.

It was established that the selectivity to carbon dioxide of the adsorbent modified by water is higher than selectivity of the adsorbent modified by acetonitrile. In the presence of water the difference in CO_2 and N_2 diffusion coefficients is more pronounced (Fig. 1). Thus, carbonaceous mesoporous CMK-5 material modified by water is more suitable for the CO_2/N_2 mixture separation.

This work was supported by the Russian Foundation for Basic Research (grant no. 16-33-00919 mol_a).

Synthesis of Spirocyclic Amino Alcohol Building Blocks Prepared via a Prins-Type Cyclization in Aqueous Sulfuric Acid

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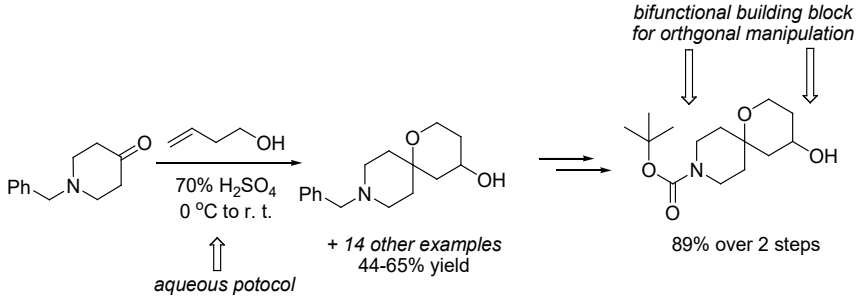
Spirocyclic motifs are valuable tools in drug design. Their use in constructing small molecule bioactive compounds delivered numerous advanced leads and clinically used compounds in diverse biotarget and therapeutic areas [1]. The privileged character of spirocycles can be intuitively linked to the more pronounced three-dimensionality of spirocyclic scaffolds compared to their flat aromatic counterparts.



In this work, we have proposed a one-step synthesis of spirocyclic scaffolds based on Prins cyclization by using sulfuric acid, N-benzylpiperidone-4 and 3-butenol. We found the best conversion of N-benzylpiperidone-4 achieved in 70% aqueous H_2SO_4 [2]. Once ability to bring about the Prins spirocyclization of azacycloalkanones in a strong mineral acid medium was demonstrated, the same protocol was applied to a range of other ketones, some of which are not basic in nature and the respective spirocyclic products were obtained in good yields. This building block has been recently used in the preparation of a library of potential GPR40 agonists, an important biological target in type II diabetes mellitus.

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An Evaporation-Assisted Liquid-Liquid Microextraction Technique for HPLC-MS/MS Determination of Pesticides in Wine

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At present, it is almost impossible to imagine a modern industrial agriculture without use of pesticides. However, even a trace amount of these substances in foods can lead to human health problems such as destruction of the cardiac, immune and nervous systems. Therefore, the pesticide residue monitoring in food and drink is an important challenge of analytical chemistry. There are many extraction and preconcentration techniques combined with different instrumental methods for determination of pesticides, but the most widely used extraction method is a liquid-liquid extraction (LLE). However, the classical LLE is difficult for automation, time-consuming and requires large volumes of toxic solvents. Another disadvantage of liquid extraction is a weak concentration of analytes from the aqueous phase to the organic phase, which reduces the limit of detection. In the current study, a novel microextraction technique for pesticides determination has been developed. It is based on dispersive microextraction with evaporation of an auxiliary solvent. The developed microextraction technique is sensitive, simple, high sample throughput and low cost, which can be used for simultaneous pretreatment of a large number of samples without any specific equipment. This method was successfully applied to the HPLC-MS/MS determination of insecticides in wine.

Scientific research was performed at the Center for Chemical Analysis and Materials Research of Research park of St. Petersburg State University.

Weak Interactions in Supramolecular Structures of Platinum(II) Isocyanide Complexes

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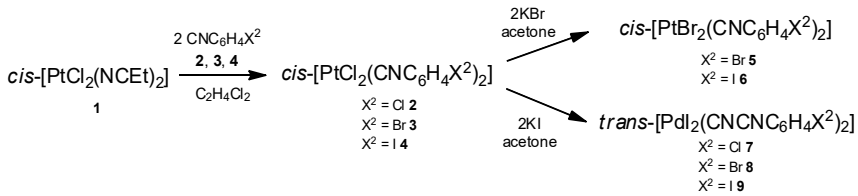
Isocyanide complexes of platinum group metals appear to be perspective building blocks in crystal engineering in consequence of square-planar environment and very slow isomerization of *cis* and *trans*-forms [1]. On the other side, the halogen bonds (XB) as other types of non-covalent interactions might be effectively used to create the supramolecular structures and useful properties in wide range of practical areas (recognition, transport and separation of anions [2], phosphorescent [3]). In this work the complexes of platinum(II) with halogen-substituted phenylisocyanides were obtained $[PtX^1_2(CNC_6H_4X^2)_2]$ (X^1 = Cl, Br, I, X^2 = Cl, Br, I).



These complexes contain both potential donor (X^2) and acceptor (X^1) of XB and demonstrate *cis-trans* isomerism in the solid state. In addition, solvates of several complexes with typical XB-donors: $CHCl_3$, CH_2Cl_2, CH_2I_2, - were received and non-covalent interactions were studied by single-crystal X-ray diffraction.

Acknowledgements. The work was supported by Russian Foundation for Basic Research (grant 14-03-31204 mol_a_dk) and Grant of Russian Federation President (МК-7425.2016.3). The authors are grateful to the Center for Magnetic Resonance, Center for X-ray Diffraction Studies, Center for Chemical Analysis and Materials Research and Chemistry Educational Centre (all belong to Saint Petersburg State University).

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Synthesis of Building Blocks for Covalent Porphyrin-Fullerene Dyads

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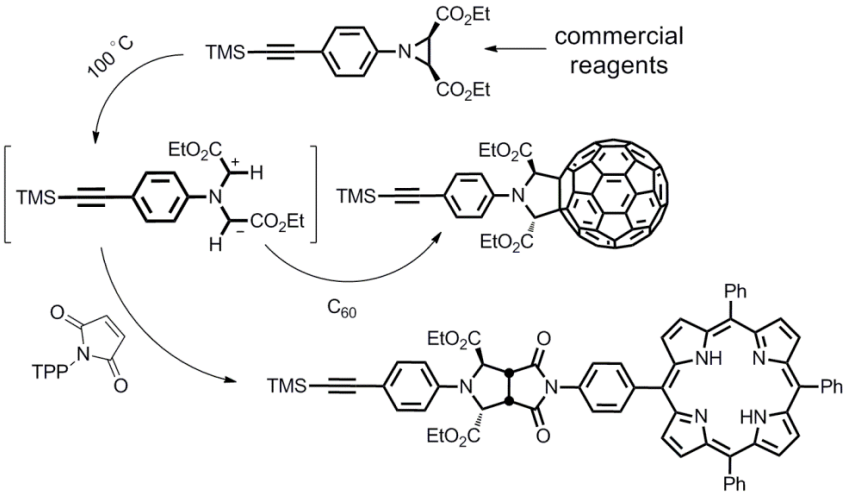
Porphyrin-fullerene dyads are considered to be promising materials for photovoltaic and photocatalytic applications [1]. Successful application of materials of this kind demands not only good match of light-absorbing electron-donor (porphyrin) and electron-acceptor (fullerene) fragments, but also appropriate linker which ensures favorable separation of the chromophores to secure fast charge separation and slow charge recombination in the dyad. In the framework of our research on pyrrolo[3,4-*c*]pyrrolyl-linked porphyrin-fullerene dyads which demonstrated formation of relatively long-lived charge separated state [2], we are heading to the modification of the initial linker with diacetylenic bridge to increase the inter-chromophoric distance targeting at the prolonged lifetime of the charge-separated state. To achieve this goal, we synthesized porphyrin- and fullerene building blocks bearing acetylenic function. Subsequent modification of these blocks will enable synthesis of the target porphyrin-fullerene dyads *via* Cadiot-Chodkiewicz heterocoupling reaction.



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Synthesis of α-Riboside Analogue Pyridine-Nucleoside Form of Vitamin B3

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Nicotinamide-β-riboside is a pyridine-nucleoside form of vitamin B3. Nicotinamide riboside was discovered as a nutrient in milk, suggesting that nicotinamide riboside is a useful compound for elevation of NAD+ levels in humans [1].

Recently, neopetrosides A and B, new naturals of the ribosides of nicotinic acid with extremely rare α-N-glycoside linkages, were isolated from Neopetrosia sp. sponge. Neopetroside A upregulates mitochondrial functions in cardiomyocytes, which allows to consider it as a model compound in the development of new drugs for the treatment of diseases associated with malfunctioning of the mitochondria [2].

Based on the fact that pyridine-nucleoside form of vitamin B3 and neopetroside A have the same biological target, and their structural forms have some similarities, it was decided to synthesize first an analog of neopetroside A with free hydroxyl on C-5` and then an α-riboside analogue pyridine-nucleoside form of vitamin B3.

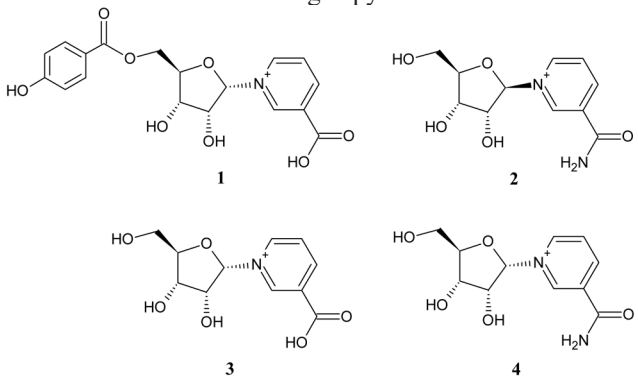

Fig. 1. Neopetroside A (1), nicotinamide-β-riboside (2), nicotinate-α-riboside (3) and nicotinamide-α-riboside(4).

The work was financially supported with RSF, grant 14-50-00126.

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Composition and Structure of Main Chemical Species in Aqueous Solutions for Laser-Induced Deposition

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Laser-induced chemical liquid-phase deposition of metals (LCLD) is one of the promising and effective methods for making pattern on dielectric substrates. In LCLD metal reduction proceeds in local volume of solution within the laser beam focal point resulting in the deposition of microsized metal structures on the surface of substrate. This approach is substantially simple, fast and precise. It is essential to fabricate high conductive tracks for such application as microelectronics and biosensing.

The aim of this work was to determine the synthesis condition for formation of conductive metallic microstructures and to investigate their electrocatalytical activity towards glucose and hydrogen peroxide. This work focused on deposition of Cu and Ni.

It was found out that the formation of the conductive electrocatalytically active electrodes by LCLD technique occurs only in solutions containing OH coordinating ligands. Coordination via other functional groups (including carboxyl, amino) does not lead to the formation of conductive structures. Conductive copper microstructures can be fabricated within specific concentration range of copper salt and organic ligand (L): the lower limit of the concentration is explained by insufficient concentration of copper ions for deposition of continuous conductive layers, upper limit is caused by polymerisation of Cu-L complex.

The topology and crystallization phase of these structures were observed by means of scanning electron microscopy and X-ray diffraction, respectively.

Acknowledgements. Authors wish to acknowledge Russian Fund for Basic Research (grants 16-33-00645 and 16-03-00436) and Saint-Petersburg State Univeristy for research grant (12.38.219.2015). The authors also express their gratitude to the Centre for Optical and Laser Materials Research, Resource Centre "Geomodel" and Chemistry Educational Centre of Research Park at St. Petersburg University.

Ambipolar Phosphine Derivatives as “Antenna” for Eu(III): Synthesis and Luminescent Properties

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A key factor in luminescence of Ln(III) is sensitization by “antenna” ligands. Asymmetrical donor-acceptor (D-π-A type) polar chromophores, which bear the p- and n-type fragments (i.e., electron rich and poor parts of the molecule), have strong absorption bands in the UV- and visible ranges and could facilitate energy transfer to the emissive level of Ln(III). Ambipolar phopsphine oxides represent a good example of D-π-A structures.

Due to the strong π-conjugation, ambipolar phosphine oxides exhibit intensive singlet emission in the range of 400-600 nm and seem to be effective sensitizers for emission ofLn(III) ions. Herein, we report the synthesis of two ambipolar phosphine oxides with unusual stereoelectronic properties (Fig. 1), Eu(III) complexes based on them and peculiar photophysical properties of these complexes.

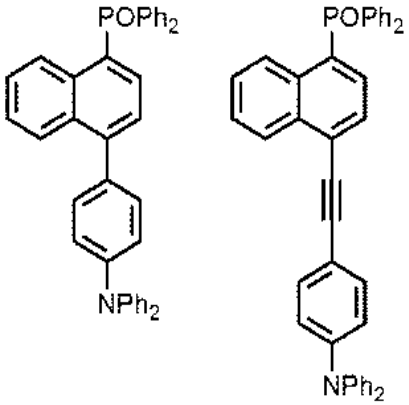

Fig. 1. Ambipolar phosphine derivatives.

The authors appreciate financial support from the Russian Science Foundation, grant 16-13-10064. All measurements were performed using the following core facilities at St. Petersburg State University Research Park: Centre for Magnetic Resonance, Centre for Optical and Laser Materials Research, Centre for Chemical Analysis and Materials Research, and X-ray Diffraction Centre.

Controlled Construction of d-f Dyads: HeteronuclearIr(III)/Yb(III) NIR Emitter

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The range of sensitizerdesigned for the NIR emitting ions Nd(III), Er(III) and Yb(III) is quite extensive. In recent years, a lot of d-block chromophores were introduced to the Ln(III) systems to improve the energy transfer from the light-harvesting antennae to the center lanthanide ions.Iridium(III) complexes represent a perspective type of building blocks for d-f dyads construction due to their tunable emission bands over the entire visible and NIR spectra, generally with relatively small changes to the coordinating ligands.

Herein, we report the synthesis of d-f dyad with cyclometalated Ir(III) complex as “d-block” and Yb(III) β-diketonate complex as “f-block” (Fig. 1).

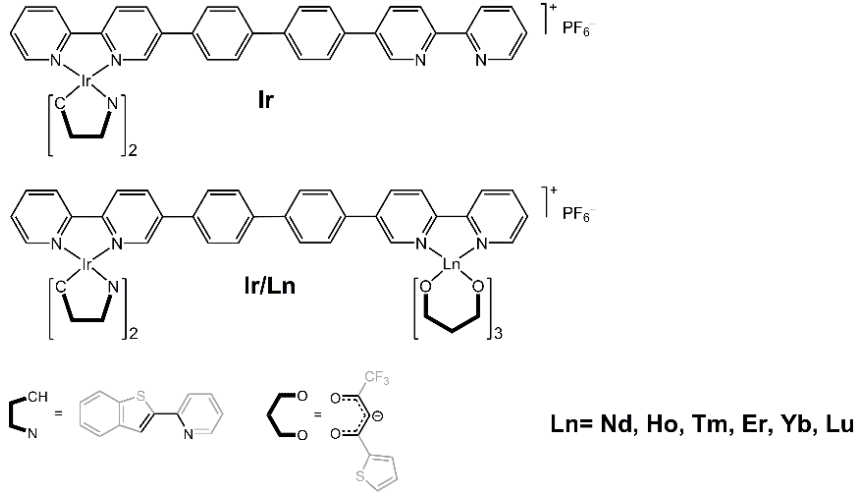

Fig. 1. Structures of the “d-block” and Ir(III)/Ln(III) dyad.

Photophysical experiments shown the energy transfer inside of the dyad obtained.

The authors appreciate financial support from the Russian Science Foundation, grant 16-13-10064. All measurements were performed using the following core facilities at St. Petersburg State University Research Park: Centre for Magnetic Resonance, Centre for Optical and Laser Materials Research, Centre for Chemical Analysis and Materials Research.

Synthesis of Monolithic Polymeric Sorbents with Molecular Imprints for Solid-Phase Extraction and Analysis of Proteins

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Nowadays synthesis of artificial biomimetic receptors attracts a lot of attention because it is a great tool in chemistry for creating different analytical systems. These synthetic materials have several advantages: the production is cheap and simple, they can be stored for a long time and they can mimic biological receptors with the same recognition ability. One of the ways to create this kind of materials is a molecular imprinting technique. It is based on a copolymerization of functional and cross linking monomers in the presence of target compound (template) followed by its further removal from the polymeric matrix. The formed cavities are complementary to the template in size, shape and arrangements of functional groups. While molecular imprinting of low-molecular weight substances is easy and well-studied, the preparation of polymer materials with imprints of macromolecular compounds like proteins is still a challenging field.

The aim of this work was the development of macroporous monolithic polymer for protein recognition. Initially, the method of molecular docking was applied to the rational choice of the suitable monomers providing the necessary molecular memory and minimized conformational changes of a model protein (bovine serum albumin, BSA). The study of interaction of a set of monomers with BSA *via* computer simulations allowed for the selection of (3-acrylamidopropyl) trimethylammonium chloride and 2-hydroxyethyl methacrylate as functional monomers and ethylene glycol dimethacrylate and poly(6)ethyleneglycol diacrylate as cross linkers. The preparation of polymers was carried in two steps. Initially, the preparation of macroporous polymethacrylate framework by *in situ* thermo-initiated polymerization in the presence of porogenic solvents was optimized. At the second step, the conditions for covering of a framework with a hydrophilic polymer layer using the monomers selected for protein imprinting were developed. The morphology and porous characteristics before and after grafting of hydrogel layer to framework were evaluated by SEM and data on hydrodynamic permeability.

Acknowledgements. The research was performed using Research Park of Saint Petersburg State University: Interdisciplinary Center of Nanotechnology, Center for Chemical Analysis and Materials Research and Center for Geo-Environmental Research and Modeling (GEOMODEL).

Molecular Simulation of Gas Hydrates Occupation: Comparison of SI and SII Structures

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To avoid the global warming carbon capture technologies should be developed and improved. The main source of carbon dioxide in the atmosphere is flue gas, which is the complex mixture of N_2, CO_2 and some other gases. One of the promising technologies for separation and purification of such mixtures is the formation of gas hydrates.

The composition of the hydrates in equilibrium with the bulk gas phase (CO_2/N_2 equimolar mixture) was obtained by the Monte Carlo method in a grand canonical (μVT) ensemble at temperature of 250 K and pressures up to 50 atm.

According to the results obtained, the cages occupancy by carbon dioxide in the SI hydrate structure is higher, than in the SII structure. CO_2 mainly occupies T- and H-cavities in SI and SII structures, respectively. Selectivity of the hydrate framework to carbon dioxide is higher for the SI structure (Fig. 1).

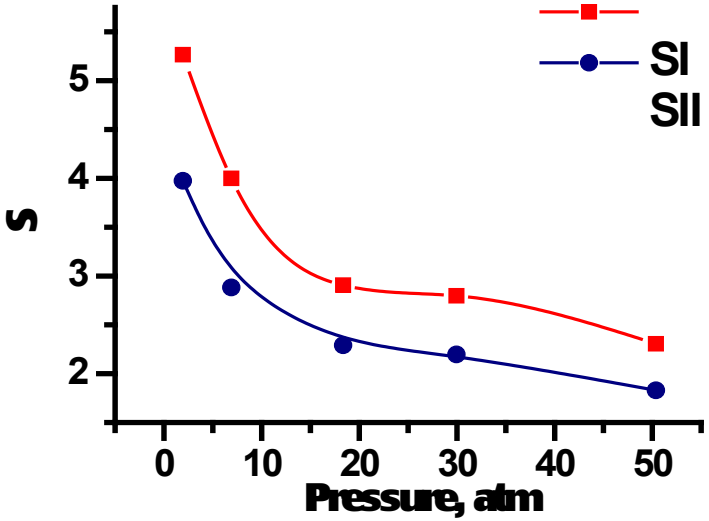

Fig.1. Selectivity of hydrate framework to carbon dioxide.

Synthesis, Characterization and Functional Characteristics of Hydroxyapatite and Ferrite Barium Based Bioceramics and Polymer Composites

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The development of magnetic materials for interstitial hyperthermia treatment of cancer is an ever evolving research field which provides new alternatives to antitumoral therapies especially in bone tissue engineering. Under the effect of AC magnetic field local point temperature rise occurs, which affect on cancer cells. This approach allows to destroy tumor cells and minimize damage for healthy cells [1].

We studied two types of functional materials: bioceramic and polymer inorganic composite. As the main components osteogenic hydroxyapatite (HAP) and magnetic barium ferrite (FB) were used, and the structure of material were formed by porogen and starch correspondingly.

Bioceramic was made by solid-state method at 850ºC based in our original approach [2]. Polymer composites were produced by the precipitation (HAP direct synthesis in presence of starch), and phase separation (liquid nitrogen was used as cooling medium) methods following by freeze drying of obtained samples. Such procedure based on the combination of two stages was not previously described.

As-prepared samples were characterized by XRD, SEM, TEM, SSA estimation, VSM. Breaking strength and modulus of elasticity were also measured.

Among all three components of as-prepared bioceramic only HAP mass increasing impact on mechanical characteristics. For polymer inorganic composites in a certain range (HAP – 32/48/64 %, FB – 8/12/16 %, Starch – 60/40/20 %) of mass ratio, formation of a complex self-organized structure was detected. The latter was consisted of HAP nanoparticles, FB nanoneedles and starch molecules and characterized by optimal functional characteristics (mechanical and magnetic).

The distinction between the products of two using methods is due not only to differences in the initial components, but also to the possibility to obtain the complex ordered structures in phase separation process.

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Phase Behavior of Aqueous Biphasic Systems Containing Dialkylimidazolium Ionic Liquids with Halide or Amino Acid Anions

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Aqueous biphasic systems containing water-miscible Ionic Liquids (IL) are considered as very perspective as a media for liquid-liquid extraction (LLE) of bioactive materials [1]. One of the important advantages of ILs is a possibility for the modification of their chemical structure and, as a result, their properties, i.e. their multifunctionality. Among the modified ILs, the aminoacidic ILs (AAILs) attract much attention [2] also because of their low toxicity and biodegradability.

The main aim of this work is to evaluate the effect of structure of ILs on the phase behavior of their aqueous-salt solutions. ILs under study here are ILs with dialkylimidazolium cation and halide or amino acid anions, [$C_n$mim][X], where n - number of carbon atoms in the alkyl chain of IL (n =4, 6, 8; [X] = Br^-, Cl^- or amino acidic anions: Leu-Leucine, Val-Valine, Lus-Lysine).

The liquid-liquid equilibrium was studied at 298.15 K for ternary systems, [$C_n$mim][X] + water + salt (K_2HPO_4 or K_3PO_4) by the isothermal titration method. The data on binodal curves were correlated by the Merchuk' equation [3]. The tie lines were received by using the data for the binodal curve and the data on water concentrations in the coexisting liquid phases. The experimental binodal curves obtained for the systems with some halide ILs mentioned above are in a satisfactory agreement with the literature data [4].

It was found that the heterogeneous region is wider in case of ILs with amino acid anions or with the shorter alkyl chain length of ILs. As expectable result, the extractive capacities increase for the studied systems containing AAILs.

The obtained results are helpful to understand how anionic structure of the ILs affect the phase behavior of their aqueous-salt solutions towards their application in LLE of bioorganic compounds.

This study was financially supported by RFBR according to the research project # 16-03-00723 a.

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A study of Methylamine Intercalation into the Interlayer Space of Protonated Layered Perovskite-Like Titanates $HLnTiO_4$ (Ln = La, Nd)

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The structure of perovskite-like titanates $ALnTiO_4$ (A = alkali metal, Ln = lanthanide) relating to Ruddlesden-Popper phases is characterized by complete ordering of A and Ln cations in two interlayer spaces separating perovskite-structured blocks. Protonated forms $HLnTiO_4$ may be produced by ion exchange in acid solutions [1]. They may be used as the initial compounds in various ion-exchange, pyrolysis and intercalation processes.

The products of organic bases intercalation into the interlayer space of perovskite-like oxides are of interest as precursors in producing monolayers. Since the monolayers are nanoscale objects with high specific surface area, they may become a basis for catalysts, photocatalysts and materials for electronics [2].

However, intercalation activity of perovskite-like titanates in reactions with organic bases is not sufficiently investigated. In particular, there is no information concerning synthesis of organo-inorganic hybrid derivatives based on $HLnTiO_4$.

The present research considers producing methylamino-derivatives of protonated titanates $HLnTiO_4$ and their properties. Particular attention is paid to selection of optimal synthesis conditions, structure of the products and their thermal stability.

Acknowledgements. This research was supported by Russian Foundation for Basic Research (grant № 16-33-60082). Authors also are grateful to Saint Petersburg State University Research Park: Center of Thermal Analysis and Calorimetry, Research Centre for X-ray Diffraction Studies, Center for chemical analysis and materials research, Interdisciplinary Resource Center for Nanotechnology.

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New Experimental Data on Synthesis and Protonation of Layered Perovskite-Pike Titanates $K_2Ln_2Ti_3O_{10}$ (Ln = La, Nd)

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The structure of layered titanates $A_2Ln_2Ti_3O_{10}$ (A = alkali metal, Ln = lanthanide) relating to Ruddlesden-Popper phases consists of triple perovskite-like blocks separated by interlayer spaces containing alkali metal cations. Protonated forms $H_2Ln_2Ti_3O_{10}$ are usually produced by ion exchange in aqueous acid solutions. During this process also intercalation of water molecules into the interlayer space occurs that as a rule is not noted in the gross formula.

Conditions of synthesis and protonation significantly affect the morphology of produced particles and phase composition (in the main, the amount of intercalated water and completeness of alkali cations substitution). Consequently, selection of appropriate conditions is of great importance for obtaining products with specified properties. For example, increasing of intercalated water amount leads to growth of photocatalytic activity of $H_2Ln_2Ti_3O_{10}$ in the reaction of reductive water decomposition [1] because the interlayer space acts as a reaction zone along with the crystal surface [2]. At the same time molecules of water expand the interlayer space that facilitates subsequent intercalation of organic compounds and creating of organo-inorganic hybrid derivatives.

The present research considers some aspects of synthesis and protonation of perovskite-like layered titanates $K_2Ln_2Ti_3O_{10}$ that are not described in the literature. Particular attention is paid to techniques of the protonation and comparison of the products.

Acknowledgements. This research was supported by Russian Foundation for Basic Research (grant № 16-33-60082). Authors also are grateful to Saint Petersburg State University Research Park: Center of Thermal Analysis and Calorimetry, Research Centre for X-ray Diffraction Studies, Interdisciplinary Resource Center for Nanotechnology.

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Structural and Electrosurface Poperties of Porous Glasses in $FeCl_3$ Solutions

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The structural, adsorption and electrokinetic characteristics of micro- and macroporous glasses (PG) of the brand 8B-NT (pore radii of 1.5 nm – MIP and 15 nm – MAP) have been studied in $FeCl_3$ solutions ($0.5\text{-}10^{-5}$ M). A study of the PG's pore morphology is an important problem, because their structure parameters, including the pore inhomogeneities, affect the sorption, capillary, diffusion, adhesive, optical, and other properties. The structural resistance coefficient (β), which reflects the contribution of the nonconducting skeleton to the electrical conductivity of the membrane, for MAP glasses was practically independent of the type of electrolyte and did not change with time. The value of β for MIP glasses changes with the transition from the HCl solution to $FeCl_3$, but returns to the practically original value for each of these solutions for multiple transitions. For both types of PG, regions of $FeCl_3$ concentrations are found at which a decrease in the specific electrical conductivity of the pore solution as compared with the free solutions was observed. This can be caused by a significant decrease in the mobilities of specifically sorbed counterions in pore channels.

The values of the electrokinetic potential were found by the methods of microelectrophoresis and streaming potential. It was found that high specificity of iron (III) ions to the surface of porous glass leads to the appearance of a positive region of the ζ-potential due to the superequivalent adsorption of counterions in the Stern layer. The position of the isoelectric point depended on the method of determining the ζ-potential, which is connected with the different structure of the electrical double layer on the open surface of the PG particles and in the pore channels of the membranes. The equilibrium data of Fe^{3+} adsorption on the surface of a PG were analyzed using Langmuir and Freundlich isotherms. It was found that Langmuir's equation best describes the sorption process on the surface of PG 8B-NT in the investigated concentration range, and the maximum adsorption of iron ions is 3.4×10^{-11} mol / cm^2.

The reported study was funded by RFBR according to the research project № 17-03-01011a. The studies were carried out using the equipment of the Resource Center of St. Petersburg State University "Methods of analysis of the composition of matter" and the Interdisciplinary Resource Center in the direction "Nanotechnology".

Synthesis and Characterization of Hexacyanoferrates of Transition Metals Doped with Magnesium as Promising Cathode Materials

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The need for energy storage systems is increasing every day. Everyone knows the systems based on lithium-ion batteries, which have a high capacity, performance cycling and stability. However, the use of these systems is complicated by high cost and fire hazard caused by the presence of organic solvent. Replacing lithium on less active magnesium can solve these problems. Moreover, it is expected that an increase in the ion charge should improve the battery's energy characteristics [1].

Hexacyanoferrates of transition metals were attracted the attention of scientists as promising the cathode materials for aqueous batteries in the last decade [2]. The structure of complex is a three-dimensional polymer network containing metals in different degrees of oxidation in the cubic lattice sites. Cyanide anions on the faces of the cube make the structure open to intercalation not only neutral water molecules, but also cations of alkaline and alkaline-earth elements. The electrochemical characteristics of these cathode materials primarily depend on the particle size and the presence of water molecules and cations in the intercalation cavities [3].

In this study, a number of hexacyanoferrate complexes of transition metals doped with magnesium ions were obtained by the method of co-precipitation in solution. This method allows to influence the particle size and obtain samples with a high degree of crystallinity. As a result, particles of metal cyanide complexes were characterized by ICP, SEM, TGA, XRD with using the Rietveld method to refine the structure of the complexes. The basic electrochemical characteristics of the received cathode materials were identified by using galvanostatic potentiometry and voltammetry methods.

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Synthesis and X-ray Study of Non-covalent Interactions in New Adducts $[Cu(I_3)(CNXyl)_3]$ and $[Cu(I_3)(CNXyl)_3]•CHI_3$

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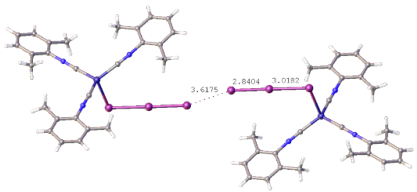
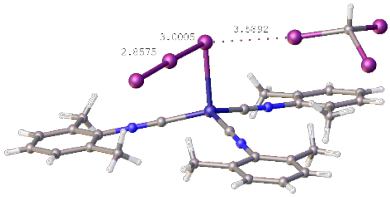
Isocyanide complexes of transition metals are convenient building blocks for the study of noncovalent interactions (in particular, halogen bonding) and the development of materials with practically useful properties on the basis of these interactions [1].

In this work complex $[CuI(CNXyl)_3]$ was synthesized by the reaction of CuI with 3 equivalents of isocyanide CNXyl (Xyl=2,6-$Me_2C_6H_3$) in acetonitrile at room temperature for 40 min and isolated in 96% yield. The compound was characterized by ESI^+-MS, ^1H NMR and IR spectroscopies.

Adducts $[Cu(I_3)(CNXyl)_3]$ и $[Cu(I_3)(CNXyl)_3]•CHI_3$ were obtained by co-crystallization $[CuI(CNXyl)_3]$ with CHI_3. The nature of non-covalent interactions in solid phase was studied by X-ray diffraction method.



$[Cu(I_3)(CNXyl)_3]$



$[Cu(I_3)(CNXyl)_3]•CHI_3$

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Dispersive Liquid-Liquid Microextraction for HPLC Determination of Meropenem in Biological Fluids

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Meropenem (Fig. 1) is a carbapenem antibiotic with a broad-spectrum in vitro activity to a wide range of bacteria used to treat a wide variety of infections. To avoid bacterial resistance or toxic side effects during meropenem treating, the determination of this antibiotic in biological fluids is highly advisable. Taking into account, that meroprenem concentrations in biological fluids are at low levels, effective preconcentration methods of the target analytes from the sample matrix is an essential step of sample preparation.

In this study we have used dispersive liquid-liquid microextraction for the determination of meropenem. Dispersive liquid-liquid microextraction (DLLME) is one of the important approaches in sample preparation. The main principle of this method involves the fast dispersion of a water–immiscible extraction solvent by means of a disperser solvent (miscible in both water and extraction solvent) in an aqueous solution. This leads to formation of the fine droplets of the extractant and the subsequent extraction of the analytes from the sample solution. The very high contact area between the extraction solvent and aqueous sample results in quick extraction equilibrium. Other main advantages of DLLME are the simplicity of operation, low cost, and high extraction recovery and enrichment factor. In present work we have used octylamine as a novel extraction solvent for DLLME. Octylamine and dispersive solvents (acetonitrile) were mixed with aqueous samples and shaken to form a cloudy solution. After that, the mixture was centrifuged to break the emulsion and the octylamine was separated to its own phase. The parameters affecting the extraction efficiency, such as volume of octylamine, type and volume of dispersive solvent, the shaking time, extraction time were investigated.

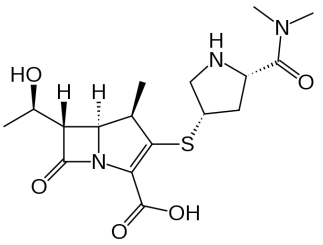

Fig. 1. Chemical structure of the Meropenem.

PLA-Base Films with Gradient Concentration of L-Cysteine

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Poly(lactic acid) have been of significant research interest due to its biocompatibility and biodegradability that leads to its broad application in medical science and biotechnology [1]. The degradation of PLA via hydrolysis or enzymatic processes leads to the formation of naturally occurring metabolites. This makes the polymer one of the best candidates for in vivo applications.

This work was aimed to show the possibility of forming gradient on the surface of PLA. The polymer was synthesized by the ring-opening polymerization (ROP) of D,L-lactide. The PLA-based films were obtained by casting of polymer solution in chloroform onto cellulose membrane. The modification of films surface by 2-aminoethyl methacrylate leads to formation the "-ene" chemistry and opportunity for thiol-ene click reaction with SH-group of cysteine (Fig. 1). A surface gradient of cysteine concentration was provided by application of protection mask with gradient fogging. Thus photoinitiated process occured only on UV irradiated regions. In order to visualize the surface concentration of cysteine the films were stained with Cy3 dye and analyzed by confocal scanning laser microscopy (CSLM). The developed procedure will be further applied for formation of gradient of cells adhesion factors.

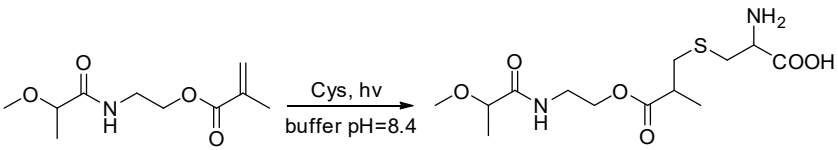

Fig. 1. Thiol-ene click reaction.

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Interaction between Aldazines and Homophtalic Anhydride. Following Transformations of (*E*)-2-arylydenamino-1-oxo-3-aryl-1,2,3,4-tetrahydroisoquinoline-4-carboxylic acids

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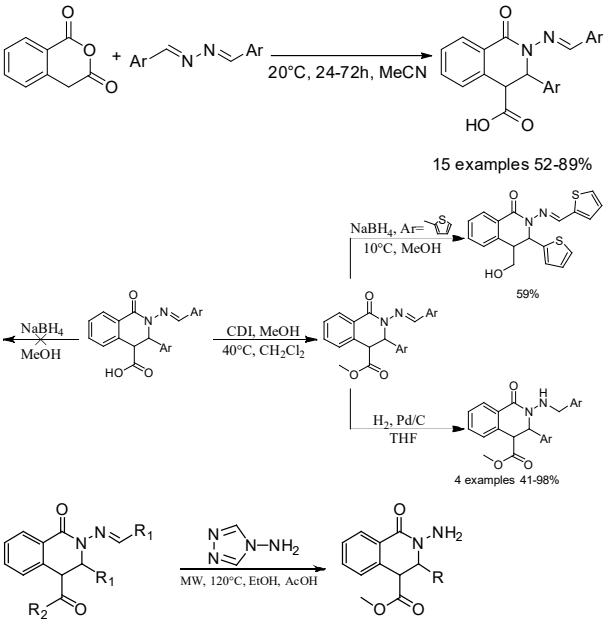
The interaction between aldazines and homophtalic anhydride realizes by Castagnoli-Cushman reaction (CCR) which was firstly described by Castagnoli N. in 1969 [1]. This reaction gives an opportunity for simple way of heterocyclic compounds synthesis [2], some of them show biological activity.

In this work we obtained 15 acids by simple procedure which is given on scheme. Our attempts to reduce C=N bond in free acids by sodium borohydride failed, but after conversion into methyl esters they were easily hydrogenated by gaseous H_2 in presence of Pd/C as a catalyst (see scheme). In compound with 2-thienyl substituent hydrogenation didn't pass, but we obtained product with reduced carboxymethyl group and remained C=N moiety by using sodium borohydride. For preparing compounds containing unsubstituted NH_2 group we proposed new method of accepting arylyden fragment by 4-*H*-1,2,4-triazole-4amine. In three samples we got the products with good yields.



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Phase Transformations of Protonated and Hydrated Perovskite Type Layered Titanate $K_{2,5}Bi_{2,5}Ti_4O_{13}$ Derivative during Thermolysis

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Layered perovskite-like oxides are solid crystalline substances formed by two-dimensional nanosized perovskite slabs interleaved with cations or cationic structural units. Until present time perovskite-like compounds are actively studied as materials with wide range of important physical and chemical properties such as superconductivity, colossal magnetoresistance, ionic conductivity, ferroelectricity, catalytic and photocatalytic activity and electrochemical properties. In recent years the development of new layered perovskite-like compounds with specified physicochemical properties using the soft chemistry methods attracts increasing attention [1].

The present research considers ability of bismuth-containing complex oxide $K_{2,5}Bi_{2,5}Ti_4O_{13}$ to undergo protonation and intercalation of water molecules into interlayer space [2]. The series of derivatives with general formula $H_xK_{2,5-x}Bi_{2,5}Ti_4O_{13}*yH_2O$ were obtained in water and nitric acid solutions. The phase transformations during thermolysis processes of obtained derivatives were studied by means of thermogravimetric analysis, simultaneous thermal analysis, HT XRD and IR spectrometry. As the result the row of new phases with layered structure was obtained and characterized.

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Colloidal CdSe Quantum Dots: New Synthetic Route, Spectroscopy and Applications

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One emerging area of nanoscience being at the interface of chemistry, physics, biology and materials science is the field of semiconductor nanocrystals, also known as colloidal quantum dots, whose unique properties have attracted great attention by researchers during the last two decades [1].

Colloidal approaches provide quantum dots of excellent quality due to the control in their size, shape, structure and composition of the material, and hence can be directly used for the respective applications.

In most articles, CdSe QDs have been synthesized at temperatures above 200 °C using trioctylphosphine oxide (TOPO) as solvent and trioctylphospine (TOP) as capping agent which are hazardous in nature.

We have developed a much cheaper and green Non-TOPO/TOP-Based synthetic route of a series of CdSe QDs in the high boiling point solvents by injection of Se powder into a Cd oleic acid solution without use of TOP. N-hexadecane was selected as the solvent. It is cheaper, environmentally friendlier, and more stable in the atmosphere than the reported solvents such as TOPO or ODE.

The CdSe quantum dots have been successfully synthesized in the temperature range 230-260 °C (with a step of 10 degrees). The increase in particle size with red shift in colour was also confirmed by the UV–Vis absorption spectra. Photoluminescence spectra were measured and the photoluminescence quantum yield was obtained. The crystal structure of the as-synthesized product was analyzed by XRD with CuKa radiation.

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Synthesis and Magnetic Properties of $Sr_2Mg_{1-x}Ni_xSi_2O_7$ and $Sr_2Mg_{1-x}Ni_xGe_2O_7$ ($0 \le x \le 0.1$)

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Silicate and germanate melilites $Sr_2MgSi_2O_7$/$Sr_2MgGe_2O_7$ and solid solutions on their basis are promising materials as rich colour pigments and phosphors.

In present research the series of nickel doped strontium magnesium silicate and germanate (Sr2Mg1-xNixSi2O7; $Sr_2Mg_{1-x}Ni_xGe_2O_7$, $0 \le x \le 0.1$) solid solutions were prepared by the high temperature solid state reaction method. The phase composition of all the compounds under study was controlled by the method of X-ray analysis and Rietveld refinement (Fig. 1).

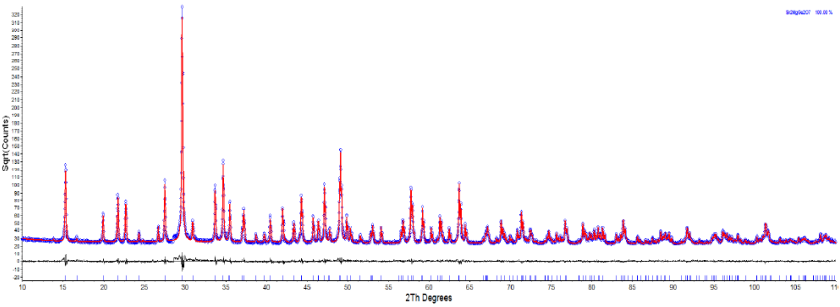

Fig. 1. Rietveld refinement of diffraction pattern for $Sr_2Mg_{1-x}Ni_xGe_2O_7$ (x = 10%).

On the basis of measuring the magnetic susceptibility of the solid solutions paramagnetic components of magnetic susceptibility (χ_{Ni}) and effective magnetic moments (μ_{eff}) of nickel atoms were calculated at various temperatures and concentrations of the solid solutions. In the report valence state of nickel atoms and their interatomic interactions in different matrixes are discussed. Magnetic methods confirmed the valence state of nickel atoms. The report discusses the reasons for the different nature of the exchange interactions between nickel atoms, depending on the type of matrix.

Scientific research was performed with the help of St. Petersburg State University Research Center for X-ray Diffraction Studies.

Synthesis and Characterization of $Na[Ga(NH_2BH_3)_4]$

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Nowadays scientists are searching for a new kind of fuel instead of hydrocarbons. The most perspective direction is the use of hydrogen as a source of energy, because its combustion is accompanied by the release of a large amount of heat, and only water is formed as a by-product. Since it is much easier to handle solid hydrogen carriers compared to liquid or gaseous hydrogen, ammonia borane and its derivatives are potential sources of hydrogen [1, 2].

In this research we synthesized a complex ammonia borane $Na[Ga(NH_2BH_3)_4]$. At first stage sodium ammonia borane $NaNH_2BH_3$ was produced by reaction between NH_3BH_3 and Na in THF solution under argon [3]. At second stage reaction between $NaNH_2BH_3$ and GaX_3 (where X is Cl or I) in THF solution under inert atmosphere at low temperatures [4] after several days results in formation of $Na[Ga(NH_2BH_3)_4]$. Compound was identified by solid state ^{11}B NMR and IR spectra. Data obtained are in good agreement with the reported values for its analog $Na[Al(NH_2BH_3)_4]$ [2].

It was found that $Na[Ga(NH_2BH_3)_4]$ is unstable at room temperature, so it cannot be used as an industrial source of hydrogen.

We are thankful to the resource centers of the St. Petersburg State University "Magnetic resonance methods of research", and "X-ray diffraction methods of research" and to Krasnova I.S. and Shelyganov P.A. for the assistance.

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The Influence of Hydrothermal VO_2 Thermal Treatment Conditions on Product Morphology and Properties

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There are several crystal modification of vanadium dioxide. VO_2 (A) (tetragonal), VO_2 (B) (monoclinic), VO_2 (R) (tetragonal-rutile), and VO_2 (M) (monoclinic-rutile) are most widely known. Monoclinic phase has layered structure that is perspective as an electrode material for Li-ion batteries. Tetragonal modification is considered as an intermediate phase between VO_2 (B) and VO_2 (R)/ VO_2 (M). Rutile modifications undergo a reversible semiconductor-to-metal phase transition (SMPT) at 68 °C turning into each other with an electrical, magnetic and optical properties change. Due to this transition rutile phases are perspective for thermosensors, thermoswitchers, IR limiters and smart coatings for windows. However, in hydrothermal process VO_2 (B) or a mixture of VO_2 (B) and VO_2 (M) is a usual product [1] and obtaining of a thermochromic rutile phase requires some additional treatment.

Mixed VO_2 (A) and VO_2 (B) powders were obtained in hydrothermal synthesis and treated at 200-400 °C in oxygen and inert atmosphere. Obtaining of VO_2 (M) was observed by XRD. Powders were analyzed by SEM. Its specific surface area was measured by BET method. SMPT characteristics were investigated by vibration sample magnetometry and impedance spectroscopy.

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Investigations are carried out in Resource Centers of St. Petersburg State University Research Park: Centre for Geo-Environmental Research and Modelling (GEOMODEL), Centre for X-ray Diffraction Studies, Centre for Innovative Technologies of Composite Nanomaterials.

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New Color Standards for Color Normalization in Optical Sensing

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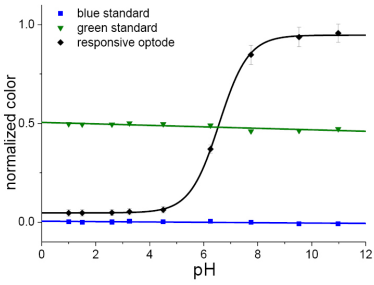
Ion-selective optical sensors (optodes) are rapidly expanding tools in various fields of science and industry. They translate the analyte activity into the optical signal due to the presence of lipophilic pH-indicator. Their signal is the result of the ion-exchange equilibrium between the optode phase and the solution.

In accordance with the modern trends of miniaturization of analytical techniques, microphotography instead of spectrophotometry is typically used to register colorimetric signal of bulk optodes. In this case, for obtaining adequate results, optode color should be normalized using color balancing algorithms, e.g. white standard. However, it was suggested that the polymeric membrane containing the same indicator as the sensors themselves is more promising as the color standard. Its color is a superposition of the colors of the protonated and deprotonated forms of the indicator, which can potentially lead to more adequate and reliable method of color normalization.

In this contribution, we report on our studies aimed at developing of the novel color standards as an alternative to the conventional white standard. These standards are based on plasticized poly(vinyl chloride) films containing lipophilic pH-indicators. Obviously, the color standard film should not change its color in response to the solution composition. To achieve that, the ion-exchange between the two phases should be suppressed by imposing constant Galvani-potential at the phase boundary. It was shown [1, 2] that this can be achieved by introducing moderately lipophilic electrolyte into the polymeric sensor phase. Its distribution between the phases stabilizes the Galvani-potential. Tetra(butyl ammonium) tetra(butyl borate) salt was used in this work. All of the tested compositions demonstrated no effect of neither qualitative nor quantitative composition of the solution in their color (see the Fig.). pH/Na^+-selective optodes based on the same matrix and containing the same indicator were calibrated using the developed standards. The resulting response curves had similar properties to the curves obtained with the conventional white standard in terms of accuracy and reproducibility of the measurements.



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Nanosized Anion Exchanger as Stationary Phase in Capillary Electrochromatography

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Nowadays a lot of different techniques are proposed for the determination of ionic and ionogenic compounds in complex samples by capillary electrophoresis. However, many of them possess low selectivity concerning to analytes with close electrophoretic mobilities, or high detection limits. Capillary electrochromatography (CEC) with stationary phase absorbed or covalently bonded on the capillary surface combines the selectivity of ion chromatography and high efficiency of capillary electrophoresis. It is one of the most perspective way to solve the problems connecting to LODs and selectivity improvement.

This work describes the application of basic nano-sized anionite (NSA), type AB-17 [1], as a physically-absorbed stationary phase for CEC efficient and selective separation of inorganic anions and organic acids. The modification procedure of capillary walls by NSA was developed. It was established that flushing of capillary by NSA aqueous suspension resulted in formation of strong physically-absorbed coating, possessing stablilty in wide pH range from 2 to 10.

The simultaneous determination of 8 inorganic anions (Br^-, Cl^-, NO_2^-, SO_4^{2-}, NO_3^-, F^-, HPO_4^{2-}, CO_3^{2-}) on the modified capillary was developed. The additive of 0,05 mM NSA in the BGE led to sufficient increase of separation efficiency and selectivity (N = 200- 1500*10^3 t.p./m, R_s = 1,0 – 12,7). Besides, the various on-line concentration techniques were applied to decrease the detection limits. For instance, field amplified sample stacking along with NSA modified capillary provided 8-30 ng/ml LODs of inorganic anions. In case of electrostacking these values were even lower (1 pg/ml – 7 μg/ml).

Determination of organic acids (formic, acetic, oxalic, tartaric, malic, citric, lactic and succinic) on the modified by NSA capillary possessed also high efficiency (N = 360 - 600*10^3 t.p./m), resolution (R_s = 2,2 – 7,8) and LODs (9-34 ng/ml and 1 - 2ng/ml in case of field amplified sample stacking and electrostacking, correspondently). The developed method of organic acids analysis was approved by quantitative determination of organic acids in wines.

Acknowledgements. The authors are grateful to the Chemistry Educational Centre, Research Park, Saint Petersburg State University for technical support. The authors also greatly appreciate financial support of RFBR grant № 17-03-01282-a.

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Transport and Physicochemical Properties of Nanocomposite Pervaporation Membranes

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Membrane processes are known as ecological, energy and resourse-saving technologies that offer many advantages compared to conventional processes such as distillation. Pervaporation as a membrane process is a promising direction of the technology of separation of industrial solutions. Azeotropic, close-boiling mixture cannot be easily separated by distillation, but can be effectively broken up by pervaporation. The key factor of the pervaporation is the material of membrane, its design and optimization allow to influence on transport and physicochemical properties.

In the present work novel mixed matrix membranes were obtained by including endofullerenes FeC_{60} into the matrix of P84 copolyimide (BTDA-TDI/MDI, copolyimide of 3,3'4,4'-benzophenone tetracarboxylic dianhydride and 80% methylphenylene diamine + 20% methylene diamine). Mass transfer through P84/FeC_{60} membranes was studied by sorption and pervaporation tests toward methanol and methyl acetate. The separation of methanol-methyl acetate mixture is an essential industrial task due to the fact that these substances take part in many chemical processes as reactants and media. In the pervaporation experiment over the concentration range of 5-22 wt% methanol in feed, all membranes showed high affinity to methanol and produced permeate concentrated in methanol.

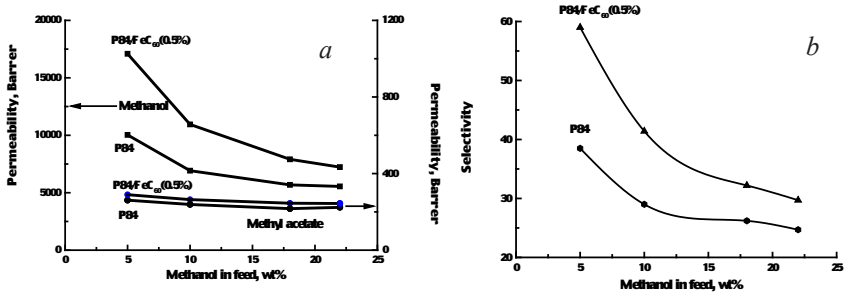

Fig. 1. Dependence of permeability (a) and selectivity (b) on methanol concentration in the feed for pervaporation of MeOH–MeOAc mixture using P84/FeC_{60} membranes.

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Synthesis of Polyacrylic-Citric Acid for Biomedical Applications

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A new acrylic based monomer with hanging citric acid groups through reaction between acryloyl chloride and citric acid was synthesized. Then, this monomer was polymerized in aqueous solutions by radical polymerizations to obtain polyacrylic-citric acid with a molecular weight and polydispersity around 2300 g mol^{-1} and 1.018 respectively. The size average of synthesised polymer was determined by DLS in aqueous solutions and it was around 10 nm. Electrostatic interactions between dodecyl amine and dodecyl amine and citric acid unites in polyacrylic-citric acid resulted in micelles with the ability of loading anticancer drugs (Fig. 1). The obtained drug delivery systems were able to efficiently transfer doxorubicin through the cell membrane. Ability of assemblies to transfer DOX through the membrane of MCF7 cells was studied by confocal laser scanning microscopy (CLSM). Also Cytotoxicity tests show that drug delivery systems are able to destroy and inactivate MCF cancer cells, efficiently [1, 2].

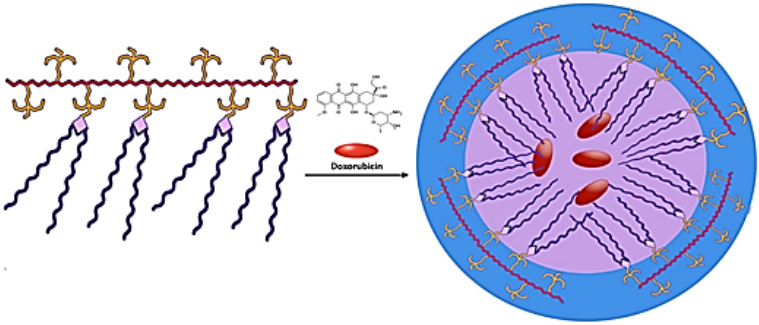

Fig. 1. Loading of doxorubicin by amphiphilic carriers.

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Stability of PEPPSI-type Metal-Organic Complexes

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Metal-organic catalysts are an integral part of chemistry in 21th century, especially as a component of cross-coupling reactions [1]. Some of them are susceptible to hydrolysis by traces of water [2]. PEPPSI complexes are metal-organic catalysts of the last generation, which are known as relatively stable. For estimation of their stability under typical reaction conditions Pd-PEPPSI complex **1** and Pt-PEPPSI complex **2**, which had been obtained according to the described procedure [3], were examined (Fig. 1). During the series of experiments, the complexes were heated at 80 ºC under air atmosphere in anhydrous and 90% aqueous dioxane solution for 10 days. Monitoring of the complexes behavior was undertaken via UV-spectrometry, TLC and HPLC analysis. The results have shown neither any changes of the spectral intensity nor by-product formation. This proves that Pd- and Pt-PEPPSI complexes have excellent stability and do not demonstrate any detectable changes. As a result, their properties allow applying them as a catalyst in various conditions including aqueous-organic solutions at elevated temperature.

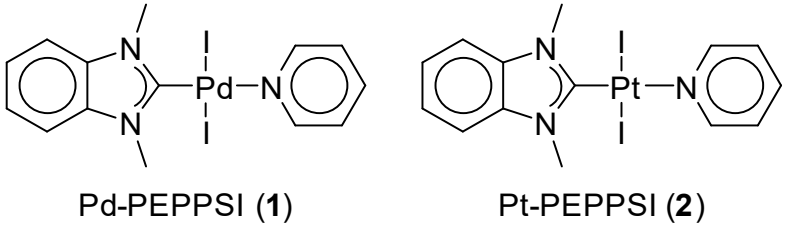

*Fig. 1. Structures of the studied complexes **1**and **2.***

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Hybrid Membranes Containing Star-Shaped Macromolecules with Fullerene Core for Intensification of Propyl Acetate Production

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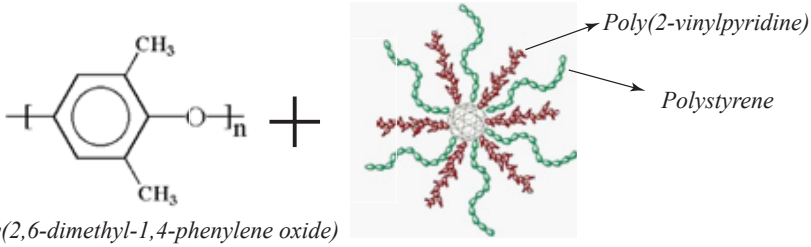
Membrane technologies are one of the most used in industry of liquids and gases separation due to energy saving and environmental protection methods of separation. Development of novel membrane materials helps to achieve an improvement of the main transport parameters, productivity and selectivity.

In the present work mixed matrix membranes based on polyphenylene oxide (PPO) have been obtained by including hybrid star macromolecules that composed of a twelve-arms star with six nonpolar arms of polystyrene (PS) and six polar arms of poly-2-vinylpyridine (P2VP) grafted onto a fullerene C_{60} core. The membranes containing up to 5 wt% filler were studied in pervaporation of the system simulating the esterification reaction of n-propanol and acetic acid.



Poly(2,6-dimethyl-1,4-phenylene oxide)

Fig. 1. Scheme of star-shaped macromolecules with fullerene core.

It was found the possibility of the control on esterification process by water removal using membranes under study to shift the chemical equilibrium of reaction. This result may be useful in connection with the prospect of the practical realization of the hybrid process "reaction + pervaporation" for propyl acetate production.

Acknowledgements. A.Yu. Pulyalina acknowledge the Russian Foundation for Basic Research (project 15-03-02131) and also Fellowship of the President of Russian Federation (project № 184, SP-1469.2015.1).

Investigation of Heterogeneous Area in the Systems with Reaction of Ethyl Formate and Ethyl Acetate Synthesis by the Gas Chromatography Method

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Today the method of gas chromatography is one of the most common and precise methods for determining the compositions of equilibrium liquid phases because it let to select easily the optimal conditions of separation depending on the task and the type of system under investigation. We used the gas chromatography method to study heterogeneous region of splitting in the multicomponent liquid-phase systems with reaction of ethyl acetate (ethanol – acetic acid – ethyl acetate – water) and ethyl formate (ethanol – formic acid – ethyl formate – water) synthesis under polythermal conditions. Data on the liquid-liquid equilibrium were obtained using gas chromatograph "Crystal 5000.2" with the following separation parameters: Porapac R packed column (1 m x 3 mm), rate of carrier gas was 60 ml/min (helium, grade A), the operating temperature of the column was 180 °C, the operating temperature of the thermal conductivity detector was 240 °C, the operating temperature of the evaporator was 230 °C. Initial solutions with compositions corresponding to the region of splitting, were prepared in chromatographic vials (5 ml) using gravimetric method with an accuracy of 0.001 g. Stirred up sealed vials were placed in a liquid thermostat at a given temperature. After the phase equilibrium reached, the samples of each phase were taken by chromatographic syringe (1 μl) and were analyzed 2-3 times using the gas chromatograph. To calculate the equilibrium compositions, internal normalization method and relative calibration were used. The error of chromatographic analysis was ± 0.005 mol. fraction. During the experiment, 150 experimental points of compositions of equilibrium liquid phases were obtained. Obtained experimental data will be useful for the development of coupled (reaction + phase transition) processes of chemical technology that require detailed information on the phase structure and singularities of the topology of phase diagrams of reacting systems.

The study was carried out using the funds of grant of Russian Science Foundation (project No. 17-73-10127).

Possibilities of the Using of some Equations of State for the Estimation the Mass Flow of Natural Gases

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The problem of quantitative estimation of the flow of natural gas (NG) is of practical and commercial importance. For example, in many cases NG is sold on the basis of mass flow that gives the opportunity for the control of general mass of consumed product. Usually the obtaining the data on mass flow is connected with direct measurements of volume flow and density. Such determination needs the use of various devices, such as multiple ultrasonic transient-time meters, conventional orifice plates and turbine meters. Evidently that such complex of experimental equipment has many disadvantages and limitations. Accordingly, the reduction in the number of such devices in the measuring stations becomes an urgent task. There are many studies on the measuring of the mass flow rate of different gases in the literature (see, e.g. [1]). Unfortunately, these devices, as a rule are suitable for low concentration gases in low velocity range. This disadvantage is critical for transmission pipelines where NG concentration and velocity are very high.

In our study we tested the method proposed by M. Farzaneh-Gord and co-workers [1] for the calculation of NG densities and estimation of mass flow on the basis of these data. The novel correlation is based on the NG gas temperature, pressure and Joule Thomson coefficients (JTC). The JTC values were calculated as the derivatives of the temperature by the pressure (process through the throttling valve at constant enthalpy). The actual densities of different NG mixtures were calculated by AGA8 EOS: the use of the equations of state (EOS) makes it possible to calculate the density, but this requires information on the temperature, pressure and composition of the mixture. In this case the measurement of NG properties and mass flow could be carried out in real time regime. The further development of the method will be based on the application different EOS for the search of optimal quantitative determination of NG flow using minimum of experimental data.

Acknowledgements. This research was supported by RFBR (17-58-560018).

Re7ference

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On the Way to the Lewis Acid/Base Stabilized Phosphanyltrielanes: Synthesis and Structure of H_3GaPCy_3

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Compounds of the type H_2MPH_2 (M=Al, Ga) are prospective precursors for the generation of group 13/15 semiconductor materials [1]. However, these compounds are very prone to polymerization. The way to stabilize them is the coordination of Lewis base (LB) or Lewis acid (LA). The LA/LB-stabilized compounds can be prepared via salt elimination reaction [2]

$$LA{\cdot}PH_2M' + XH_2M{\cdot}LB = LA{\cdot}PH_2MH_2{\cdot}LB + M'X,$$

where LA = $W(CO)_5$, $M(C_6F_5)_3$; LB – substituted phosphine; M' = Li, Na; M = B, Al, Ga; X - halogen.

The compound H_3GaPCy_3 (Cy - cyclohexyl) is precursor for preparation of XH_2GaPCy_3. In contrast to its analogues, H_3GaPCy_3 has high (up to 130 ºC) thermal stability and is even stable on air [3]. The molecular structure of H_3GaPCy_3 has attracted our attention, since according to [3] it features one anomalously short Ga-H bond distance of 1.35 Å (two other Ga-H bond distances are 1.53 and 1.54 Å). According to the CSD database [4], the average value of Ga-H distance among the 21 compounds of the type H_3GaLB is 1.43 Å, which casts doubt on the previously reported structure. In order to solve this discrepancy, we have repeated X-ray structure determination of H_3GaPCy_3.

H_3GaPCy_3 was synthesized by the reaction between $LiGaH_4$ and PCy_3 in diethyl ether at -78 ºC, after filtration ether was removed under vacuum. The saturated solution of H_3GaPCy_3 in dry toluene was kept for two days at -30 °C, yielding colourless plates, suitable for the X-ray structural analysis. Gallium has expected tetrahedral geometry with Ga-H distances 1.45, 1.46, and 1.48 Å, in contrast to the earlier report [3]. Thus, the structure of H_3GaPCy_3, refined in present work (R-factor is 3%, which is significantly less than 7.2% in [3]), does not exhibit anomalously short Ga-H bond distances.

This work was supported by the SPbSU-DFG grant 12.65.44.2017. We thank the resource centers of St. Petersburg State University "X-ray diffraction methods of research" and "Magnetic resonance methods of research".

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Research of the Critical Phenomena in the Liquid-Phase Splitting System Propionic Acid – Ethanol – Ethyl Propionate – Water at 30°C

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Development and deployment in industrial production of processes with supercritical fluids represents an actual and interesting task. Processes with critical transitions it is used in various industries, since pharmaceutics and finishing with production of perfumery production, they are used in production of fuel, in a supercritical fluid chromatography, and also for creation of supercritical reactionary environments. Knowledge of phase balance and the critical phenomena is for this purpose necessary.

This work is devoted to research of the liquid-phase splitting system, namely receiving experimental data about the critical phenomena with the corresponding creation of binodal curves and surfaces with the corresponding arrangement on them critical points. As object of research the system propionic acid – ethanol – ethyl propionate – water is chosen at 30 °C and atmospheric pressure. The analysis of system was carried out by method of isothermal titration.

Research of the critical phenomena for two ternary systems and five quaternary systems with various ratio of concentration of propionic acid and ethyl alcohol was conducted. As a result of research there were afforded 7 compositions of critical phenomena. In terms of obtained experimental data there were constructed critical states at triangles of Gibbs-Rosebaum and "critical curve" (Fig. 1) at concentration tetrahedron of compounds.

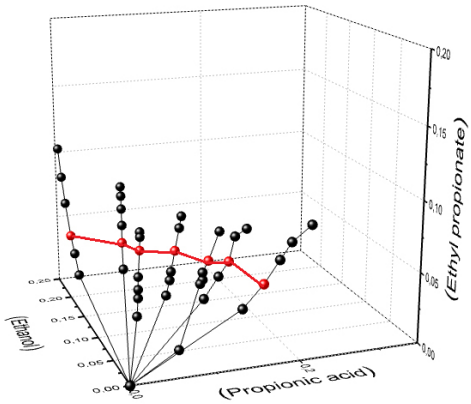

Fig. 1. Critical curve at concentration tetrahedron of compounds.

Solid State Structure of Complex of Ammonia Borane with Tetraglyme

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Molecular complex of ammonia borane with tetraglyme of 2:1 composition was obtained as a side product of $CsNH_2BH_3$ preparation. According to CCDC database it is the first complex of ammonia borane with acyclic polyether. Structure of complex was determined by single-crystal X-ray diffraction measurements (Fig. 1) and computation methods.

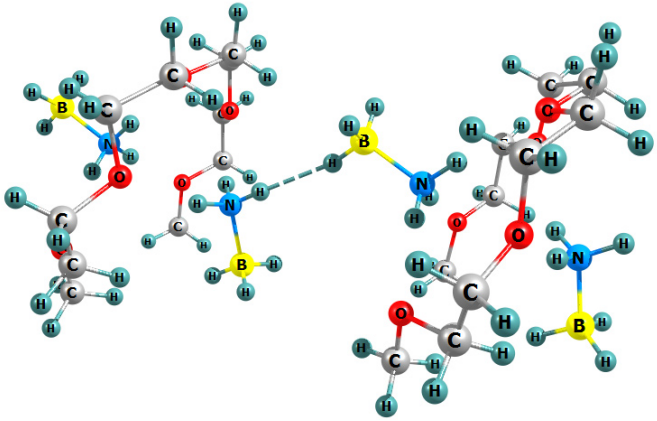

Fig. 1 Molecular structure of $C_{10}H_{22}O_5$•$2BH_3NH_3$ in the crystal. Two molecules connected by N-H—H-B dihydrogen bond.

It is interesting to note that there is one short contact (1,94 Å) N-H---B-H (see Fig. 1) between adjacent $C_{10}H_{22}O_5$•$2BH_3NH_3$ complex particles. This dihydrogen bonding is found to be shorter comparing with similar interaction in ammonia borane crystals (2.02-2.32 Å)[1].

In present work we compare features of hydrogen bonding in complexes of ammonia borane with crown-ethers and tetraglyme.

This work was supported by Science Foundation grant 14-13-0015. We thank Computer Center Resource Center of SPSU for computational time and A. Virovets (University Regensburg) for conducting X-ray diffraction measurements.

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Synthesis Magnetite Sorbents Based on Zeolite and Magnetite Nanoparticles

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Magnetic sorbents are used in many chemical processes. Due to their nanoroporous structure and magnetic properties, they are applied as magnetic sorbents for cleaning of drains water, collect oil from the surface of reservoirs and in medicine, as transport for drug delivery. There are many methods for synthesizing magnetite.

In this work, we synthesized the samples using three different techniques: one-stage precipitation, two-stage precipitation and mechanical mixing of the finished reagents. Analysis of the test samples showed that the material with the optimal set of characteristics-magnetic properties, catalytic activity, sorption ability for example of heavy lead ions and the properties of acid-base centers, can be achieved using single-stage precipitation of magnetite nanoparticles in the presence of a zeolite matrix.

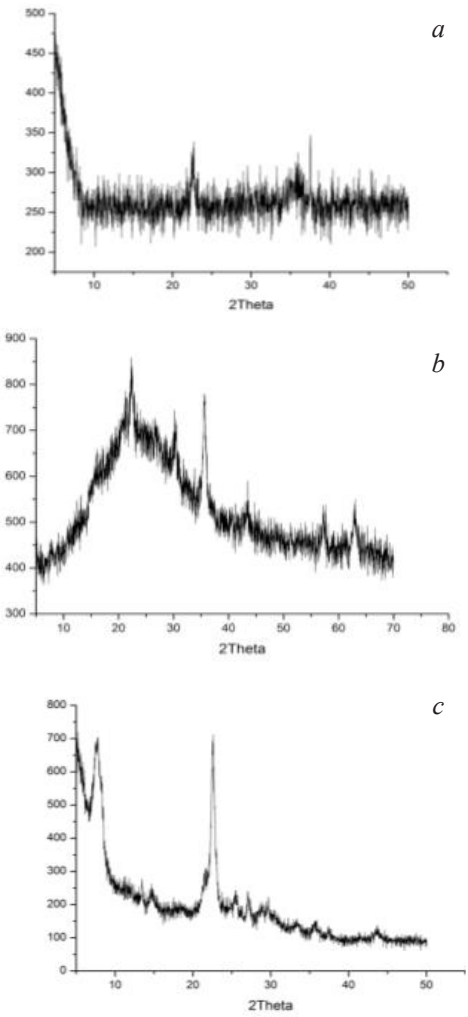

Fig. 1. X-ray diffraction patterns of the samples under study (a) one-stage precipitation; (b) two-stage precipitation; (c) mechanical mixing of the finished reagents.

Mass Spectrometric Study of Langmuir-Blodgett Films Based on Lanthanide Stearates

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The researcher's interest in the electronic properties of thin films containing metal atoms [1, 2] has not decreased in recent years. The magnetic centers in nanoscale objects can lead to the presence of a large number of different physico-chemical properties in such structures. Thin-film structures obtained by the Langmuir-Blodgett method based on transition metals or lanthanides salts and of fatty acids cause a particular interest. To construct a chemical model of interaction in such structures, it is necessary to clearly represent the structure of such objects. A combined mass spectrometric study of Langmuir-Blodgett films based on lanthanide stearates was carried out to solve this problem.

The films based on lanthanide stearates were obtained by the Langmuir-Blodgett method by applying a solution of stearic acid in hexane to the surface of a water solution of the lanthanide salt. These films were collapsed, and then dispersed in acetonitrile in an ultrasonic bath.

The formation of lanthanide mono- and distearates (depending on the metal contained in the film) was proved by the LDI-MS and ESI-MS method.

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Excited States of Eu-Au Heterometallic Luminescent Complex with5-(4-ethynylphenyl)-2,2'-bipyridine Bridging Ligand:DFT-Based From-the-ground-up Approach

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Heterometallic compounds comprising atoms of d- and f-elements connected by a bridging ligand are a versatile platform for the design of efficient luminophores with desired properties. The targeted optimization of luminescent properties requires a detailed insight into the functions of the building blocks, from which these complexes are assembled. In this work we demonstrate a from-the-ground-up approach to the investigation of excited states of a Eu-Au heterometallic luminescent complex (Fig. 1).

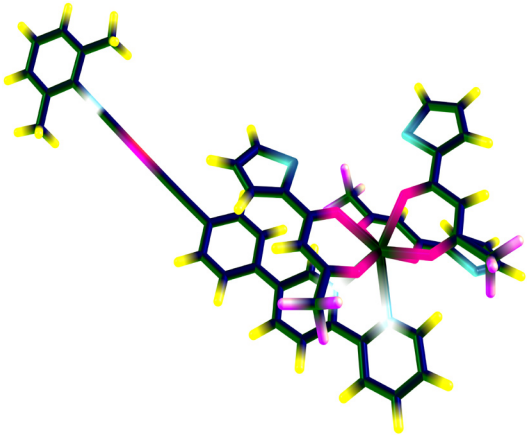

Fig. 1. Structure of the Eu-Au heterometallic complex studied in this work.

TDDFT calculations were performed to obtain the excited states of the above species; the results of these calculations were analyzed using NTO formalism.

The calculations were performed using the facilities provided by the Computational Resource Center (Research Park, St. Petersburg State University).

This work was supported by the Russian Science Foundation (grant no. 16-13-10064).

Synthesis of Copper Containing Nanoparticles by Microwave Heating

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In this work we synthesized copper containing nanoparticles by microwave heating in a PEG-600 solution. Also it was tried to produce a bimetallic nanoparticles (n/p) by adding cobalt nanoparticles to the medium of reaction. More over the reduction of Cu^{2+} in a PEG-600 solution was researched by optical spectroscopy.

The copper reduction reaction scheme was proposed based on information from spectral analysis.

It was determined that cobalt nanoparticles were not a seed crystal of growth for copper particles, although little islet of copper was found on cobalt (Fig. 1). Copper nanoparticles grew on their own seed crystal in the solution (Fig. 2).

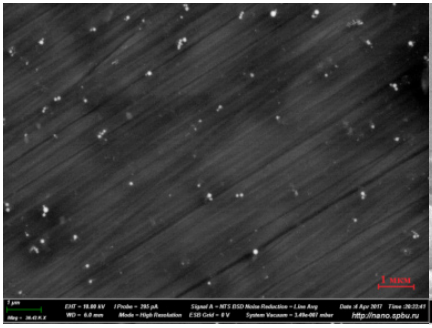

Fig.1. SEM-image of cobalt-copper n/p.

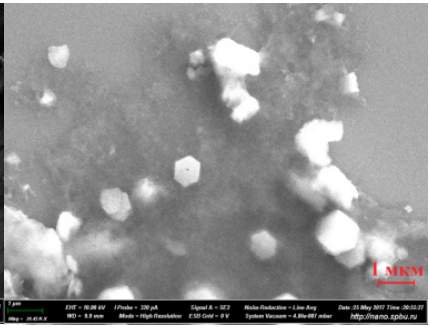

Fig.2. SEM-image of copper n/p.

Monodisperse Hydrosol of Detonational Nanodiamond Coagulation in KCl and $BaCl_2$ Solutions

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Continuous increase in industrial production of detonation nanodiamond (DND) is caused by intensive expansion of its practical application areas. Microporous agglomerates of DND with dimensions from tens to several hundred nanometers are formed as a result of strong explosives mixture detonation in a closed volume and a non-oxidizing medium. Recently developed methods of deagglomeration [1-3] allow one to obtain monodisperse DND hydrosol (particle size – 4-5 nm).

For the first time, the electrosurface properties of a monodisperse DND sol in KCl (10^{-4}-10^{-2}) M solutions in the pH range 3.0-11.0, as well as the aggregate stability of the sol in a wide range of KCl and $BaCl_2$ concentrations at pH 5.0 were studied. Some results of stability study are shown in the Fig. 1.

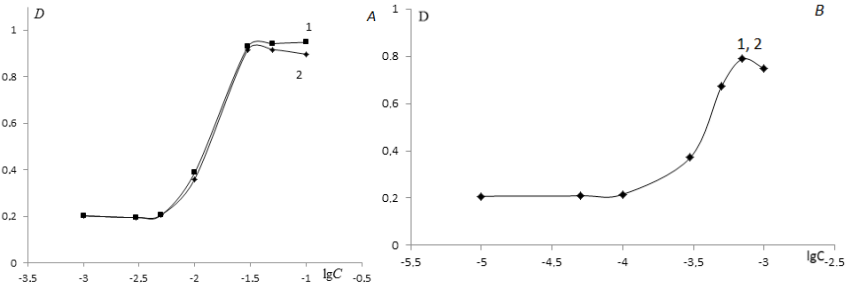

Fig. 1. Dependences of the DND hydrosol absorbance on concentrations of KCl (A) and $BaCl_2$ (B) solution. Observation time is 3 minutes (1) and 5 minutes (2).

Stability and coagulation of a monodisperse DND sol can be explained both in terms of the classical and expended DLVO theory. Coagulation of the DNA sol in NaCl and BaCl2 solutions at pH 5.0 occurs in the primary potential minimum via the barrier mechanism.

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Synthesis and Thermal Properties of Hydroxyapatite Nanoparticles with Different Morphology

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Currently, most of polymer-inorganic scaffolds for bone tissue engineering are based on hydroxyapatite (HAP) nanoparticles [1]. This is due to the fact that natural HAP is the main component of human bone tissue, and synthetic NPs demonstrated the ability to in vivo degradation and recrystallizing under the action of enzymes. Note that this process can be controlled by varying the degree of NPs crystallinity. In the other hand the process of polymer-inorganic composites preparation may be accompanied by the formation of various structures based on HAP NPs which can be affected on materials degradation.

So, the present work includes the hydrothermal synthesis of NPs with various axial ratios; characterization by XRD, TEM methods, SSA estimation, and FTIR spectroscopy; and the study of thermal properties of as-prepared NPs by TGA and DSC.

Synthesis of HAP NPs was carried out under hydrothermal conditions in the presence of organic molecules of various nature (etidronic, salicylic, tartaric, succinic acids, o-phenanthroline and catechol, SDS, PVP, stearin) and at the different temperatures. The use of this method is due to the possibility of obtaining a highly crystalline product. The final particle sizes ranged from 35 to 150 nm in length and from 8 to 33 nm in width.

HAP nanospindles (180 °C), nanorods (240 °C) and nanoneedles (180 °C, SDS as a capping agent) (37, 74 and 135 nm in length, 24, 26 and 33 nm in width) were chosen to further experiments.

The TGA results showed a several stages weight loss at the temperature range of 30–150, 200–300 and 400–600 °C, which characterize the processes of evaporation of adsorbed water. For nanoneedles, a weight loss was observed at the temperature range of 600–800 °C, which may be due to decarboxylation and dehydroxylation processes. It was also found for this sample that the peak at 700 °C could be due to the presence of a NPs highly structural organization [2].

So, the HAP NPs with various shape and sizes were synthesized, its thermal stability up to 600 °C was established. In addition, the formation of a NPs lamellar structure was also demonstrated.

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Separation Performance of Novel Polyheteroarylene Membranes

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Membrane technology is one of the most promising in the sphere of separation of liquid and gas mixtures due to such advantages as eco-friendliness, low energy consumption, and possibility of automation of the process. Pervaporation is the most useful, simple and cheap method for separation of liquid mixtures especially azeotrope, nearly boiling point and thermally non stable mixtures. The range of available industrial membrane materials is limited thus the development and investigation of novel polymer materials are the primary task.

The aim of the present work is the fabrication of non-porous membranes based on metal-polymer complexes with Cu(I) of polybenzoxazinoneimide (PBOI-Cu(I)) and imide-containing polyamic acid (PAA-Cu(I)), and investigation their transport properties in separation of methanol (MeOH) - methyl tertiary butyl ether (MTBE) mixture. MTBE is the fuel additive which increases the octane number. The industrial method for the production of MTBE has one disadvantage: product contains methanol, and purification of MTBE is the important goal.

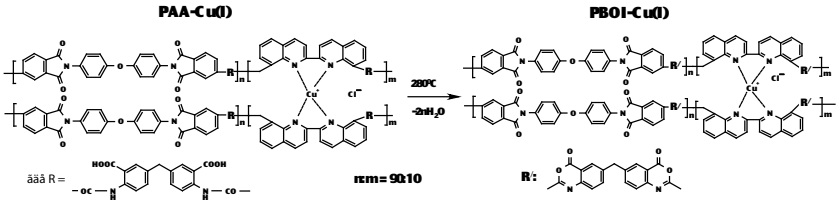

Fig.1. Scheme of PAA-Cu(I) to PBOI-Cu(I) transformation.

In pervaporation of methanol – MTBE mixture membranes under study permeate preferably methanol and can be used for effective purification of MTBE from methanol impurities.

Acknowledgements. Dr. A.Yu. Pulyalina acknowledges the Russian Foundation for Basic Research (project 15-03-02131) and also Fellowship of the President of Russian Federation (project № 184, SP-1469.2015.1).

Voltammetric Determination of Sulfur-Containing Amino Acids Using Nanostructured Electrodes

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Sulfur-containing amino acids such as cysteine, homocysteine and sulfur-containing tripeptide – glutathione are ubiquitous in physiological fluids. They play an important role in antioxidation protection and metabolism. It has been reported that levels of these thiols are essential – concentration changes in tissues may be related to such serious diseases as arteriosclerosis, leukemia, cancer, Alzheimer's and/or Parkinson's disease [1, 2].

This project is devoted to development of highly selective determination of sulfur-containing amino acids and their derivatives using voltammetric approach. For this purpose, we offer to use electrochemical sensors based on electrodes modified with nanostructures of noble metals and transition metal oxides. Modification of electrodes with nanostructures is performed by layer-by-layer technique.

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Palladium(Ii)-Mediated Addition of Aminothiazaheterocycles to Coordinated Isocyanides

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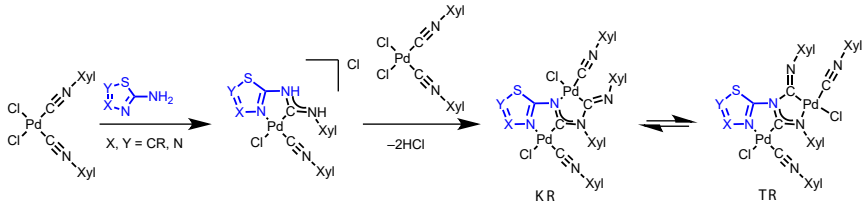
It is well known, that reactivity of isocyanides can be significantly changed with their coordination to a metal center. For instance, this allows an addition of weak nucleophiles to a triple CN bond, which is unlikely for free isocyanides. It was found recently in our research group that palladium(II) isocyanide complexes tend to react with α-aminoazaheterocyles with the formation of diaminocarbene complexes. These species are nucleophiles themselves and able to react with another isocyanide molecule yielding binuclear products [1].



Scheme 1. Pd^{II}-mediated addition of aminothiazaheterocycles to xylylisocyanide.

In this work, we found that the reaction of palladium(II) *bis*-xylylisocyanide complex with various aminothiazaheterocycles (thiazol-, thiadiazol-, and isothiadiazol-2-amines) gives the mixture of two binuclear regioisomeric products (**KR** and **TR**, Scheme 1) which are subject to reversible isomerization into each other in a solution. The isomeric ratios of products depend on the structure of starting aminothiazaheterocycle. The obtained complexes were characterized by set of physicochemical methods: HRESI-MS, FTIR, 1D and 2D NMR spectroscopies, and single-crystal X-ray diffraction.

This work was supported by Russian Science Foundation (project 14-43-00017P). Physicochemical studies were performed at the Center for Magnetic Resonance, Center for X-ray Diffraction Studies, Center for Chemical Analysis and Materials Research, and Chemistry Educational Centre (all belong to Saint Petersburg State University).

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Self-organization of Langmuir-Blodgett Films on the Surface of an Aqueous Subphase Containing 3d-Metal Ions and the Study of their Physicochemical Properties

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Langmuir-Blodget films represent the special kind of supramolecular structures organized by amphiphilic molecules containing metal ions and hydrophobic fragments contacting with different phases (the metal ion borders on the aqueous phase, the organic «tail» borders by air). These films may be applied as new sorbents of biologically active substances used for their determination by HPLC method [1].

In the report the results of study of the physicochemical properties of Langmuir-Blodgett films formed by 3d-metal stearates will be presented. These films were synthesized from the aqueous subphase by dropping a solution of stearic acid in hexane on its surface. The chemical composition of the obtaining films was determined by mass spectrometry (LDI), and the morphology of the resulting collapsed films was studied by the SEM method.

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Solubility and Solid Phase Formation in Ternary Systems CdX_2 – S – DX (X=Cl, Br, I; S=dimethylsulfoxide, N,N-dimethylacetamide; DX=1,4-dioxane) at 298 K

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At present there is no general theoretical concept which allows us to predict the processes occurring in ternary systems including binary solvent and electrolyte and the effect of these processes on the structure of compounds presented in equilibrium with liquid phase. Therefore, the study of this kind of systems is essential for the further development of Solution Chemistry. Furthermore, the compounds formed in these systems can serve as effective catalysts, precursors for the synthesis of metalorganic frameworks, drugs and so on.

The report will present the results of study the solution-solid phase equilibria in ternary systems which contain cadmium halides, aprotic organic solvent (dimethylsulfoxide and N,N-dimethylacetamide) and 1,4-dioxane. The influence of halide ion on the form of the solubility isotherms and the structure of equilibrium solid phase was analyzed. We noticed the solvating ability of the second solvent in mixtures with 1,4-dioxane increases. This phenomenon was explained on the basis of data on the structure of a binary solvent. Compositions and structures of individual and mixed solid solvates were also identified and analyzed from positions of the theory of hard and soft acids and bases [1] and concepts of donor-acceptor interactions in the systems under consideration [2, 3].

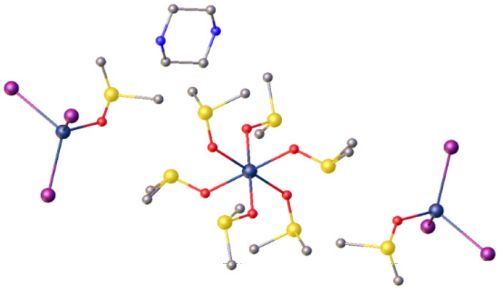

Fig. 1. Structure of mixed solvate of cadmium halide with DMSO and dioxane.

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Active Templates for Surface-Enhanced Raman Spectroscopy Based on AgAu@C Nanoparticles

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Creating of templates which can be active in surface-enhanced Raman spectroscopy is a very important issue in case of detecting low concentrations of such dangerous substances as toxins. We developed templates based on AgAu@C nanoparticles deposited by laser irradiation from metalorganic complex and tested them on a rhodamine 6g as a model substance. Also we investigated the adsorption processes of rhodamine 6g on synthesized samples. The results of such experiments are presented in Fig. 1 (a - SERS-measurements, b – adsorption curves).

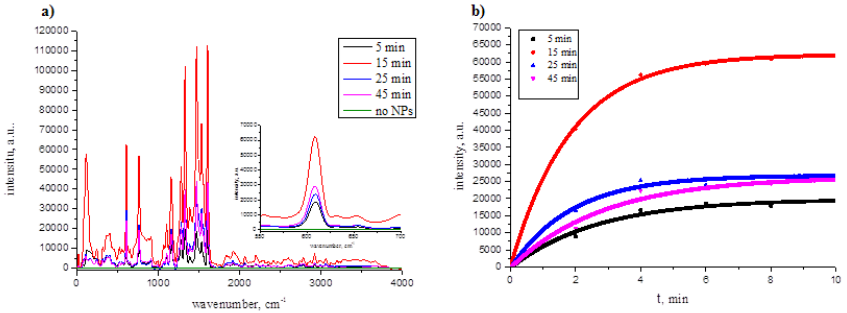

Fig. 1. a) SERS-measurements of rhodamine 6g on synthesized samples; b) adsorption curves.

It was found out that samples with NPs, deposited during 15 minutes, show the best results.

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Polymerization of Droplets under Flow Using Photoinitiated Azide-Alkyne Cycloaddition

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Photochemistry is recognized as an underused synthesis tool. However, absorption of a mole of photons of UV light provides as 130 times greater energy as compared to ambient condition. It would overcome energetic barriers for many chemical reactions [1].

The main advantages of flow photochemical reactors over conventional batch systems are; consistent light penetrations, controlled exposure times, precise temperature control and removal of the photochemical products from the irradiated area. These features typically result in higher conversions or yields, improved selectivity, enhanced energy efficiencies and reductions of solvent volumes and consequently waste [2].

The Cu(I)-catalyzed azide–alkyne cycloaddition (CuAAC) reaction is one of the most widely used 'click' reactions. Within the framework the possibility of using a copper-catalyzed azide-alkyne cycloaddition (CuAAC) reaction for photocontrolled polymerization of pre-synthesized monomers was performed under irradiation with UV-light in the flow mode. Thus, the polymer beads with alkyne-azide functionalized surface was prepared according to a modified reported procedure [3].

The possibilities, limits of applicability of this approach, as well as details of the experimental work will be presented in the poster report.

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Membranes Based on Polysulfone for Pervaporation of Binary and Multicomponent Mixtures

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Currently the membrane technology is actively developed and widely used for purification, concentration, fractionation of liquid and gas mixtures. One of the perspective membrane methods is pervaporation. This process is used for the separation of mixtures of low-molecular substances. This method attracts the attention of the chemical, petrochemical and biochemical industries as an alternative process to traditional separation methods (for example, distillation or liquid-liquid extraction) due to its characteristics: harmless, compact equipment, simplicity and flexibility in operation and low-energy. It is possible and widely applied to separate azeotropic mixtures, mixtures of isomers and also close-boiling or thermally unstable substances by pervaporation. Nowadays there is a great variety of membranes based on polymeric and inorganic materials. Among them the polymers take an important place as they have good mechanical characteristics, film forming properties and high water selectivity. In the present research polysulfone (PS) was investigated as a polymer material for pervaporation separation of binary and multicomponent mixtures.

The aims were to develop dense and supported membranes based on polysulfone and to study their physicochemical and transport characteristics. The physicochemical properties of the membranes were investigated by the immersion sorption method and measurements of contact angles. Transport characteristics of obtained membranes were studied by pervaporation for separation of azeotropic mixtures (ethanol-water, 1-propanol-water, 1-propanol-propyl acetate-water) and of multicomponent mixtures for the potential use of these membranes in a hybrid or combined process «esterification reaction + pervaporation». It was shown that the supported membrane with a selective layer of polysulfone deposited on porous support MFFK had the best transport properties.

Critical Phenomena in Acetic Acid – Amyl Alcohol – Amyl Acetate – Water System Under Polythermal Conditions

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The investigation of the critical phenomena observed in systems that have both of chemical and phase transformations is of interest of researchers. The study of such systems expands thermodynamic knowledge and helps to improve the process of organic synthesis.

The system explored is the acetic acid – amyl alcohol – amyl acetate – water one. Amyl acetate was synthesized by etherification and purified in distillation columns. The experiment was carried out under polythermal conditions, e.g. 303.15, 318.15, 333.15 K. The solubility and the critical area were studied in ternary and quaternary systems by the isothermal titration method, or the «cloud-point technique» method. The data obtained was used in the Gibbs-Rosebom triangle to see the direction of the binodal and the location of the critical points. The formation of the concentration tetrahedron of compounds has allowed investigating the shape of the critical curve. The graphics received under different temperatures were compared and there was regularity between increasing in temperature and increasing in solubility (Fig. 1). In the course of all studies of the critical area, a pale blue opalescence was observed.

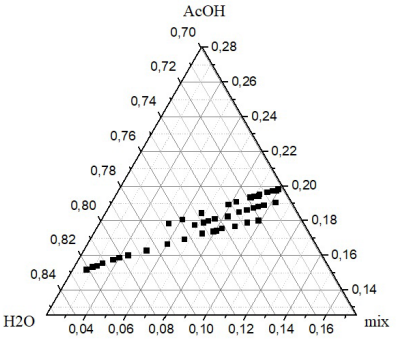

Fig. 1. The solubility in acetic acid-amyl alcohol-amyl acetate-water system at 303.15, 318.15, 333.15 K.

Support: Maria Toikka is grateful to the Russian Science Foundation (grant 17-73-10290) for the support of this study.

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Synthesis and Adsorption Properties of Fe_3O_4@AlOOH Nanoparticles: Removal of Congo Red Dye from Aqueous Solutions

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Nowadays a lot of studies are devoted to magnetite (Fe_3O_4) nanoparticles (NPs) because of their magnetic, electric, and adsorption properties [1]. Usually the precipitation procedure in inert atmosphere to prevent surface oxidation is used to obtain Fe_3O_4. In this study we report the synthesis of 'core-shell' nanoparticles Fe_3O_4@AlOOH to protect magnetite from oxidation and aggregation and improve its absorption properties. There are many applications for γ-AlOOH in medicine, food industry, for wastewater treatment and gas emissions due to its porous structure, thermal stability and resistance to hydration. The regulation of AlOOH-shell crystal structure and thickness was made by variation of temperatures (from 140 to 240°C in increments of 20°C) and pH values (4, 7, 9) in hydrothermal synthesis. Thus, optimal synthesis conditions were found.

The structure of obtained NPs was determined by XRD, TEM, FTIR spectroscopy, SSA estimation, DLS measurements. The magnetic properties of as-prepared samples were studied by VSM, the characteristics of hysteresis loops were found, and all the samples under study demonstrated superparamagnetic behavior.

Three types of NPs with different structures (Fe_3O_4, AlOOH and Fe_3O_4@AlOOH) further were used as a Congo red (CR) adsorbent. The absorption kinetics and adsorbed CR vs NPs mass dependences were studied to find the optimal conditions for absorption process. The adsorption isotherms were recorded for all types of NPs in the dye concentrations range of 0,1-2 mg/ml. The process is normally described by the Langmuir isotherms and the maximum adsorption capacity is 1,4 mg/mg for AlOOH, 1,0 mg/mg for core-shell NPs and 0,6 mg/mg for Fe_3O_4. The Fe_3O_4@AlOOH adsorption properties are close to AlOOH, but NPs with magnetite-core also can be taken from the solution via magnetic field (saturation magnetization at room temperature is equal to 60 emu/g). Thus, a possibility of synthesis core-shell nanoparticles Fe_3O_4@AlOOH for sorption applications was demonstrated.

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Synthesis and Characterization of Nanoflower $Bi_2O_2CO_3$-$ZnFe_2O_4$

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Among semiconductors Bismuth subcarbonate $Bi_2O_2CO_3$, which is structurally close to the aurivillius family, is composed of alternate $Bi_2O_2^{2+}$ and CO_3^{2-} layers, with the plane of the CO_3^{2-} group orthogonal to the plane of the $Bi_2O_2^{2+}$ layer. $Bi_2O_2CO_3$ has long and widely been used for various medical and heal the care purposes [1]. $ZnFe_2O_4$ is a chemically and thermally stable semiconductor material, which is suitable for wide applications including photocatalyst, imaging, drug delivery, and hot-gas desulfurization [2]. Some studies have focused on the fabrication of $Bi_2O_2CO_3$-based composite catalysts, including ($Bi_2O_2CO_3/MoS_2$, $Bi_2O_2CO_3/Bi_2WO_6$, …). In the present work, in this study BOC nanoflower were coupled with ZFO nanoparticles to prepare magnetic BOC-ZFO nanocomposites using one-step hydrothermal method. The nanoparticle was characterized with FT-IR, XRD, UV-Vis, SEM and EDX analysis. XRD and SEM (Fig. 1 (a-b)) results confirm the successful synthesis of nanoflower BOC-ZFO structure.

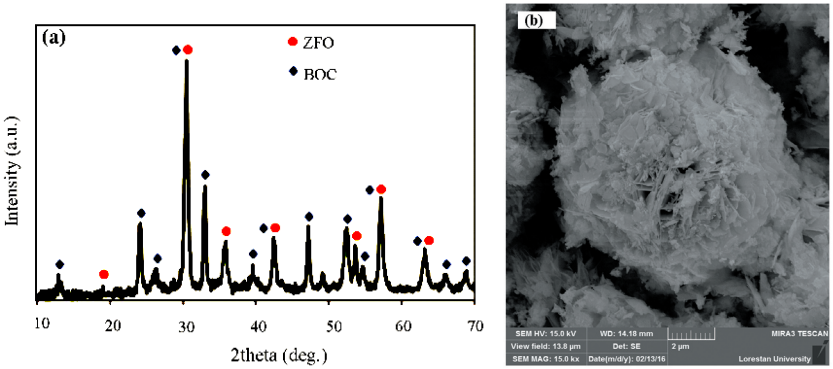

Fig. 1. (a-b) XRD and SEM of $Bi_2O_2CO_3$-$ZnFe_2O_4$.

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B.Geo- and Astrophysics

The Application of Multiple Linear Regression Algorithm to the Microwave Radiometer RPG-HATPRO Data in the Problem of Liquid Water Path Retrieval

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The analysis of liquid water path (LWP) values obtained by built in operational algorithm for the RPG HATPRO instrument has shown that LWP retrieval bias has random character due to presence of spurious input data. That makes the interpretation of the results difficult. In order to solve that problem the multiple linear regression algorithm (LREA) has been applied to RPG HATPRO data for LWP retrieval since this algorithm is assumed to be less sensible to spurious input data. The retrieval errors have been estimated on the basis of numerical experiments. The algorithm's response to input data failures has been investigated for LREA. The bias estimations have been made for this algorithm using cloud free observation periods. Also, two retrieval algorithms LREA and a built in operational quadratic regression algorithm (QREA) of LWP retrieval supplied by the manufacturer of the RPG HATPRO microwave radiometer have been compared to the "reference" algorithm based on the inversion of the radiative transfer equation.

The New Method Processing of Seismic Data for Study Geological Structure of Lake Baikal

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Lake Baikal is the main link of one of the largest zones of active continental rifting. The interest of formation and history of the development of this lake has increased due to the study of regional and global climate change in recent years.

Large volume of geological and geophysical work was carried out on Lake Baikal in the previous decades. The data of multichannel seismic profiling (1992) have decisive significance for clarifying the structure of the Baikal. The results of this seismic profiling after modern methods of processing and interpretation are presented in this work. The main aim of the work is study the processes associated with the migration of hydrocarbons according to the data of multichannel seismic profiling to assess the ecological state in the central ecological zone of the Baikal territory.

Modern processing was performed in the software package "CubeTechnology" and consisted of the method multifocusing «spherical mirror», migration and spectral decomposition by the RGB. Obtained data after reprocessing and interpretation clarified the characteristic of geological structure of Lake Baikal:

- the boundaries of the main reflecting horizons are traced, including the bottom simulating reflector related with gas hydrate (BSR);
- the structural map of roof of the acoustic foundation was constructed;
- the thickness of the sedimentary cover was estimated.

The author thanks the Head of the laboratory of methodological developments in the field of interpretation of seismic data Karpinsky Russian Geological Research Institute S.A. Gritsenko and the scientific supervisor T.S. Sakulina for help in the process of performing the work.

Analysis of the Observation of Atmospheric CO_2 Concentrations in the Ambient Air at the Peterhof Station over a Four-Year Period (2013-2016)

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The main target of the research was to analyze the CO_2 annual variations and growth rate at the Peterhof station, compare our results with independent measurements and modeling results and observe the variations of carbon dioxide diurnal cycle. High accuracy measurements of CO_2 concentrations in the ambient air are being carried out at Saint Petersburg State University by Los Gatos Research Greenhouse Gas Analyzer 24r-EP from 2013.

CO_2 has pronounced annual cycle with summer minimum and winter maximum and the peak to peak amplitude: in Peterhof 24 -31 ppm (6-8%); in Teriberka 16-21 ppm (4-5%); in Tiksi ~ 20 ppm (~ 5%). The characters of CO_2 annual cycles for all four years of measurements are in a good agreement with each over: the highest concentrations are specific for cold seasons, when the least concentrations are specific for warm season.

The growth rate of CO_2 at the Peterhof site estimated for 2013–2016 is (2.44±0.20) ppmv/yr, which is in good agreement with Mauna Loa trend (2.55±0.11) ppmv/yr for 2013–2016 and global growth rates (2.60±0.26) ppmv/yr for 2013– 2016.

From 2013 to 2016 the peak to peak amplitude of diurnal cycle of CO_2 concentrations in a warm season has been gradually decreasing, e.x. in June - from 50 ppm to 30 ppm (from 13% to 8%). In our research we find out that for 2013-2016 the peak to peak amplitude of diurnal cycle of CO_2 has strong relationship with the air temperature with correlation coefficient $R = 0.78$.

Investigation was supported by Russian Science Foundation (grant No14-17-00096). Authors thank Geomodel Research Center (SPbU) for providing the observational facilities.

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Investigation of the Width of the Spiral Structure of Disk Galaxies

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Spiral arms are one of the prominent features of many disk galaxies. As a site of the ongoing star formation, the spiral structure appears as regions of the enhanced surface brightness in the smooth underlying stellar disk. The overall appearance of the spiral structure (the shape, contrast, number of arms) differs significantly from galaxy to galaxy, proving the measurement of its parameters to be a hard task. These measurements, on the other hand, are of the great importance, since they can shed the light on the mechanism of the spiral pattern formation.

One of the most interesting parameters of the spiral structure is the width of spirals. The goal of this work is to develop a method for the spiral width measurement, and to apply it to a sample of spiral galaxies. The main idea of our method is to approximate the arms with a set of logarithmic spirals then to slice the arms with the lines perpendicular to the spirals and fit the fluxes across the lines with skewed gaussians. Before slicing the galaxies all of their images were masked thoroughly which was followed by photometric decomposition using DECA package [1]. The decomposition was implemented in order to distinguish the spiral structure to work with it directly and to obtain parameters needed for comprehensive exploration of the structure (bulge to disk ratio, exponential scale).

In order to apply our method, we compiled a sample of face-on spiral galaxies based on the Galaxy Zoo [2] and HyperLeda [3] databases. The images of the objects (around 200 items) were downloaded from the Sloan Digital Sky Survey (SDSS) database [4] in different spectral bands.

After the widths were found they were checked for any correlations within the set and also some of their properties were investigated such as asymmetry of profiles, etc. The techniques developed are to be used on larger sets of objects and the results to follow are of great interest for studying morphology of galaxies and developing theories of galaxy formation and evolution.

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The Effect of Atomic Clock Noise on Searching of Narrow-Band Gravitational Signal in Pulsar Timing

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Pulsar timing was suggested for detection of low-frequency gravitational waves ($10^{-9}Hz < f_{gw} < 10^{-7}Hz$) by Sazhin in 1978 and independently by Detweiler in 1979. Pulsar timing can be used for detection of different types of signal. In particular, it can be used for detection of monochromatic narrow-band signal, that is generated by a scalar field. Such scalar field is described in Chmelnitsky&Rubakov and suggested to be a possible candidate to warm dark matter.

A classic scalar field with mass 10^{-23}-10^{-22} eV is considered as warm dark matter. It acts as an ideal liquid with oscillating pressure, and these oscillations cause the oscillations of gravitational potential at frequency m, which can be detected using pulsar timing. The effect of these oscillations on pulsar timing is comparable to the effect of a monochromatic gravitational wave with characteristic strain $h_c \approx 2 \cdot 10^{-15} (10^{-23}\ eV/m)^2$ and frequency $f = 5 \cdot 10^{-9}\ Hz \cdot (m/10^{-23} eV)$. But unlike usual gravitational-wave background, in case of warm dark matter the signal will be narrow-band and monochromatic and the angle correlation coefficients will not depend on angular distance between pulsars.

The most important noise, arising during the observations, is clock noise, caused by errors in time standard. Both signal and clock noise have monopolar correlations, and it is this type of noise we are studying in this project.

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The Study of Cloud Condensation Nuclei Properties of Pollen Grains

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Atmospheric aerosol particles could influence the climate directly through scattering and absorbing solar and planetary radiation and also indirectly by acting as cloud condensation nuclei (CCN) and modifying cloud forcing and hydrological cycle. The least understood components include the primary biogenic aerosols (PBAs), such as pollen grains, that represent a significant fraction of the total aerosol component in atmosphere. A number of prior studies have showed that PBAs have the high ability to act as CCN and ice nuclei [1, 2]. But also under high humidity pollen grains can rupture to form submicron subpollen particles (SPP) that can serve as CCN under appropriative atmospheric conditions too [3]. The researches of CCN properties allow to find a connection between the sources of aerosol particles and condensation activity that depends on their size, chemical composition and hygroscopicity. The influence of chemical composition can be described using the effective hygroscopicity parameter κ.

In this study the CCN ability of 3 different types of SPP typical for boreal forest biom in the size range 20-300 nm under supersaturation (SS) level within 0.1-1.1% was analyzed. For this aim the tandem of special CCN spectrometer and Condensation Particle Counter (CPC) was used. The critical supersaturation S_C (i.e. the point at which the growing droplet can spontaneously grow to form a cloud droplet) and hygroscopicity parameter κ were determined for birch, pine and rape samples.

Acknowledgements. This work was supported by the Geo Environmental Research Center “Geomodel” of the Saint Petersburg State University.

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The First Outcomes and Further Plans of Incorporating GEC into the Chemical Climate Models

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Coupling between global electric circuit and microphysical processes within the cloud is not fully-realized so far. In frame of this investigation the impact of the atmospheric electricity to global climate through the changing of ionospheric potential difference (IP) between surface ground and the bottom boundary of ionosphere based on the model data was carried out. We have incorporated parameterization of the ionospheric potential developed by Eugene Mareev [1] into the chemical-climate model SOCOLv2 [2] and have found that ionospheric potential strongly depends on the some cloud parameters such as: cloud top, bottom and thickness as it was proposed. The comparison of the obtained IP with real data of the fair-weather electric field (Carnegie curve) has shown the similar variation. Also we included By-component of the interplanetary magnetic field (IMF) to counting of the autoconversion rates for the understanding the coupling of the IMF and low atmosphere parameters through the global electric circuit (GEC). The correlation between surface pressure and variation of By-component IMF at high latitudes (>75°S) was found and compared with previous results [3, 4]. The first outcomes of this investigation and proposals to the future work will plan to present in scope of the conference.

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The Study of Ionospheric Total Electron Content Variability Using the Signals of COMPASS/Beidou Geostationary Navigational Satellites

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With the development of GNSS (Global Navigational Satellite Systems) and SBAS (Satellite Based augmentation systems) constellations, the coherent multi-frequency L band transmissions are now available from a number of geostationary satellites. These signals can be used for ionospheric total electron content TEC estimations in the same way as widely used GPS/GLONASS signals. At the same time, geostationary satellites have the advantage of a fixed ionospheric pierce points, in comparison with the moving pierce points for GPS / GLONASS satellites broadly used for TEC estimation, which allows continuous TEC monitoring along a given direction in the ionosphere.

The purpose of this work is to study the possibility of using the signals of geostationary COMPASS / BeiDou satellites for continuous TEC monitoring, as well as the analysis of the day-to-day variability of TEC in the ionosphere of the middle and equatorial latitudes under calm and disturbed heliogeophysicsl conditions, especially during recent geomagnetic storms and sudden stratospheric warmings.

As an example we present the essential asymmetry in the ionospheric TEC response to geomagnetic disturbances in the northern and southern hemispheres during the strongest in the current solar cycle St. Patrick's day 2015 geomagnetic storm, caused by a complex combination of processes responsible for the occurrence of positive and negative ionospheric disturbances.

We also present intensive positive TEC anomalies in equatorial and mid latitude ionosphere at midday hours for minor and major final sudden stratospheric warmings (SSW) of February and March, 2016. The observed anomalies lasted for about one week after SSW peak and had the amplitudes comparable to those typically observed during moderate geomagnetic storms. This result shows the importance of the atmosphere - ionosphere coupling for description of the ionospheric electron density distribution.

Our results demonstrate the convenience of using geostationary COMPASS/ Beidou satellites for monitoring TEC in the ionosphere under various heliogeophysical conditions.

Polarimetric Observations of Blazar AO 0235+164

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Currently, one of the leading problem of both theoretical and observational astrophysics is determination and investigation of active galactic nuclei (AGN) nature. These extragalactic objects demonstrate such exotic properties as fast and sharp variability across the electromagnetic spectrum, non-thermal form of the spectral energy distribution (SED), high and variable polarization degree up to 60-70% and etc., so the great numbers of observers groups pay their attention to AGN monitoring, and observational laboratory at Saint Petersburg State University is among them.

AO 0235+164 is one of the most intensively studied BL Lacertae objects (AGN subclass). In the given paper the polarimetric data is presented; the correlation between photometric and polarimetric data is found; the method of analyzing developed by V.A. Hagen-Thorn and S.G. Marchenko [2] are used and the conclusions on the blazar behaviour are done.

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Simultaneous Source Separation via Hyperbolic Vector-Median Filtering

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By standard technique of marine seismic surveys, a second shot is fired after the medium's response from the previous shot is recorded, during which the source cannot be used. Therefore, a lot of working time is wasted inefficiently. This problem can be solved using several sources with time delayed signals. The ability to separate the signal from simultaneously operating sources allows for multiplying the speed and efficiency of work.

The use of seismic sources with time-separated signals requires the solution of a complex problem of their separation. This problem can be solved by various methods, such as spatial inversion, encoding of pulses, median filtering, etc.

Median filtering (MF) is well-known for its ability to remove spiky noise in a seismic profile after NMO or with relatively flatter events. MF has been successfully utilized in the deblending process [1]. This work demonstrates the use of a hyperbolic vector median filter instead of a conventional MF to remove blending noise. Fig. 1 shows the result of the operation of such filter.

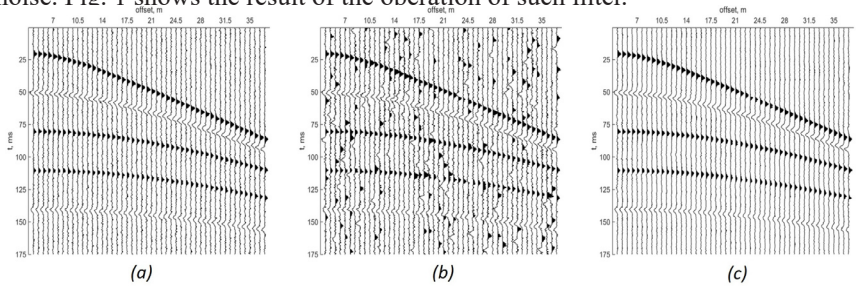

Fig. 1. Synthetic example in common midpoint domain. (a) Unblended data for source #1. (b) Blended data. (c) Deblended data for source #1.

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An Ice Core Chronology Based on Orbital Tuning of Air Content Records: a Case Study of the Dome Fuji (Antarctica) Ice Core

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Paleoclimate data is the main thing scientists need to understand natural climate variability and future climate change. The ice cores from deep Antarctic boreholes provide this data and give us an opportunity to analyze a long climatic record with a relatively high time resolution. One of these records, air content in ice (V), is supposed to have a strong link with the local summer insolation. This assumption has allowed researchers to build new ice core chronology based on this link. The dating method proposed by Raynaud et al., 2007 and further developed in Lipenkov et al., 2011 includes the selection of suitable insolation curve and the calculation of time delay between air content and insolation time series using Continuous Wavelet Transform (Torrence&Compo, 1998). To date, this method was effectively applied to Dome C and Vostok ice core records (Raynaud et al., 2007 and Lipenkov et al., 2011, respectively).

Our study proves that continuous wavelet transform (CWT) is the most suitable tool for tuning the preliminary dated air content records on the calculated local insolation time series. The uncertainties associated with applying this technique to the experimental air content records have been thoroughly investigated. The new dating method was for the first time applied to constructing the orbital time scale for the Dome Fuji (77°19'S, 39°42'E) ice core, using a composite air content record obtained from this site.

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The Use of Quasiorthogonal Sweeps in Vibroseis Survey

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In modern seismic survey, the vibrational method becomes more and more popular. Traditionally, the widely used and most studied signal is the linear chirp. There are some problems when using the signal, such as strong jitter in the vicinity of the minimum and maximum frequencies in amplitude spectrum and the so-called "low-frequency problem".

Using pseudorandom sweep (PRS) solves these problems. A pseudorandom sweep can be generated based on a pseudorandom sequence. An essentially new feature of working with PRS is the possibility of separating wave fields from several simultaneously operating vibrators. It is necessary that signals from different vibrators have a low level of crosstalk or correlated at times that are not of interest in seismic studies. In these terms, signals are quasiorthogonal [1]. Fig. 1 shows a segment of a phase-modulated signal with m-sequence, its autocorrelation and cross-correlation between two signals based on different m-sequences.

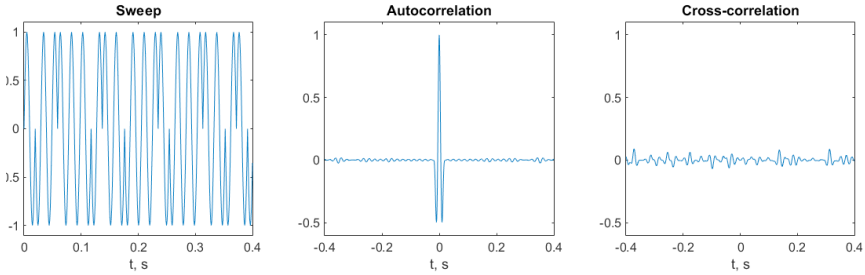

Fig. 1. Phase-modulated signal with m-sequence and its correlation functions.

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C. Mathematics and Mechanics

Topology of Two-Frequency Quasi-Periodic Regimes in Control Systems

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We study the topology of forced two-frequency quasi-periodic regimes in a class of control systems [1] (non-autonomous nonlinear systems of differential equations in $\mathbb{R}^n$) using a direct approach as follows. Instead of focusing on the corresponding invariant tori [2] in the extended phase space, we study the projection of such a tori onto coordinate space, or, equivalently, the closure of the set $\cup x(t)$ (complete trajectory) on which the quasi-periodic solution $x(\bullet)$ winds. Denote this set by M. Restricting to the case of two frequencies, one can however observe a rich topology: in $\mathbb{R}^3$ such a set may be any surface of genus g or even have more complicated structure.

Since a two-frequency quasi-periodic function $x(\bullet)$ can be represented as $x(t)=\Phi(\omega t)$, where $\omega=(\omega_1,\omega_2)$ is the frequencies vector and $\Phi(\bullet,\bullet)$ is a periodic with respect to the lattice $\mathbb{Z}^2$ function, it is natural to consider Φ as a "parametrization" (not necessary one-to-one) of M. One of the results to will be announced is a theorem that in a topologically typical situation the set of critical points of such a parametrization has measure zero.

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On Boundary Value Problems for the Wave Equation with Conditions on the Entire Boundary

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Wave equations play an important role in describing processes in physics. Some applications lead to emerging of specific problems which need a new approach to be solved. For the first time, such a problem related to my talk emerged in [1] and later a similar problem has been studied in [2].

The problem is to find the solution u to the wave equation

$$\frac{\partial^2 u}{\partial t^2} = a^2 \sum_{i=1}^{n} \frac{\partial^2 u}{\partial x_i^2}, x \in \mathbb{T}^n, t \in [0, \tau], a > 0; \quad (1)$$

$$u\big|_{t=0} = g_0(x); \quad (2)$$

$$\left(Au + B\frac{\partial u}{\partial t} \right)\Big|_{t=\tau} = g_1(x), \quad (3)$$

where A,B are (pseudo) differential operators on $\mathbb{T}^n$, with orders 1 and 0 respectively.

Theorem. *a) The problem (1)-(3) will be Fredholm solvable if and only if operator family*

$$\sigma(D)(x,\xi) : l^2(\mathbb{Z}) \to l^2(\mathbb{Z})$$

$$\sigma(D) = \sigma\left(\frac{1}{ai}A + B\right)(x + m\tau\xi, \xi)T^{-1} + \sigma\left(-\frac{1}{ai}A + B\right)(x + m\tau\xi, \xi)T$$

is invertible for all $(x,\xi) \in S^*\mathbb{T}^n$, *where* $T\omega(m) = \omega(m+1)$;
b) If the principal symbols $\sigma(A), \sigma(B)$ *of A,B are constant in x, then the problem (1)-(3) will be Fredholm solvable if:*
1) $\sigma(B)(\xi) \neq 0$ *for all* $\xi \in S^{n-1}$

2) $\dfrac{\sigma(A)(\xi)}{\sigma(B)(\xi)} \notin \mathbb{R}$ *for all* $\xi \in S^{n-1}$

The proof of this theorem is based on a reduction of problem (1)-(3) to the boundary and the results obtained in [3].

Acknowledgements. The author is grateful to G-RISC for support, this research was partly performed at Leibniz University of Hannover.

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Takens' Method for an Autonomous Bicycle with Control

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Takens' method is a family of approaches for the analysis of time series generated by nonlinear deterministic dynamical systems. It typically allows to reconstruct an unknown dynamical system by constructing a new state space. The reconstruction preserves the properties of the dynamical system that do not change under smooth coordinate changes.

The talk introduces the nonlinear control system of an autonomous bicycle [1]:

$$\begin{aligned} \dot{\sigma} &= u_\sigma \\ \dot{\alpha} &= \kappa_\alpha \\ \tilde{M}\begin{bmatrix} \dot{\kappa}_\alpha \\ \dot{\upsilon}_r \end{bmatrix} &= \tilde{F} + \tilde{B}\begin{bmatrix} \dot{u}_r \\ \dot{u}_\sigma \end{bmatrix} \end{aligned} \qquad (1)$$

where α is the roll-angle, α is the parametrization of the steering-angle,
υ_r is the velocity of the rear-wheel along the contact line,
$\tilde{M} = \tilde{M}(\alpha,\sigma)$, $\tilde{B} = \tilde{B}(\alpha,\sigma,\upsilon_r)$ are 2x2 matrices,
$\tilde{F} = \tilde{F}(\alpha,\sigma,\upsilon_r,\kappa_\alpha)$ is a 2 dimensional vector function,
and u_r, u_σ are the controls.

System (1) may be represented as a differential equation of the following form:

$$\dot{v} = F_0(v) + \sum_{i=1}^{2} F_i(v)u_i(t) \qquad (2)$$

Here F_i, $i = 1..2$ are nonlinear functions, and u_i, $i = 1..2$ are the controls.

Differential equation (2) generates a cocycle over the space of admissible controls. For this system a modification of Takens' method for a such cocycle system is considered [2].

After choosing a suitable phase space and a space of controls for the cocycle Takens' method gives reliable reconstruction results of the dynamics for typical systems.

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Usage of Convolutional Neural Networks for Dynamic Images Analysis

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Neural networks have significant value as they are applied for data processing in many areas like economics, robotics, medicine.

It seems interesting to apply neural networks for detecting objects in dynamic images (series of frames) and forecasting their trajectories. In the article different parabolic trajectories are represented as an example. Also there is another point of interest – the original way the data are preprocessed to be used as training sets for neural network.

For further development, received information can be used for detecting various rockets or missiles, their trajectories, launch and landing sites and also the type of the rocket.

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Oscillating Loss of Stability of Trivial Solution for Boundary-Value Problem with Linear Deviate in Boundary Condition

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Let us consider nonlinear boundary-value problem with linear deviate in boundary condition

$$u' = \beta\ddot{u} - \gamma u(t-\tau) + F(u) \qquad (1)$$

$$u'(0,t) = 0, \quad u'(1,t) = \alpha u(x_0, t-\tau) \qquad (2)$$

Parameters $\alpha \epsilon \mathbb{R}$, $\beta, \gamma > 0$, $\tau \geq 0$ $x_0 \in [0,1]$ and in zero smooth function $F(u)$ has at least the second infinitesimal order.

To research the stability of trivial solution of problem (1), (2), it's necessary to find the eigenvalue with vanishing real part on the left side, i.e. the greatest among the rest. When all eigenvalues are in the left part of complex plane and one pair of them are on imaginary axis, there is an oscillating loss of stability of zero balance state. Our task was to find critical values of initial parameters, when there is the stability loss of trivial solution of problem (1), (2).

The research was carried out by means of special software. All calculations were performed on a large number of independent streams of CPU.

As a result of numerical research there were found some critical values of initial parameters, when zero balance state of problem (1), (2) is collapsing vibrationally.

This work was supported by the Russian Science Foundation (project nos. №14-21-00158).

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On Fredholm Property of *G*-operators Associated with Morse-Smale Diffeomorphisms

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The object of this study are *G*-operators associated with a Morse-Smale diffeomorphism $g : M \to M$, where M is a 2-dimensional closed surface. Diffeomorphism g satisfies the following properties (see [3]):

1. the set of non-wandering points on M is finite and hyperbolic;
2. diffeomorphism g requires the transversality condition.

G-operators are presented in the form of a finite sum

$$D = \sum_k a_k(x) T^k : \; H^s(M) \to H^s(M), \qquad (1)$$

where $a_k(x) \in C^\infty(M)$, T is a shift operator associated with g: $Tu(x) = u\left(g^{-1}x\right)$, while $H^s(M)$ stands for the Sobolev space of smoothness s.

Operators of the form (1) are also known as weighted shift operators and they often appear in dynamical systems and probability theory, see [1, 2].

The Fredholm property of such operators depends on the smoothness exponent s of the Sobolev space (e.g., see [4]). So, the problem is to determine, for which exponents s operator (1) is Fredholm.

We obtained the following two results:

1. Explicit conditions are obtained for operators with constant coefficients to be Fredholm for s fixed.
2. For arbitrary operators of the form (1), we describe the dependence of their Fredholm property on s.

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Global Climatic Phenomenon «El- Niño» Neural Networks Forecasting Possibility

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«El- Niño» is the equatorial Pacific Ocean surface temperature increasing, which is the cause of many environmental and economic disasters. The effect of «El- Niño» was particularly strong in 1997-1998: a huge tornado in the USA (24,000 dead, $ 34 billion of economic losses), rains in the Chilean Atacama Desert, the catastrophic floods in Africa and the consequent increased mosquitoes breeding led to an epidemic of cholera in Kenya. It is also expected that «El- Niño» was the cause of hurricanes «Debbie» in Australia and «Matthew» in USA in 2017.

«El- Niño» is not easily predictable. This phenomenon doesn't lend itself to statistical forecasting and the simulation model can't give a qualitative result, since all the factors influencing the forecasting object are unknown. But prediction becomes possible with neural networks using.

The proposed method has 2 stages:

1. Neural network approximation of main factors of «El-Niño» occurrence process based on other climatic factors.
2. «El-Niño» classification based on main forecasted factors.

We also hypothesized the correlation between the dynamics of geomagnetic storms and «El- Niño». We verified this assumption and used geomagnetic storms data in forecasting. We assume that this dependence was not previously studied in details.

The results provide that «El-Niño» can be predicted by the proposed method. The presented results are intermediate and we formulated the further plans of accuracy improvement based on it.

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Bifurcations of Nonhomogeneous Solutions for the Erosion Equation

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Experimental research in the field of beam technologies are based on the series of surface erosion models, and the most common among them is the Bradley Harper model [1]. In work [2] the model which takes into account the nonlocality of the sputtering was considered.

In the aforementioned work the nonlocal erosion equation in the case of sufficiently small spatial deviation was considered. A basic version of the equation has the following form:

$$u_t = du_{xx} + hcw_x + hb_1 w_x^2 + hb_2 w_x^3 \qquad (1)$$

where $u = u(t,x), w = u(t,x+h), \quad h,c,b_1,b_2 \in R, \ |h| \ll 1$.

Let $h \neq 0, b_1^2 + b_2^2 \neq 0, d > 0$. The equation was studied in the normed form with periodic boundary conditions given by

$$u(t,x+2\pi) = u(t,x). \qquad (2)$$

In the given work the stability conditions for a flat surface and spatially nonhomogeneous solutions of the erosion equation were defined. Wave solutions of the spatially nonlocal erosion equation linearized in a neighborhood of a zero equilibrium state were constructed. It was shown that in case when a flat profile loses stability, then the solutions bifurcate from the equilibrium state in the form of high-mode traveling waves. Also, asymptotic formulas for the corresponding solutions were obtained, and the stability conditions for them, i.e. the conditions of their physical realization were found. These results were obtained by using invariant manifolds method and Poincare-Dulac normal forms theory and also asymptotic analysis methods.

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Mandreling of Shape Memory Alloy Sleeve as Simulated by COMSOL Multiphysics Software

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Shape memory alloys (SMA) are used as materials for thermomechanical couplings. In order to make the process of design and producing of such couplings more efficient correct methods of calculation should be applied. In the present work an attempt has been performed to use the COMSOL Multiphysics software for modeling of the mandreling process of shape memory alloy sleeve.

Mandreling was considered at a temperature below the final temperature of the reverse martensitic transformation, when the sleeve was completely in martensitic state. At this temperature, the stress-strain diagram of SMA looks like a stress-strain diagram of an elasto-plastic material with hardening. Therefore, the following hardening function, connecting stress σ and strain ε, was selected to approximate the experimental data for TiNi SMA:

$$\sigma = 60\varepsilon + 95(1 - e^{-4.2\varepsilon}) + \frac{10}{1 + 55(\varepsilon - 0.33)^2} - 1.4307175.$$

The sleeve was 30 mm length, with inner diameter d_i = 22.5 mm and outer diameter d_o = 30 mm. The mandrel diameter d_m, which was larger than d_i, was varied. Dependence of the d_i on d_m after finishing of mandreling was obtained.

Distribution of von Mises stress in the sleeve during the mandreling process is presented in Fig. 1.

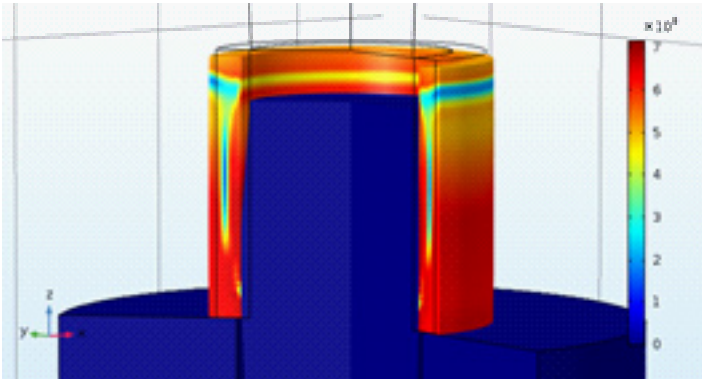

Fig. 1. Distribution of von Mises stress (in Pa) during the mandreling process. The dark blue elements are the mandrel and the bottom support.

Scientific research was performed at the Research park of Saint Petersburg State University Computing Center.

Numerical Investigation of Cavitating Flows with Liquid Degassing

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Cavitation is a phenomenon of bubbles (cavities) formation in liquid due to pressure drop. Cavitating flows play an important role in a wide range of applications. For example, cavitation is one of the key problems in designing of pumps, hydro turbines, ship's propellers, etc. Special attention is paid to cavitation erosion and to performance degradation of the hydraulic devices (noise, fluctuation of the mass flow rate) caused by formation of the two phase system with an increased compressibility.

One more important problem accompanying the above phenomenon is liquid degassing. It is known that the concentration of dissolved air in water at normal conditions is usually from 8% to 14% [1]. Determination of the degassed air content is important for the forecast of the device efficiency. Models for degassing in turbulent cavitating flows are not presented in the literature or in simulation codes. Therefore, development of a model for simultaneous cavitation and liquid degassing is the important fundamental and applied task.

A degassing model formulated in the present study provides a coupling between the dissolved gas diffusion process and the local characteristics of the turbulent cavitating flow (pressure and vapor volume fraction). The model is based on an analytical solution of the diffusion equation in a spherical cell corresponding to a single bubble. Henry's law is used to formulate a boundary condition for gas concentration at the bubble surface.

Numerical simulations of the three-dimensional unsteady flow of a cavitating liquid in a channel have been conducted. The geometry of the channel and the physical properties of the liquid were selected in accordance with the experimental test bench developed in the research center of Robert Bosch GmbH in Germany [2].

The obtained results are in satisfactory agreement with the experimental data and demonstrate the efficiency and robustness of the formulated model and the numerical algorithm.

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Hausdorff Dimension in Non-Metrizable Bornological Spaces of Control Theory

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In dimension theory it is customary to assume that the desired space Z has a metric structure. In the case of a metric space, there is a well-known formula for Hausdorff dimension [1].

$$dim_H(Z) = inf\{d \geq 0 \mid \mu_H(Z,d) = 0\} = sup\{d \geq 0 \mid \mu_H(Z,d) = +\infty\},$$

where $\mu_H(Z,d)$ the Hausdorff d-measure of space Z.

The talk describes the situation where this construction is impossible because of the non-metrizability of the original space. In this case, it is useful to introduce a bornological structure on the initial space Z. In [2] a method was described that allows one to define the Hausdorff dimension in bornological spaces. To do this, it is necessary to consider disks D in bornological spaces. Then we can define the element of a net

$$d_D(Z) = lim_{D'} dim_H(Z \cap X_D, X_{D'})$$

and Hausdorff dimension in bornological space

$$dim_{H,bor}(Z) = lim_D d_D(Z) = lim_D lim_{D'} dim_H(Z \cap X_D, X_{D'}).$$

As many result, in the talk estimates of the Hausdorff dimension were obtained for the case of bornological spaces. Some application for calculating the dimension of certain systems, for example, including the Henon system, in the bornological spaces are given.

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Stability Analysis of Recurrent Neural Networks for Time Series Based System Control in Aviation

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In aviation performance indicators represent states of captured, linked sub-systems, so the inner-workings of the system are recognizable shown in time-discrete time series [1]. The ability of recurrent networks (RNN) to model these temporal data and act as dynamic mappings makes them ideal for application to complex control problems. Because such networks are dynamic, however, application in control systems, where stability and safety are important, requires certain guarantees about the behavior of the network and its interaction with the controlled system. Both the performance of the system and its stability must be assured [2].

Therefore a transportation of the common RNN state space description $x(t+1) = F(Wx(t) + Du(t) + b)$ with the state vector x and the control *vector* u*, where* W, D and b are real weight matrices and F(.) is continuous and differentiable, *to a feedback control system*

$$f(x,u) = x(t+1) = Px(t) + \phi(t,r*x(t),u(t)),$$

which we may consider as an interconnection of a linear part and a nonlinear part*:* $Px(t) + q\xi(t)$ with $\delta(t) = r*x(t)$ and $\xi(t) = \phi(t,\delta(t),u(t))$, where *P, q* and *r* are constant real matrices, *x* is a state vector and $\phi(t,\delta,u)$ is real. This time-discrete dynamic system is usable to apply several studies regarding stability and dynamical behavior for both linear and nonlinear part [3]. A general method involves Lyapunov functions, which is applied for both the autonomous stationary net considering the state *x* and the control system considering state *x* and input *u* and satisfying the stability of the control structure. In addition investigations considering input sets causing periodical effects and their stability are applied.

With the received knowledge of stability with respect to input values and network parameters a guidance from inside the network can be derived to optimize the process of system controlling and receive undetectable optima.

Parts of the results were derived in cooperation with the Saint Petersburg State University (SPbU) within the G-RISC research exchange program.

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Bifurcations of Spatially Inhomogeneous Solutions of a Boundary Value Problem for the Generalized Kuramoto-Sivashinsky Equation

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In this paper, the generalized Kuramoto-Sivashinsky equation

$$u_t = -b_1 u_{xx} - b_2 u_{yy} - d_1 u_{xxxx} - d_3 u_{xxyy} - d_2 u_{yyyy} + c_1 (u_x)^2 + c_2 (u_y)^2,$$

where $u = u(t,x,y)$, $b_1, b_2, d_1, d_2, d_3 \in R, d_1, d_2, d_3 > 0$ with homogeneous Neumann boundary conditions

$$u_x(t,0,y) = u_x(t,\pi,y) = u_{xxx}(t,0,y) = u_{xxx}(t,\pi,y) = 0,$$
$$u_y(t,x,y) = u_y(t,x,\pi) = u_{yyy}(t,x,0) = u_{yyy}(t,x,\pi) = 0$$

is considered.

This equation represents a model of surface pattern formation during ion beam sputtering. This technological process is of interest due to it has a wide range of applications in a modern microelectronics (nanoelectronics), particularly in semiconductor processing of materials. Mathematical models are based on Sigmund's theory of sputtering [1]. It is shown that the inhomogeneous surface relief structures can occur when there is an exchange of stabilities of the equilibrium states. Stability analyses of spatially homogeneous equilibrium states are given, as well as local bifurcations are studied in the case their stability changes. The method of invariant manifolds coupled with the normal form theory was used to solve this problem. For the bifurcating solutions the asymptotic formulas are found. From applications to physics (nano- and microelectronics) point of view of most interest are spatially inhomogeneous solutions. They described an inhomogeneous relief on the surface of semiconductor materials under ion bombardment. It is shown that from a mathematical point of view the question of the auxiliary system of ordinary differential equations which is commonly called the Poincare-Dulac normal form. It is confirmed that the formation of nanoscale patterns on the surface can be considered as self-organization phenomena.

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Modified Foerster Model in Human Population Dynamics

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Size of human population on Earth has a huge impact on economy, social situation and ecology.

Growth of the population is affected by many, often random factors, such as natural disasters, wars, technological breakthroughs and social changes.

Surprisingly, there exists a simple model which approximates well the population data of the past two millennia. This model was proposed by H. Von Foerster [1]. In Russian literature these results were popularized by S. P. Kapitsa [2].

However, the model predicts approaching infinity in the nearest future, which is impossible. In fact, decrease in growth of the population is observed instead.

In our study we try to summarize results of past researches and propose a modification of the Von Foerster model in order to make it consistent with novel data.

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About One Boundary Problem in Mechanics of the Rotary System

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Following, we have a nonlinear boundary value problem is considered

$$u_{tt} + (g_1 u_t + g_2 u_{t,xxxx}) + (1 - i\omega)u_{xxxx} + u_{xx}(a_1 \int_0^1 |u_x|^2 dx + a_2 \frac{d}{dt} \int_0^1 |u_x|^2 dx) = 0 \quad (1)$$

$$u(t,0) = u(t,\pi) = u_{xx}(t,0) = u_{xx}(t,\pi) = 0 \quad (2)$$

where $u = u_1(t,x) + iu_2(t,x)$ – complex-valued function; g_1, g_2, ω, a_1 and a_2 – these are some positive constants. This problem appears in the mechanics of the rotary systems and describes the transverse vibrations of rotating rotor of a constant cross-section from a viscoelastic material whose ends are pivotally fixed. This equation is given in a renormalized form. In particular ω is the normalized rotation speed (f.e., [1-3]).

This problem (1), (2) has the zero state of balance. So, the following assertion is valid:

Theorem 1. The solution $u \equiv 0$ is asymptotically stable, if $\omega < \omega_0$ and loses stability at $\omega_0 < 0$

At $\omega = \omega_0$ the critical case is realized. In particular, $\omega_0 = \min \omega_k$ where $k=1,2,...$ and $\omega_k = \frac{g_1 + g_2(\pi k)^4}{(\pi k)^2}$.

In case, if $\omega > \omega_0$, in particular $\omega > \omega_k$, where ω_k is the element of the sets $\{\omega_n\}$, is true

Theorem 2. The boundary problem (1), (2) has the non-trivial singlemode periodic solution of the form

$$u(t,x) = \eta_k exp(i\sigma_k t) sin(\pi n x),$$

where $\eta_k^2 = \frac{2}{a_1} * \frac{\omega^2 - \omega_k^2}{\omega_k^2}$, $\sigma_k = \omega \frac{(\pi k)^4}{g_1 + g_2(\pi k)^4}$.

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Elliptic Theory for a Generalization of Non-Commutative Torus

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We consider a class of operators of the following form:

$$D = \sum_{\alpha\beta\gamma\delta\varepsilon} a_{\alpha\beta\gamma\delta\varepsilon} x^{\alpha} \left(-i\frac{d}{dx}\right)^{\beta} E^{\gamma} T^{\delta} \mathcal{F}^{\epsilon} : \mathcal{S}(\mathbb{R}) \to S(\mathbb{R}), \qquad (1)$$

where

- $\alpha + \beta \le N$;
- $Eu(x) = e^{ilx} u(x)$ is product with an exponential factor;
- $Tu(x) = u(x-k)$ is shift operator;
- $(\mathcal{F}u)(x) = \int e^{-ix\xi} u(\xi) d\xi$ is Fourier transform;
- $\mathcal{S}(\mathbb{R})$ is Schwartz space of rapidly decreasing functions on the line.

This class is a generalization of Connes class of operators on the non-commutative torus [1].

The symbol of operator (1) is the following expression

$$\sigma(D) = \sum_{\alpha\beta\gamma\delta\varepsilon} a_{\alpha\beta\gamma\delta\varepsilon} x^{\alpha} \xi^{\beta} z^{\gamma} \mathcal{T}^{\delta} F^{\epsilon} \in \left(C\left(\mathbb{T}^3\right) \rtimes \mathbb{Z}^2\right) \rtimes \mathbb{Z}_4,$$

where

- $\alpha + \beta = N$;
- $\left(C\left(\mathbb{T}^3\right) \rtimes \mathbb{Z}^2\right)$ is the crossed product of the algebra $C\left(\mathbb{T}^3\right)$ of continuous functions on 3-dimensional torus by group $\mathbb{Z}^2$, associated with the shift operator action. This space is also an algebra. Therefore, we can define the double crossed product $\left(C\left(\mathbb{T}^3\right) \rtimes \mathbb{Z}^2\right) \rtimes \mathbb{Z}_4$ [2].

Theorem.

1)For operators D_1, D_2 of the form (1) the following composition formula holds:

$$\sigma(D_1, D_2) = \sigma(D_1)\,\sigma(D_2)$$

2)If operator D is elliptic, i.e. its symbol $\sigma(D)$ is invertible, then the Fredholm property holds for this operator in Sobolev spaces on the line (cf. [2]).

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A Global Attractor in a Multivalued Dynamical System for a Two-Phased System with Heating

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In this work we study the asymptotic behavior of solutions of Maxwell's equations coupled with the heat equation for the Stefan problem in 3-dimensional space describing a microwave heating process:

$$\epsilon(x)E_t + \sigma(x,\theta)E = rotH, \quad (x,t) \in \Omega \times (0,T],$$
$$\mu(x)H_t + rotE = 0, \quad (x,t) \in \Omega \times (0,T],$$
$$A(\theta)_t - \nabla(k(x,\theta)\nabla\theta) = \sigma(x,\theta)|E|^2, \quad (x,t) \in \Omega \times (0,T],$$

where Ω is a bounded, open, simply-connected domain of $\mathbb{R}^3$with a regular boundary and $(0,T]$ is a time interval. We consider an initial boundary value problem for this process. It is assumed that $\epsilon(x), \mu(x), \sigma(x,\theta), k(x,\theta)$ are known functions. A phase change process is accounted with the enthalpy operator A.

This kind of a heating process is widely used in medicine, biology and many different fields of industry [2].

The existence of a weak solution of the system is shown in [1], but the uniqueness of such a weak solution is not proved. In the presentation it will be shown [3] how to introduce a multivalued dynamical system based on weak solutions of this system. The existence of a global attractor for this multivalued dynamical system is proved. Some numerical calculations for the temperature behavior are carried out.

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D. Solid State Physics

The Processes of Charge Transfer at the Insulator-Semiconductor Interface under the Irradiation of Helium Ion Beam

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During last decade scanning ion microscopes (SIM) started to be widely used for investigations of the surface morphology as well as to manufacture nanostructures by means of resist-based lithography and local material sputtering. Though the image formation in SIM is similar to that in scanning electron microscope (SEM), the interaction of ions with materials has distinctive features due to ion opposite charge and higher mass. Special conditions can be selected to create the balance between primary and emitted particles for research of insulators in SEM, but the accumulation of charge in insulators under the ion irradiation in SIM is inevitable. Of particular importance in applications are the investigations of thin dielectric films on a silicon (Si) substrate. However, there are no experimental data on the accumulation of charge in these structures under the action of ion beams.

Secondary electron (SE) emission from thin films of silicon nitride (Si_3N_4) on Si was investigated with a helium scanning ion microscope Zeiss ORION. It was found that SE yield decreased with increasing of number of incident ions because of charging and reached non-zero value (Fig. 1) at a certain relation of film thickness and energy of ions. It was established that non-zero value of SE signal was proportional to electronic energy loses of helium ions (He^+) in Si substrate and, accordingly, could be explained by electron emission from substrate to dielectric film. Additionally, special technique was developed for measuring energy distribution of SE (SEED) excited from insulators. Reliable data of SEED of Si_3N_4 was obtained.

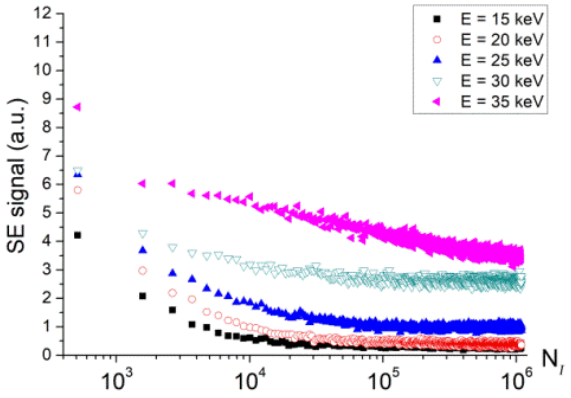

Fig.1. SE signal as a function of incident ions for 220 nm Si_3N_4/Si.

Investigations were performed at the Interdisciplinary Resource Center for Nanotechnology (IRC-NT) of the Research park of Saint Petersburg State University

Optical Properties of ZnO/ZnMgO Quantum Well Structure

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Nowadays, the study of the optical properties of wurtzite type ZnO crystal and related nanostructures are of a great interest due to the unique combination of the optical and electrophysical properties of zinc oxide. As a wide direct band gap semiconductor with a large exciton binding energy of 60 meV, ZnO attracts a worldwide attention for its applications in the short-wavelength optoelectronic devices, such as light-emitting diodes (LEDs) and laser diodes (LDs).

In this work, ZnO/ZnMgO heterostructure with two quantum wells (QW) of thicknesses 2.7 nm (QW-1) and 7.1 nm (QW-2) grown with the molecular-beam epitaxy (MBE) method in the direction of the polar axis is investigated (Fig. 1). We have studied the luminescence and reflection spectra in the region from 3.0 to 3.8 eV (Fig. 2). The luminescence spectra have been obtained in the temperature range 5 – 200 K.

We analyze our data in order to identify the narrow and wide QWs contributions in the light emission from the heterostructure under study. The effect of built-in electric fields produced by the interface strains on the energy position of QW luminescence is discussed.

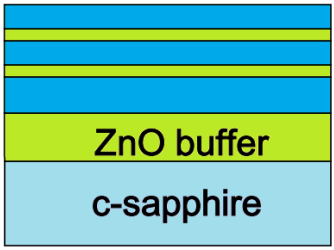
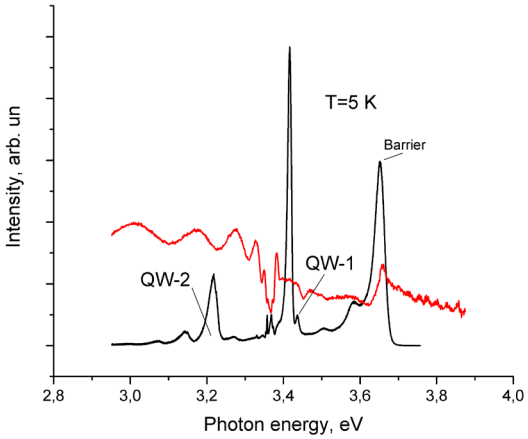


Fig. 1. – $Zn_{0.85}Mg_{0.15}O$ *barrier* – *ZnO quantum wells.*

Fig. 2. – *reflection spectrum* – *luminescence spectrum.*



Exploring Optical Properties and Characteristics of $Cs_2BiAgCl_6$, $Cs_2BiAgBr_6$ Halide Double Perovskites

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In recent years, lead-based halide perovskites attract a great attention as a class of semiconductor materials with a variety of applications in the fields of photovoltaics and optoelectronics. This structure ($APbX_3$, A = Cs, CH_3NH_3 or $HC(NH_2)_2$, X = I, Br or Cl) performs high efficiency of light absorbance in the visible range, high mobility of carriers and long diffuse lengths [1]. In addition, perovskites have low cost of fabrication and can be simply synthesized with methods of wet chemistry. During several years of studying these materials, power conversion efficiency of perovskite solar cells has increased from 3% to 22%. Despite its great potential, lead-based halide perovskites have a short lifespan and deteriorate rapidly after exposure lo light, humidity and high temperatures [2]. A major issue is toxicity − the presence of lead limits widespread and commercialization of this material.

One of solutions for these problems may be the substitution of lead by a combination of two heterovalent atoms with the formation of a double perovskite structure $Cs_2B_1^{3+}B_2^{1+}X_6$, where X = Cl^- or Br^-, B_1 = Bi^{3+}, Sb^{3+}, In^{3+}, Au^{3+} and B_2 = Ag^+, Cu^+, Au^+ or In^+. In present work, we have synthesized and investigated optical properties and characteristics of $Cs_2BiAgCl_6$ and $Cs_2BiAgBr_6$ halide double perovskites in the form of powder and single crystals.

Acknowledgements. The present study was performed within the Project "Establishment of the Laboratory "Photoactive Nanocomposite Materials" No. 14. Z50.31.0016 supported by a Mega-grant of the Government of the Russian Federation. This work was supported by RFBR 17-53-50083 m_a project. This work was carried out using equipment of SPbU resource centers "Nanophotonics", "Geomodel" and "X-ray Diffraction Studies".

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Effect of Helium Ion Beam Treatment on the Etching Rate of Silicon Dioxide

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Silicon dioxide (SiO_2) is one of the key dielectrics in microelectronics. For instance, thin films of SiO_2 are widely used in different metal-oxide-semiconductor (MOS) structures. Therefore possibility of local control of thickness of film with high spatial resolution is actual practical task. In paper [1] it was demonstrated that ion implantation enhances etching of SiO_2 in water based hydrofluoric acid solution. Thus local ion implantation and subsequent etching in water based acid solution allow us to create structures with predefined geometry from SiO_2.

In our work we used helium ion microscope for performing local ion implantation. After etching we observed formation of wells with help of atomic-force microscope in exposed areas. Comparison of results of etching process of exposed and unexposed areas allowed us to calculate relative etching rate. Using Monte-Carlo simulation [2] we estimated radiation induced defect density. Then we plotted the dependence of the etching rate on defect concentration (Fig. 1).

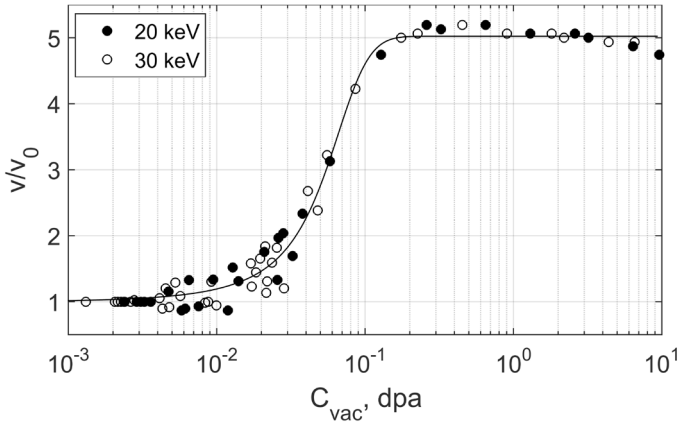

Fig. 1. The dependence of the relative etching rate on defect concentration (defect per atom).

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Mechanism of Interaction of Ar^+ Ions with Atoms in Ta_2O_5 Films

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Owing to the preferential sputtering of O, bombardment of Ta_2O_5 by Ar^+ ions is one of suitable ways to produce two-layered system Ta_2O_5/TaO_x being of practical relevance as memorizing layer for ReRAM [1]. However, oxygen deficiency of TaO_x causes a strong dependence of device properties on the x in TaO_x. At the same time, TaO_x exhibits different properties depending on the value of x, which is important from the point of view of functionalization of devices. This can result in a lower breakdown field and higher leakage current [2]. So far, there is a considerable lack of information on the effect of Ar^+ ion sputtering-induced oxygen deficiency on properties of Ta_2O_5.

This work is devoted to careful analysis of the oxide chemical composition after different sputtering steps, which allowed us to establish the mechanism of the interaction of the Ar^+ ions with the atoms in TaO_x films. The different x was realized using in-situ Ar^+ ion sputtering of the sample.

The X-ray photoelectron spectroscopy and the near edge X-ray absorption fine structure in two modes (by monitoring the partial electron yield (PEY) using an MCP with a retarding grid, and the total electron yield (TEY) from the sample when the drain current from the sample was measured) were implemented at each step of etching. All the measurements were performed at the RGL-station on the Russian-German beamline at the BESSY II synchrotron light source of the Helmholtz-Zentrum, Berlin. In order to establish the Ta chemical states observed after each sputtering step Cassa XPS software was employed for peak fitting of Ta 4f XPS spectra. Such complex approach allowed to study the redistribution of valence and conduction band states of TaO_x depending on the value x.

It is important that formation of a metallic Ta layer was established. The sputtering induced formation of metallic Ta suggests Ta_2O_5 as a feasible candidate for not only insulating applications but, also as a material suitable for the fabrication of nanometer-sized conductors by direct oxide decomposition. Ar^+ ion sputtering-induced evolution of Ta_2O_5 can be divided into three stages. At the first step Ta valence changes slightly from Ta^{5+} to Ta^{4+} and Ta^{5+} states mixture and local symmetry stays constant. The second step is associated with phase change during which Ta valence remains constant and polyhedron structure mainly consisted of octahedral TaO_6 transforms to the new one with pentagonal pyramid TaO_5 as dominating structural unit. At the third step Ta valence strongly alternates and metallic Ta is observed.

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The Study of Dislocations in HVPE Gan by Electrophysical Methods

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GaN is a promising direct-wide-gap semiconductor for high power and optical electronic applications. GaN crystals were grown by heteroepitaxial methods due to absence of suitable substrates and as results, crystals have a high density of grown-in defects. In the most cases these defects have a negative effect on recombination properties of crystal. However, it was shown that a-screw dislocations could be effective radiative centers at 3.18 eV [1]. Unfortunately, the complete model of carrier recombination is still absent. Electrical measurements will be help to establishing quantitate parameters of this type of dislocation. The aim of this work is an investigation of an impact of freshly induced dislocations on electro-physical properties of GaN Schottky diodes.

In the first part of this work electro-physical properties of 4 GaN samples with different dopant concentrations were investigated by current-voltage (I-V), capacitance-voltage (C-V) methods and deep level transient spectroscopy (DLTS) for choosing the most suitable crystal for further research. The special undoped GaN crystal with free electron concentration N_d=3*10^{16} cm^{-3} and thickness d=7,9 μm, which grown by hydride vapour phase epitaxy (HVPE), was chosen for local plastically deformation by scratching.

We had compared two different parts of the same sample. A basal plane one of them was scratched by diamond scriber with a period of h=100±20 μm and length l=5±0,5 mm. Another one was not subjected to any plastically treatments. After that, Au was deposited by thermal evaporation on these two samples (initial and scratched) from special mask. I-V and C-V measurements shown that freshly induced dislocations changed some parameters of diodes. In addition, it was noticed that parameters of the scratched sample could be various deeply by the time. We supposed that changes of electro-physical parameters associated with introducing different sets of dislocation, which create new energy levels in the band gap and new ways and mechanisms of carrier recombination. Results of electrical measurements and model of carrier recombination will be presented on conference.

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Influence of Doping with Rare Earth Ions on ZrO_2 Optical Properties

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The study of dielectric materials doped with rare earth ions has been attracting great attention due to possible photonics and biophotonics application. ZrO_2 is an important photonic material and has been widely studied during last couple decades. It's unique properties, such as high refractive index, wide band gap and low phonon energy (470 cm^{-1}) [1], which increases the number and the probability of radiative transitions in rare earth doped samples, makes ZrO_2 one of the most promising oxides to be used as a host material for Stokes and anti-Stokes luminescence [2]. It is also known that doping ZrO2 with rare earth ions leads to absorption in extrinsic region [3]. The general aim of this work is to investigate how doping with different rare earth ions influence optical properties of ZrO_2 in cubic phase.

In present work several samples of ZrO_2 in cubic phase doped with Y^{3+}, Yb^{3+}, Er^{3+} and simultaneously with pair of Er^{3+} and Yb^{3+} were synthesized and characterized. Diffuse reflectance spectra and spectra of Stokes and anti-Stokes luminescence of all samples were studied. In addition, photostimulated defect formation in samples doped with different rare earth ions was investigated and comparative analysis of that process was made. Overall, this work includes synthesis, characterization and research of how type and concentration of dopants affect optical behavior of ZrO_2 in cubic phase doped with different rare earth ions.

Acknowledgements. The present study was performed within the Project "Establishment of the Laboratory "Photoactive Nanocomposite Materials" No. 14.Z50.31.0016 supported by a Mega-grant of the Government of the Russian Federation.

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Sucrose as a Molecular Crystalline Matrix for Alloyed Semiconductor Nanocrystals

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Semiconductor nanocrystals today are probably one of the most intriguing cases of modern solid state materials. Their unique properties powered by quantum-size effects appointed them as a fundamental material for photonics. Nanocrystals are now widely used for developing optoelectronic devices such as light emitting diodes and even advanced color displays [1, 2].

However, nanocrystals have severe limitations for operating conditions, defined by the lack of stability. Overcoming these limitations is a vital task. Among the most effective ways to do so is by enclosing nanocrystals in some protecting matrix. This matrix should be able to isolate nanocrystals from the destructive external impact but at the same time preserve their essential optical properties. Crystalline matrixes show promising results in this challenge [3]. However, materials that have been used so far were ionic crystals NaCl [4], LiCl [5], KCl, KBr [3]. They have free ions in their crystal-forming solutions that cause the aggregation of nanocrystals. To evade this, using molecular crystals can be the answer.

We have studied the possibility of using sucrose as a molecular crystalline matrix for nanocrystals incorporation. Obtained mixed macrocrystals containing alloyed CdZnSe/ZnS were investigated for their physical and optical properties and proved to be quite promising for certain environmental conditions.

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NMR Study of Nanocomposites Based on Ferroelectrics KDP and DKDP

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Researching of nanostructured composite materials, in particular, nanoporous matrices with dielectric and metal particles embedded into pores is one of the most interesting directions of modern science. The physical properties of small particles change due to the size effects associated with the size and geometry of the pore grid. As a result, the characteristics of the particles under confinement may differ significantly from the corresponding bulk materials. Size effects strongly affect the temperature and type of phase transitions. The NMR method which is highly sensitive to local changes in physical properties in the matter [1] has been successfully applied to the research of nanoporous structures with metallic and dielectric particles embedded into pores. Our aim is to study the influence of size effects on the ferroelectric phase transition in KDP and DKDP embedded into nanoporous matrices in comparison to bulk samples by nuclear magnetic resonance.

A fine grounded powder KDP and DKDP, powder KDP embedded in a porous glass with pore sizes of 7-8 nm and powder DKDP embedded in a synthetic opal with a diameter of silica spheres of 220 nm are investigated. All measurements were performed using a Bruker Avance 400 pulse NMR spectrometer. ^{31}P NMR spectra were studied in the temperature range from 80 K to 293 K. It was demonstrated that in conditions of confined geometry a phase transition does not occur in this temperature range due to the influence of size effects.

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Development of a Sensitive Setup for Measuring the Hall Effect in low-Mobility Materials

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We report on the development of a highly sensitive AC Hall effect setup for measuring charge carrier mobilities in organic semiconductors. The signal-to-noise ratio has been improved significantly by modulating both the magnetic field (from -1 to 1 T at a frequency of up to 100 Hz) as well as the current through the sample. The Hall voltage is detected at the difference frequency. This scheme allows us to separate the Hall voltage from Johnson noise, probe misalignment voltage and thermoelectric voltage. The setup was compared to conventional DC Hall effect measurements using n- and p-doped silicon samples. Measurements of hole mobilities in low-mobility organic semiconductors demonstrate the high sensitivity of the setup: charge carrier mobilities in the range of 1 $cm^2 V^{-1} s^{-1}$ were observed. We will discuss how this setup can be used to characterize semiconducting polymers with applications in solar cells.

Effect of Severe Plastic Deformation and Annealing on Microstructure, Mechanical and Electrical Properties of Al-0.4Zr alloy

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Conductors based on aluminum alloys are widely used for various industrial applications, including electrical engineering [1]. In the latter case it is very important to have the combination of high electrical conductivity, strength and heat resistance for long-term operation. After a special heat treatment Al-Zr alloys demonstrate a good heat resistance due to formation of the secondary phase nanoparticles (Al_3Zr) [2]. Methods of severe plastic deformation allow significant improving the mechanical properties of Al-based alloys due to formation of ultra-fine grained or nanocrystalline structure [3].

In this work, for the first time, influence of severe plastic deformation by high-pressure torsion (HPT) and subsequent annealing on microstructure, mechanical properties and electrical conductivity of Al-0.4Zr alloy has been investigated. Microstructure of samples was studied by electron back-scattering diffraction and transmission electron microscopy. Strength and ductility were tested by uniaxial tension, microhardness was measured by Vickers method, electrical conductivity was measured by four-probe method.

Analysis of results has showed that the HPT treatment leads to formation of ultra-fine grained (UFG) structure, but there is no precipitation of secondary phases. The UFG structure provides an increase of strength by ~1.6 times without sacrificing ductility (>17 %), however the level of electrical conductivity decreased by ~20 %. The effect of additional increase in strength (by ~25 %) and electrical conductivity (by ~10 %) of the HPT-processed samples due to their annealing in the temperature range 423–503 K has been found. Changes in the contributions of different mechanisms to hardening and electrical resistivity due to modifying microstructure have been analyzed.

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Temperature-Programmed Desorption Spectra of CO_2 Remaining on TiO_2 Rutile Surface after Photooxidation of Carbon Monoxide

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Titanium dioxide is one of widely investigated UV photocatalysts [1]. The photocatalytic oxidation of organic compounds by TiO_2 has attracted much interest. In particular the photooxidation of CO on TiO_2 is considered as the simplest one to study processes on catalysts surface and as ecologically significant reaction. Earlier we have shown that products of CO photooxidation, CO_2, remains on the surface and may be removed by heating up to 500 K [2]. A feature of temperature-programmed desorption (TPD) measurements of CO_2 was revealed by us that the position of the maximum of CO_2 TPD peak, T_m, shifts to lower temperature with desorbing CO_2 amount.

In present work TPD spectra of CO_2, remaining on the dehydroxylated TiO_2 surface as a result of UV-VIS irradiation of titania in $CO - O_2$ mixture, are analyzed. Experimental details and methods are similar to those described in [2]. Various amounts of CO_2 on TiO_2 surface were produced by varying the duration of irradiation (high pressure Xe arc lamp, 150 W) in $CO - O_2$ mixture.

Main TPD peak of CO_2 appears in the $T > 400$ K range, has a symmetric shape and was assigned to carbonate species. Shift of TPD CO_2 peak with amount, which is character to the second-order kinetic of desorption, actually may be considered as first-order desorption with two types of precursor states: 1) "over an empty site" and 2) "over a filled site" [3]. CO_2 desorption resulted from a migration of carbonates species along the surface (via the state "over an empty site") and subsequent interaction (desorption from precursor state "over a filled site").

The present study was performed within the Project "Establishment of the Laboratory of Photoactive Nanocomposite Materials" financed by a Grant (No. 14.Z50.31.0016) from the Government of the Russian Federation. We are grateful to the Resource Centers "Nanophotonics", "Centre for X-ray diffraction Studies" and "Centre for Innovative Technologies of Composite Nanomaterials" of St. Petersburg State University for the sample characterization.

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NEXAFS Study of Fish Bones and Hydroxyapatite

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Bone is a composite material composed of organic (primarily collagen) and inorganic (bioapatite or hydroxyapatite (HA), $Ca_{10}(PO_4)_3(OH)_2$) components, as well as lipids and water. The theoretical and experimental investigations shows the existence in bone tissue a close relationship between its hierarchical organization and local electronic structure of its mineralized phase exists [1, 2]. The 3D-superlattice (3DSL) model predicts the presence of size-dependent spectral changes in electronic structure of mineralized phase within bone relative to the band structure of HA. These effects can be investigated by studying the NEXAFS Ca2p-spectra of the pure HA deposited layer and bone nanocrystallites with strict energy calibration of all Near Edge X-ray Absorption Fine Structure (NEXAFS) Ca2p-spectra by the first narrow peak in the second diffraction order of F1s-spectra of solid K_2TiF_6 (683.9 eV [3]) registered in continuous energy scale with Ca2p-spectra of investigated sample.

Current study continue the resent investigation of atomic, chemical and mineral composition of Antarctic ice fish hard tissue and biomineralized formation [4, 5] and include investigation of NEXAFS C1s-, N1s-, P2p-, and Ca2p-spectra of bones and other biominiralized formation isolated from different types of fishes as well as HA with strong energy calibration. All NEXAFS-spectra were measured in TEY mode with an energy resolution about 0.05 eV at synchrotron source BESSY II using radiation from the Russian-German dipole beamline.

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Manipulation of Electronic Structure of Graphene Grown on Ir(111) by Pb Atoms Intercalation

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Graphene is a two-dimensional hexagonal crystal structure composed of carbon atoms. Due to its unique properties, graphene for more than ten years attracts the attention of scientists all over the world [1]. The dispersion dependence in graphene near the Dirac point has a linear nature [2], so that electrons and holes in graphene move like massless particles (for example photons). Due to this, the graphene is considered to be a perspective material for use in nanoelectronics.

One of the major methods of graphene preparation is chemical vapor deposition (CVD). This method can only take place on the surface transition metals, such as Ir(111), but because of the interaction between graphene and substrate there are differences between electronic structures of graphene, obtained on Ir(111), and electronic structure of free graphene. Intercalation of heavy metals between graphene and substrate (for example Pb) can be used for manipulation of graphene electronic structure.

In this work we studied graphene on iridium before and after lead intercalation. This system is interesting by the possibility of forming a topological phase [3]. The obtained systems were studied by angle-resolved photoemission spectroscopy (ARPES) and low energy electron diffraction (LEED). Our results show the possibility of effective tuning of the Dirac point position and band gap value by intercalation of Pb atoms underneath graphene.

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NEXAFS Study of Selected Natural Biopolymers

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Cellulose and chitin are the most abundant biopolymers on the earth: first is the main constituent of plants, serving to maintain their structure, and is also present in bacteria, fungi, algae and even in invertebrate animals, second is known to occur as a component of the cell wall in fungi and diatoms, and is also found in diverse skeletal structures of at least 19 animal phyla [1]. These biopolymers and their derivatives are used in many industrial applications and new material synthesis. Thus the investigation of their electron structure is the actual problem.

In current study absolute absorption cross sections spectral dependence in Mb and the X-ray transition oscillator strength distributions in near C1s-edge X-ray absorption fine structure (NEXAFS C1s-spectra) of these biopolymers were determined and interpreted using building block concept. Oscillator strength is the fundamental parameter which characterizes the process of X-ray beam and matter interaction and can be calculated in different approximation [2] as well as determined experimentally by the integration of absolute partial absorption cross section. Thus it is used for testing theoretical models which describe X-ray photoabsorption process.

The NEXAFS spectra of investigated material were studied on the Russian-German dipole beamline [3] of Synchrotron Centrum BESSY II by Total Electron Yield (TEY) mode with usage of specific film filter and multi-stage spectra processing. The biopolymers samples were given from the Collection of Biomineralogy & Extreme Biomimetics Group (Institute of Experimental Physics, TU Bergakademie Freiberg).

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Graphene Synthesis via Segregation of Carbon Atoms through Co Film on Graphite

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Graphene is one of the most promising materials designed to set a new vector for the development of modern electronics. A key obstacle to the massive introduction of graphene into nanoelectronics is the lack of highly efficient and cost-effective methods of synthesis at low temperatures. Widely used methods such as CVD or thermal decomposition of SiC have their weak points, so other methods are investigated. One of such methods is based on the segregation process, when carbon atoms float to the surface and arrange into graphene.

Recently we shave studied growth of graphene by segregation on thin metal (Ni, Gd) films deposited on a HOPG substrate [1–3]. In the present work, a cobalt film is taken, since graphene on Co has more ordered structure than on Ni, while temperatures of graphene growth on Co and Ni are quite similar. It is shown that the mechanism of graphene growth is the same, but the temperature regime is higher than for Ni film. Another point of interest studied in the work is the comparison of graphene growth on single crystal graphite and on HOPG.

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Understanding the Electronic, Chemical and Structural Changes of Perspective Cathode Materials for Na-Ion Batteries at Different States of Electrical Charge/Discharge

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Lithium-ion batteries are widely spread in present appliances and find application as energy source for electric vehicles and grid energy storage application. Herewith, lithium raw materials have high cost, which increases constantly; in this connection it is necessary to find the same efficient but less expensive raw material. Na-ion batteries are regarded as the best alternative to the Li-ion batteries due to: 1) Na-ion radius is similar to Li-ion; chemistry of Na de/intercalation is similar to Li chemistry; 2) Na raw materials widely spread and have low cost. Nevertheless, Na-ion batteries are characterized by reduced capacitance and operating voltages. It was established that when the $LiMO_2$-alike compounds (M - transition metal; $NaCoO_2$, $NaNiO_2$, $NaMnO_2$ and etc.) are used the reversibly insert Na ions occur, however, with limited capacity and rate capability [1]. In this regard, the development of advanced cathode materials, providing high capacity, with structural stability, reversibility and high capacitance for Na-ion batteries is an extremely demanding task.

The work is focused on the investigation of the evolution of the perspective cathode materials $NaMn_{0.8}Cu_{0.1}Mg_{0.1}O_2$ and $NaFeMnO_2$ for Na-ion batteries in different phases of the first charge/discharge cycle. NEXAFS spectroscopy (Near Edge X-Ray Absorption Fine Structure) was used to examine changes in the local structure of each transition metal element. Also to establish the influence of oxidation processes and to get information from deeper layers of the cathode material the fluorescence spectroscopy was used.

It was established the absence of structural changes in bulk of cathode materials in the first charge/discharge cycle, but at the same time these materials have strong dependence of local structure at the surface due to the oxidation process.

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Cathodoluminescence and Core Structure of A-Screw Dislocations in Gallium Nitride

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Currently III-nitrides due to their wide bandgap and high temperature stability are frequently used for the production of light-emitting devices (LED) working as white light sources and high-power devices. Economically most suitable way to manufacture such semiconductors is to grow them heteroepitaxially on sapphire. Significant differences both in lattice constants and in thermal expansion coefficients between semiconductor and substrate lead to a very high density of threading dislocations (10^{10} cm^{-2} for edge and 10^{8} cm^{-2} for screw dislocations), which reduce significantly LEDs efficiency.

In opposite to that, recent investigations [1, 2] showed that freshly introduced dislocations in GaN could be effective UV light emission centers. In particular, it was found that a-screw dislocations exhibited strong luminescence band at 3.15-3.18 eV (DRL) whereas their intersection nodes luminesced with the other energy of 3.3eV (IRL) (Fig. 1a, b) [2].

In this report we present for the first time results of the study of the a-screw dislocation core structure by means of transmission electron microscopy (TEM). Dissociated character of the cores and extended node formation were found (Fig. 1c). The obtained structural data are discussed together with spectral properties of DRL and IRL.

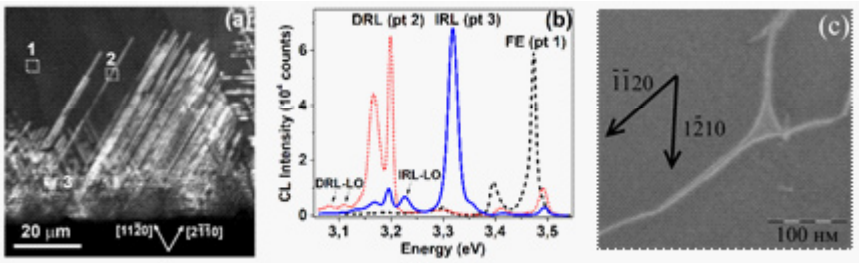

Fig. 1. (a) CL panchromatic image near the scratch (black bottom stripe) on c-plane of GaN; (b) CL spectra taken at the positions of electron beam marked in (a) as 1, 2, 3 [2]; (c) Splitted dislocation node in basal plane (0001) of GaN in STEM.

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Atomic Structure of Bimetallic Nanoparticles PtCu in Metall-Carbon PtCu/C Electrocatalysts for Low-Temperature Fuel Cells

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Composite materials containing noble metal nanoparticles have been extensively studied, since they are promising catalysts for the electroreduction reaction of oxygen in low-temperature fuel cells [1, 2]. Platinum-containing nanoparticles are of the greatest interest due to the high thermodynamic stability of platinum, which makes it possible to obtain stable particles of small size. In this work, electrocatalysts PtCu/C with core-shell structure of PtCu nanoparticles were synthesized by two methods: simultaneous and sequential chemical reduction of Cu^{2+} and Pt(IV) in carbon suspension, prepared on the basis of ethylene glycol–water solvent. The comparative analysis of atomic structures of PtCu nanoparticles in "as prepared" materials and obtained after thermal treatment at different temperatures, was performed by Pt L_3- and Cu *K*-edge extended X-ray absorption fine structure (EXAFS) using the technique for determining local structure parameters of the absorbing atoms, which have the nearest surrounding consisting of Pt and Cu atoms [3,4]. The spectra were measured at the μSpot beamline of the BESSY-II Synchrotron Radiation Facility (Berlin, Germany).

The values of structural parameters of Pt and Cu local atomic structure in studied materials derived from EXAFS enabled to construct 3D models of bimetallic nanoparticles in PtCu/C electrocatalysts. The models were constructed by simulations of the atomic clusters, which correspond to the values of the local atomic structure of Pt and Cu atoms [5]. These models enabled to reveal the relationship between synthesis and thermal treatment conditions and distributions of Pt and Cu atoms over the volume of PtCu nanoparticles in the studied electocatalysts.

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CdTe/ZnMnTe Quantum Well Structures – Reflectivity and Light Emission

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Quantum well (QW) structures which contain iron group component with the partially filled 3d-shell reveal the peculiar optical and magnetic properties. The intracenter 3d-luminescence is observed in these structures along with the exciton luminescence. The intensities of luminescence related to excitons and 3d states depend on the energy transfer between the extended electron band states and 3d-states.

We have studied the CdTe/ZnMnTe quantum well structures whose compositions are understandable from Fig. 1. Note, that the barriers are formed either by the periodically located ZnTe and MnTe thin layers (sample 1), or by the uniform solid solution ZnMnTe (sample 2).

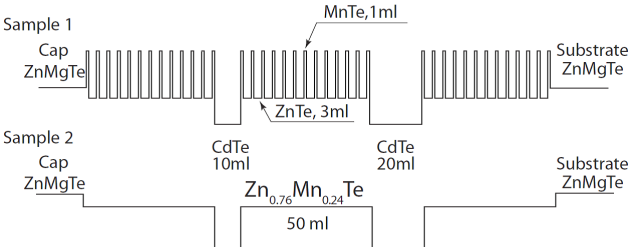

Fig. 1. Scheme of the electron energy profiles in samples 1 and 2.

The low temperature light emission spectra from samples 1 and 2 are depicted in Fig. 2

We analyze the reflectance and luminescence spectra and their dependences on the temperature and excitation conditions.

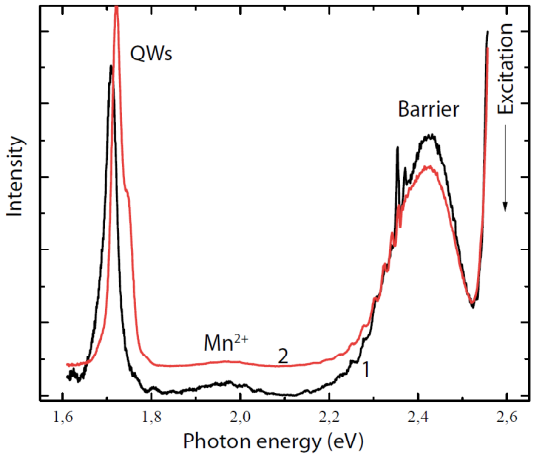

Fig. 2. Luminescence spectra from samples 1 (1) and 2 (2), T = 5 K.
Mn $^{2+}$– intracenter 3d-luminescence of the manganese ions.

Topological Surface States in Rare Earth Doped Topological Insulators

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During recent decades active research into fundamentally new structures – topological insulators (TIs) – is one of the priority areas in the physics of nanosystems. Such materials are distinguished by the presence of a bulk band gap and surface conduction states. An intriguing feature of TI is the «protection» of surface states from scattering. Such electronic structure configuration of these TI defines the researchers' special expectations for their application [1].

Magnetic metal-doped TIs are characterized by exotic properties. The study of V-, Mn-, Fe- or Cr-doped TIs presented the possibility of realizing a ferromagnetic order [2, 3]. A magnetic field breaks TRS lifting the Kramers degeneracy between up and down spins, and can open a band gap at the Dirac point. Such behavior allows the possibility of experimentally observing the quantum anomalous Hall effect (QAHE). Moreover, it is theoretically justified that Majorana fermions existence and topological superconductivity is possible in such structures [4].

The idea of doping topological insulators with rare earth (RE) metals is due to the exceptional properties of these elements. First, the magnetic moment of RE metals is much larger, so it is expected an intensification of the magnetic features in these compounds. Secondly, RE elements have a large mass. This feature means that they are able to make a significant contribution to the effects of the spin-orbit interaction. Finally, it is worth noting that the valence of Gd, Er and Dy is equal to the bismuth valence. This leads to the absence of electronic doping effects in Bi chalcogenides simplifying the analysis of samples. Such effects open wide possibilities for the application of these structures: from topological superconductivity to directly using in the realizing of a quantum computer.

In this work RE metal-doped (Gd, Er, Dy) compounds based on $BiSbTe_3$ was analyzed. The studies were carried out by the ARPES method. Behavior of topological surface states formed the Dirac cone was studied. The photoe-mission spectral analysis was done from the point of magnetic features search in the explored samples. Special interest is the analysis of the band gap existence, which should be formed in such structures due to the ferromagnetic order.

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Synchrotron Spectromicroscopy Study of Top-Down MAWCE Silicon Nanowire Arrays Covered by MOCVD Tin Oxides

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Silicon nanowires (SiNWs) are prospective nanomaterials which show a high intensive visible photoluminescence. Moreover, SiNWs arrays can be covered by tin oxides, e.g. with the use of metal-organic chemical vapor deposition (MOCVD). This attracted high research attention due to the range of common possible applications: e.g. light emitting devices developed under silicon technology [1] and gas sensing devices based on tin oxides unique properties.

Application of Photo Electron Emission Microscopy (PEEM) method due to its capability of measuring the X-ray absorption near-edge structure (XANES) from nanometer regions allowed us to obtain data about the atomic and electronic structure for the whole surface of the nanowires. Thus, the possibility of applying the method was demonstrated for complex-morphology dielectric materials.

The results of the studies show that tin oxides nanocrystals covering layer is blind and its electronic structure reveals noticeable influence of the oxygen vacancies on electronic structure. These surface defects led to sub-band formation in a covering layer band gap close to conduction band bottom. Traces of metallic tin were observed as well.

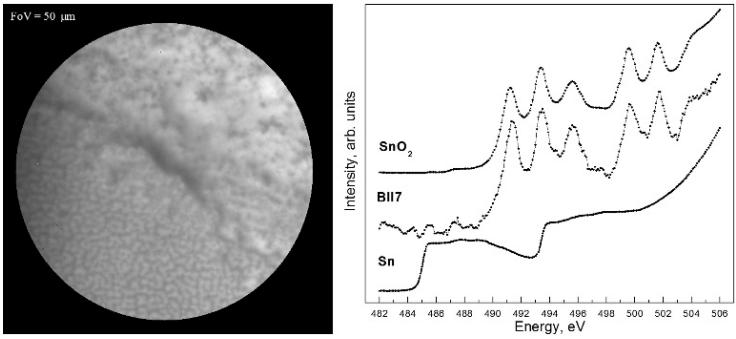

Fig. 1. Left: PEEM image of the formed composite Si NWs-tin oxides. Right: reference spectra set with XANES Sn $M_{4,5}$ signal taken from whole PEEM image (sample BII7).

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Adsorption of Silicon Atoms on the Surface of the Au/W(110)

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Trends in the development of modern nanoelectronics are determined by devices based on silicon. For several decades the main one was aimed at scaling semiconductor devices with increasing performance and reducing power consumption of microcircuits. Within this approach, the development and creation of new nanostructures does not lose its relevance. Calculations based on the density functional theory have shown that silicon atoms can form an ordered two-dimensional hexagonal corrugated structure – silicene – that can have a wide range of applications in nanoelectronics. In addition, silicene can be synthesized and converted using the basic technologies of the semiconductor industry, thereby simplifying the process of integration into existing electronics.

The present work is devoted to the study of the possibility of forming an ordered silicene-like structure, on the Au/W(110). On the one hand, there is a possibility of low-temperature migration of silicon on the W(100) surface with the formation of a surface tungsten silicide WSi. On the other hand, the Au/W(110) system is well investigated and has a well-ordered structure. It is expected that the interaction of the gold monolayers with tungsten will reduce the probability of Si-Au alloy formation and at the same time the condition for the migration of silicon atoms on the gold surface will be fulfilled, due to the residual influence of the tungsten substrate, resulting in the formation of an ordered structure based on silicon [1].

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Investigation of Efficient Upconversion Nanocomposite Materials

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In the last few years, the interest to the photon upconversion (UC) materials is strongly increased due to their crucial role in reaching the high performance of various devices such as biomarkers, lasers, and other optical devices. Recently, UC phenomenon has been recognized as a promising wavelength-shifting effect for increasing efficiency of sunlight-powered devices, such as photovoltaics and photocatalysts.

The UC is a process of converting multiple photons with lower energy (longer wavelength) into a single photon with higher energy (shorter wavelength). In practice, the promising way of using this phenomenon is to create the upconversion nanoparticles (UCNs) which consist of the host matrix doped with lanthanide ions. Rare earth elements are selected due to their abundant and unique energy levels that lead to sharp luminescent emission. Equally important is the selection of the host matrix with ion dense packing and low phonon energy to get the highest upconversion efficiency. Among these, the most often-used UCNs for today are $NaYF_4$ matrices co-doped with Ln^{3+} ions. In this work, we propose to use metal-organic frameworks (MOFs) as alternative host material. In fact, the study of the mechanisms of charge/energy transfer in this compound might discover a new way for its application as a photosensitive material.

The goal of this work was to synthesize alternative porous hybrid host material, and to study the UC process in them. For this purpose, was chosen the MOF-76 including the rare-earth metal (Yb and Er) oxide clusters and 1,3,5-benzenetricarboxylic acid as an organic linker.

The phase composition, structure and morphology of synthesized compounds were characterized by XRD, SEM, adsorption-desorption measurements. The study of photoluminescence and upconversion photoluminescence of all samples under investigation was carried out using a FluoroMax Plus Spectrofluorometer (Horiba Scientific, USA). Photoluminescence spectra were obtained at room temperature. The dependences of upconversion luminescence efficiency on the dopant concentration and the density of pumping power (975 nm diode laser) were obtained and analyzed.

Acknowledgements. The present study was performed within the Project "Establishment of the Laboratory "Photoactive Nanocomposite Materials" No. 14.Z50.31.0016 supported by a Mega-grant of the Government of the Russian Federation.

E. Electromagnetic and Acoustical Processes

Low-frequency Radiation of a Charge Moving along the Axis of Circular Corrugated Waveguide

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Radiation of a charge in periodical waveguides was analyzed mainly for the cases where wavelengths are comparable to the structure period. This radiation (known as Smith-Purcell radiation) plays a significant role in microwave electronics. However, it is interesting to study as well the case of relatively long-wave radiation, where wavelengths are much greater than the structure period. For investigation of this radiation, it is efficient to apply so-called equivalent boundary conditions (Vainshtein-Sivov conditions) [1]. According to this approach, the exact boundary conditions on complex periodic surface are replaced by some equivalent conditions which must be fulfilled on smooth surface. The exact field coincides approximately with the field obtained with use of the equivalent boundary conditions (starting from some small distance from the structure). This analysis was partially performed in the paper [2], but a series of important questions was not considered.

In this work radiation of a point charge moving uniformly along the axis of the circular vacuum waveguide which has a corrugated metal surface is investigated. The corrugation has rectangular form. The period and the depth of the structure are assumed to be small compared to the wavelengths and the waveguide radius. This allows applying the above-mentioned equivalent boundary conditions. Expressions for the full field components and the wave field components are obtained. The typical numerical results are demonstrated. It is shown that the wave field has only one TM waveguide mode. The amplitude of this mode is comparable with amplitude of Cherenkov modes in dielectric waveguide. It is also established that radiation is generated if the velocity of charge is more than certain threshold value, and the magnitude of the wave field components increases with increase of the charge velocity.

The obtained results can be applied for the generation of gigahertz and terahertz radiation, as well as for development of new method of wakefield acceleration.

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Asymmetrical Current Distribution in Bus Bar Systems

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While low frequency alternating current is flowing through conductor harmful effect such as skin effect is appearing. Because of this, the effective resistance of the conductor increases and, as a consequence, it's heating [1].

When near located conductors carrying alternating currents are in proximity to each other, induced currents are flowing in one conductor by the magnetic field of the other. These currents affect the current distributions in the cross section of the conductors and effective resistance is increasing in addition to the skin effect.

While computer modeling the current distribution in three-phase bus bar system with phase shift 120°, it was found that the distribution of current density has asymmetry [2]. Systems with two and three conductors were investigated. Explanation of asymmetrical distribution was given. As an illustration finite-element modeling in COMSOL was used.

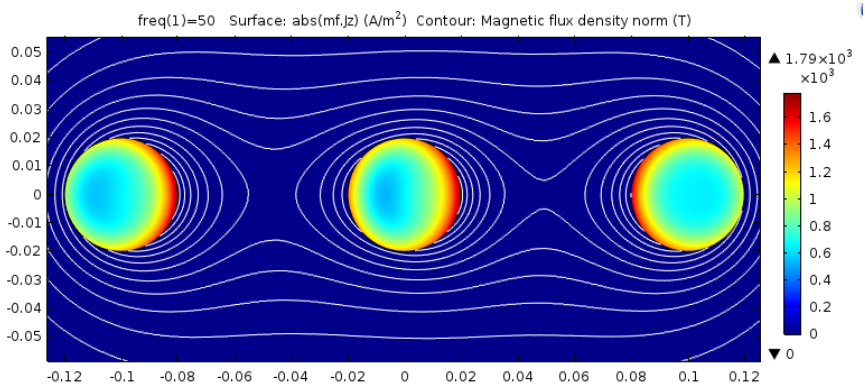

Fig. 1. Current density distribution and lines of magnetic field in three-phase system.

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The Structure of Mode Groups in Dielectric Waveguides with a Quadratic and Stepwise Refractive Index Profile

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Dielectric waveguides are nowadays considered as the perfect physical medium for transferring large data streams over long distances. However, in-creasing the efficiency of this channel requires to regard the possibility of using modal groups for increasing the signal level and improving the signal-to-noise ratio.

When solving the problem of propagation of a light pulse in a wave-guide, it is customary to consider modes [1], which can be obtained easily for a waveguide with a parabolic refractive index [2]. Modes with close propagation constants can be united into mode groups, i.e. these modes propagate with close speeds. In the case of parabolic refractive index, the modes in a group have equal propagation constants. The question arises whether in a waveguide with an arbitrary profile it is possible to distinguish such groups approximately, estimating the range of the propagation constants within the group.

A waveguide with a stepwise refractive index is of particular interest because of its wide practical application, but an analytical expression for the modes in it is difficult to work with, so one can try to find the expression of the modal group numerically using the characteristic equation [3], which will set up a spread of propagation constants for each modal group.

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Researching of Cylindrical Pipe Sound Emission

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In this work we discus sound emission process of pipe, with one opened end. Second end is closed with a solid heat conducting cover. Thermophone excite an acoustic field inside the pipe. On the surface of rigid cover placed thermophone's active element. The thermophone is a broadband nonresonant source of sound, the generation of sound waves is provided due to the thermoacoustic effect. Equal condition for excitation of half-wave longitudinal resonances in pipe and corresponding them standing sound waves is achieved by installing thermophone.

This work is theoretical preparation for experimental studies of the contribution of Schlichting acoustic flows to energy dissipation in the boundary layer of the inner surface of the pipe. As shown in [1, 2], Schlichting acoustic vortexes appears in the boundary layer because of interaction of standing sound waves with the inner surface of the tube. It should be noted that even in standing sound waves of high intensity, the acoustic Reynolds numbers of the emerging vortices are $Re_B << 0{,}1$. Physically, this means that an effective process of dissipation of sound energy takes place on the emerging vortices.

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Space-Frequency Coherence Functions of High-Frequency Fields in the Transionospheric Stochastic Channel of Propagation

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The two-position two-frequency coherence function is the core quantity in studying the pulse signal propagation in a stochastic medium, or constructing the scattering function of the stochastic channel of propagation. When studying the coherence functions for the particular case of the high-frequency EM field transionospheric propagation, it is of importance to take account of the effect of the inhomogeneous distribution of the electron density in the background ionosphere.

Unlike in the traditional treatment, where a real inhomogeneous layer of the background ionosphere is replaced by an effective homogeneous layer characterized by the same value of the Total Electron Content (TEC) as in the real inhomogeneous ionospheric layer, the effect of the inhomogeneous background ionosphere is explicitly investigated. This allows for describing the real coherence properties of the stochastic field at any height above the Earth's surface. Additionally, if necessary, this also allows for determining the properties of the equivalent homogeneous layer, which generates the coherence functions on the Earth's surface of the same properties as those obtained when solving the propagation problem through the stochastic ionosphere with really inhomogeneous layer of the background electron density, i.e. describes the range of validity of the traditional technique of the approximation of the homogeneous layer of the background ionosphere.

Obviously, it is solely of interest to deal with the case when the fluctuations of the ionospheric electron density give rise to the regime of strong scintillation of the field intensity. This is investigated here on the basis of the diffusive Markov's approximation. In the recent paper [1] the appropriate Markov's equations for the coherence functions were solved numerically. Here the analytic solution for the first coherency function is constructed for given models of the inhomogeneous background ionosphere (semi-analytic). These solutions are then compared to the known solution for the case of the homogeneous layer of the background ionosphere having the same value of the TEC.

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Universal Ultrasonic Transducer for Measuring the Acoustic Wave Velocity

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Nowadays the majority of the devices, used for measurement of the velocities of both longitudinal and transverse waves have high precision. However upon transition from measurements of one type of waves to another, replacement of converters is required, and so the speed with which measurements are performed isn't always satisfactory. When carrying out some researches there is a need of quick and simultaneous measurement of speeds of both longitudinal and transverse waves.

This work considers acoustic system, which allows measurements of distribution of the longitudinal and transverse waves extending on the same section of a sample to be made, where emitter and the receiver of ultrasonic fluctuations are both made of two couples the piezoceramic plates of different cuts, which are pasted previously to subject of control (Fig. 1). It is found out that the creation of similar acoustic installation is possible, as well as the optimal variant of construction is picked up.

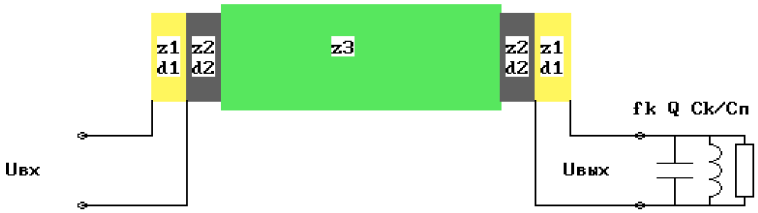

Fig. 1. Schematic of Plate-type piezoelectric transducer.

The Structure of the Polar Cap Patches Based on TEC Measurements

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HF (high-frequency) communications within the high latitude region is of growing importance for civil airlines operating transpolar routes, as these may form the shortest path between significant destinations, reducing travel time, cost and carbon emissions.

The complexity and variability of the high-latitude ionosphere structure is induced by the presence of the localized regions of enhanced electron density in the F region - patches and arcs [1]. Parameters of the patches of enhanced electron density (number, speed, trajectory and intensity) strongly depend on geophysical condition. They are typically of about 500 km in dawn to dusk direction but they range from 200 to 1000 km and exhibit electron-density enhancements of up a factor of 10 above background [2]. Electron density gradients associated with large-scale structures within the polar ionosphere form tilted reflection surfaces for HF radio waves. Consequently HF radio signals propagating through this region often arrive at the receiver over paths well displaced from the great circle direction. Such large deviations of the arrival direction have serious implications for the operation of communication and radiolocation systems operating within the HF band.

Very useful method describing of the electron density distribution in the ionosphere is based on the total electron content (TEC) measurements [3]. An approach providing the mapping of the plasma structures in high latitude ionosphere and defining their main parameters using TEC observation is presented in this paper. This method allows to assess the dynamics and statistics of the polar cap patches, which could be used in HF wave propagation channel modelling.

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Numerical Study of Properties of Viscous Waves, Generated by Plane Finite Sources

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The research contains numerical study of nonlinear viscous waves, generated by finite planes, harmonically oscillating in viscous fluid. We have solved nonlinear time-dependent Navier-Stokes and continuity set of equations for incompressible fluid. We used adhesion boundary condition and demanded that oscillation velocity equal zero at an infinite distance to the source. Amplitude of oscillation velocity was small (hence Mach number was small).

Effect of the source finite size along the oscillation direction has been studied as the one to form geometric dispersion of the wave's propagation velocity. Pressure field and oscillation velocity field depending on the distance to the plane source have been studied. It has been shown that pressure gradients appear and increase near the source edges relatively to constant pressure gradient I the medial area of the plane source. Horizontal component of oscillation velocity is formed near the edges. It causes curvature of classical liner trajectories of fluid particles in a transverse viscous wave.

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Research of Room Temperature Influence on the Time of Standard Reverberation

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In practice to make an estimation of room acoustic characteristics, an estimate is made for the standard room reverberation time with Eyring formula [1]

$$T_r = \frac{k_{cp} V}{\beta' S + 4\alpha V}, \qquad (1.1)$$

where $\beta' = -\ln(1-\bar{D})$ is the reverberation coefficient of the room; α – the dimensional attenuation coefficient (DAC) of sound waves in the volume of gas filling the room; k_{cp} is a constant coefficient; S – area of the walls, floor and ceiling of the room; V is the volume of the room; $\bar{D}$ – the average (diffuse) coefficient of sound absorption (CSA) by the surface limiting the room.

The parameters α, and the coefficient k_{cp} depend on the air temperature and, as a consequence, the time of the standard reverberation T_r also depends on the temperature. The variability of the SLAC α value can be taken into account if we use Kneser's formula [2] for calculations. In rooms with flat walls, on the surfaces of which there are no special absorbers of sound waves, sound absorption is provided by dissipation of energy in the acoustic boundary layer of a solid surface. This makes it possible to use the method developed by BP Konstantinov [3] for calculations of the average bullpen. A numerical estimate of the effect of temperature on the value of T_r was made using the example of the reverberation chamber of the Krylov State Research Center.

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Study of the Ionospheric Total Electron Content during Magnetic Storm

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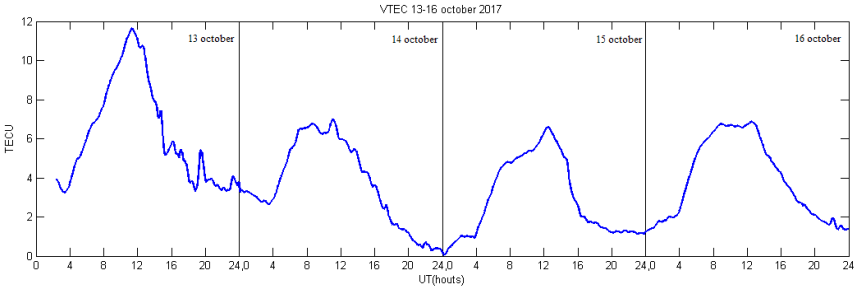
In this paper we investigated the effect of a magnetic storm on the electronic concentration of the ionosphere of the Earth. The main parameter determining the electron concentration is the TEC (total electron content). Knowledge of TEC allows solving various problems for improving the quality of the signal passing through the ionosphere of the earth. As practice shows, the higher the TEC value, the more the signal is distorted, and also by means of TEC it is possible to track outbreaks in the sun and other disturbances in the ionosphere [1].



Employing the receiving and registering facility for GPS signals, on 13 October 2017, monotonic strong increase of vertical TEC (VTEC), then recession and rapid irregular changes of VTEC continuing until 3:00 next day were recorded. According to the Internet portal http://tesis.lebedev.ru, a magnetic storm started on 13 October 2017 3:00 and ended on 15 October 2017 18:00. Peak activity of the magnetic storm was from 13.10.17 12:00 to 14.10.17 3:00, which is seen on the graph. Also on the graph, a positive and negative phase of the magnetic storm is observed.

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Observing of Macroparticles Method for Transverse Beam Dynamics Calculation in Dielectric Waveguide

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Method of macroparticles is most simple way to calculate beam dynamics [1]. Electron bunch is passing throughout dielectric waveguide with speed of light and generates Cherenkov radiation (wakefield) which can be used as accelerated field [1, 2] or THz radiation [3]. Wakefield can be divided on longitudinal field E_z and transverse field F_r. Transverse field includes asymmetric HEM-modes with amplitudes depend on radial bunch dismission (offset). The most important question of this scheme is beam dynamics caused by F_r. It is reason of collision between particles of bunch and dielectric wall.

In this work we explored employment of this method for calculation of bunch dynamics which pass throughout dielectric waveguide. We investigated the limitations on the application of this method. There are some parameters we used for analysis these limitations: number of macroparticles *N*, longitudinal beam size *sigmaZ*, transverse beam size *sigmaR*, wavelength λ radial offset *offset*. We carried out numerical calculation and compare it with analytical transverse field inside bunch received by integral convolution between Green-function and Gaussian-bunch distribution (Fig. 1). As a result, we present data tables (Fig. 2), which help to choose correct number of macroparticles.

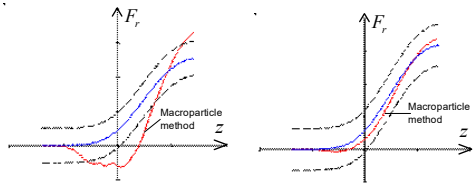

Fig. 1. Comparison transverse field calculated by integral convolution and by macroparticles method. Results can be located inside borders: a) macroparticles method is inaccurate -0 b) macroparticles method is accurate -1.

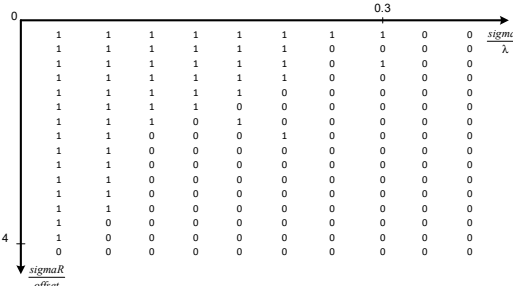

Fig.2. Calculation results for N=100.

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A Network Protocol Stack for the nRF24L01+ Transceiver

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The 2.4 GHz transceiver nRF24L01+ allows to create WLAN easily. The official documentation [1] and experiments with the SDR radio receiver claim that the nRF24L01+ transceiver doesn't allow to realize a reliable transmission of data packets between nodes deleted from each other on distance more than 100 meters. Also, the existence of barriers between nodes carries to the considerable losses of packets. That's why there is a need to develop the network layer for microlocal networks based on nRF24L01+ that will support relaying and routing packets (Fig. 1).

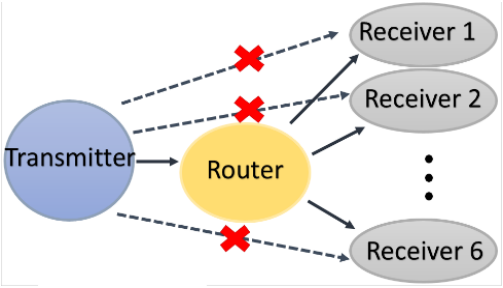

Fig. 1. Network structure.

With the purpose to simplify setup and monitoring the module the software written in C language was created. One of the software's advantages is that it does not spend many resources (16Kb). The library maintains the majority of functions of the transceiver, for example, setup of frequency channel, speed of the transceiver, power output and so on [2]. Also, there is an initialization of SPI.

After setting parameters (using functions from the developed software) the next stage is a compilation of a routing table for the transmitter consisting of channel numbers and their addresses - they will be transferred through the broadcast channel. Then the transmitter should select through which channel it will send data. If there won't be a receiver address in the local routing table then the transmitter will send a packet to the router. The router automatically will move from the receiver to the transmitter mode and will send a packet to a final node or to the next router.

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Experimental Study of Ionic Wind in Row of Needles-Plate Electrode System and its Application to Heat Transfer Enhancement

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The work aims at the experimental study of ionic wind in needles-plane electrode system and its parameters. A horizontal grounded plate of size 190x100x6 mm is also used as a heat source, so the heat flow enhancement is estimated as well. An air flow is produced as local axisymmetric jets from each needle interact. Voltage, polarity, inter-electrode and inter-needle gaps are varied. Air velocity distributions are obtained by the Particle Image Velocimetry method and then processed with the Matlab programming tools. An experimental setup is assembled to ensure maintaining the plate temperature at the constant average level of 360 K. The local temperature distribution across the plate surface is registered with an infrared imager. With the grounded plate temperature fixed, the dependences of heat power drained from the plate surface vs. the electric power consumed by corona discharge have been obtained. When using the multiple needle electrodes, a complex air flow is produced with localized thin (2-3 mm) and fast (up to 8 m/s) ionic wind jets, which allows cooling heated objects quite efficiently. The maximum heat removal is observed if high voltage electrodes are spread across the entire heated plate surface. When corona electrodes are placed compactly, a discharge self-extinction effect is observed, which results in lower high-voltage power consumption. The heat power, removed from the plate due to the ionic wind, was greater by an order of magnitude than that removable via natural convection and exceeded the electric power spent on sustaining the corona discharge by 1-2 orders of magnitude. With increasing voltage, the outgoing heat power grows, whereas the cooling efficiency, which is defined as the ratio of the outgoing heat power to the consumed electric power, drops. The efficiency is measured and compared for several electrode system configurations.

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Influence of Transverse Beam Dynamics of Bunch Train on Cherenkov Radiation in Dielectric Waveguide

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We explored a new method of producing THz radiation based on Cherenkov radiation (wakefield) created by relativistic bunch train in dielectric waveguide. The usage of dielectric waveguide relates to accelerating schemes [1] and new THz sources [2, 3]. The bunch train is sequence of relativistic electron bunches. It is possible to select only one TM0n mode in radiation while other TM modes are damped. This selection is realized by setting distances between bunches which include even number of half wavelength.

THz radiation has three main parameters: frequency, amplitude, length of wave pocket and monochromaticity. Length of wave pocket is limited by waveguide length and group velocities of TM-modes. The transverse instability caused by strong deflecting force F_r lead to radial dismission of bunches. As a result, the bunches with growing radial offset excite asymmetric HEM-modes. The presence of HEM-mode reduces the monochromaticity of radiation. We present results of calculation for THz structure for generation radiation with range 400-800 GHz (Figs.1, 2).

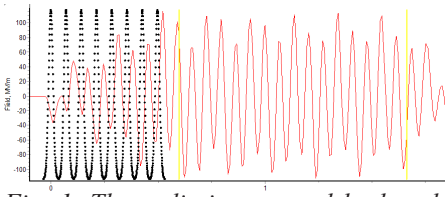

Fig. 1. The radiation created by bunch train passing in dielectric waveguide from right to left.

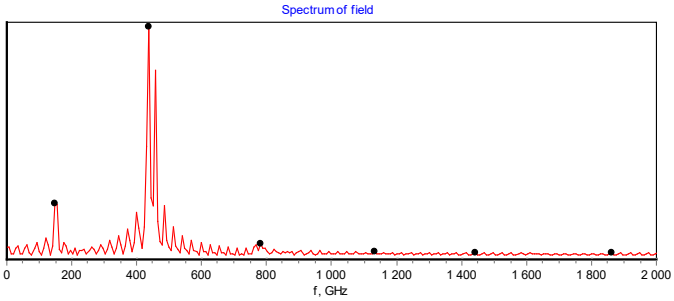

Fig. 2 Spectrum of radiation.

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The Influence of Ion Wind on a Karman Vortex Street Behind a Circular Cylinder

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The paper studies the influence of ion wind, caused by a corona discharge, on an external fluid flow. The electrode system consists of the grounded circular cylinder and two high-voltage wires. The simulation uses the unipolar model of the corona discharge.

It was shown that the weak ion force, which acts in a small domain near the high voltage wire, could dramatically change the flow structure and characteristics of Karman vortex street. The concept of ion wind efficiency was introduced. The ion wind in given electrode system creates a force, which is perpendicular to the air flow direction and allows suppressing the vortex street. The detachment angle decreases upon application of high voltage, which causes the periodic vortices to disappear. The vertical force oscillations stop, and the drag force is markedly reduced.

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High-Precision Measurement of Speed and Direction of Wind

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The measurement of speed and the direction of wind is one of the most important problems of meteorology. Therefore the problem of creation of anemometers – airflow measurement device is relevant. There are several types of anemometers: cup, wing, thermal and ultrasonic. The main problem of mechanical anemometers is the inertance of moving parts. Ultrasonic anemometers (Fig. 1) use change of time delays between the transfer and reception of an ultrasonic signal depending on a wind speed projection to the axis connecting the transmitter and the receiver of ultrasound. However in the market they have too high cost therefore development of cheaper analogs having a high precision of measurements is expedient.

Fig. 1. Ultrasonic anemometer.

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Investigation of Edge Waves

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Waves, which propagate along free edge of semi-infinite plate, are called edge waves. The study of edge waves is based on two-dimensional theory of plates, which describes only first (or fundamental) edge wave in long-wave range. The theory of plates was also used in mechanical engineering, construction of buildings, hydroacoustics and other fields.

The problem of diffraction of a plane hydroacoustic wave on infinitely narrow crack between two elastic plates lying on the liquid is one of classical problems [1]. This problem with proper choice of coordinate axes (Fig. 1) is two-dimensional. Further, in the solution of the formulated problem, we have to deal with regularization and analysis of boundary-contact integrals that is of interest from mathematical physics point of view. The resulting solution is investigated on condition $\mathbf{kh}\to 0$, where **k** and **h** denote wavenumber and plate thickness respectively. As a result, it was found that effect of scattering from a crack is weak and is not accompanied by significant energy consumption. Also, the main components of the diffraction field are cylindrical and surface waves.

We consider the three dimensional problem with the cross-section shown on Fig. 1. As known [2] edge waves can propagate along the crack. The goal of our research is to study the excitation of edge waves by a point source applied to the edges. We start with the case of free plate (no fluid). In this case edge waves are the analogues of well known Rayleigh waves on the free surface of an elastic body.

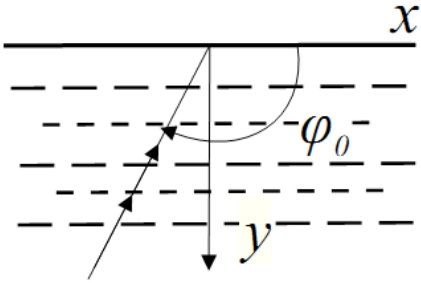

Fig. 1. The choice of axes directions.

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Experimental Research of 3d Structure of Streamer Propagation

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The aim of this study is experimental research of 3D structure of single positive streamer propagation in air in the sphere-plane electrode system. A new method is proposed for reconstruction of 3D structure using images from two cameras. Two series of experiments have shown the average angles of branching to be practically the same. No correlation is detected between branch lengths and branching angles.

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Investigation of the Velocity and Pressure Fields of a Quasiplane Viscous Wave Depending on the Mach Number

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Nonlinear viscous waves excited by planar surfaces that oscillate in harmonic order are numerically investigated. A nonlinear non-stationary equation for the motion of a viscous fluid (Navier-Stokes) with no-slip conditions at the source surface and inversion of the oscillate velocity to zero at infinity in the range of Mach numbers 0-10 is solved. The fields of pressure and oscillate velocity are investigated as a function of the distance from a finite plane source whose dimensions vary in the range (1 - 50) of the thickness of the boundary layer. It is shown that near the surface of the source and at a distance from the median line there is a quadratic pressure increase with increasing Mach number with an accuracy of 8%. Near the edge of a finite flat source a horizontal component of the oscillate velocity is formed - the viscous wave ceases to be purely transverse. It is shown that with an increase in the Mach number, the envelope of the field of the oscillate velocity becomes steeper. The modulus of the horizontal component of the oscillate velocity not only depends on the Mach number in a complicated manner, but its vector changes direction.

An Empirical Model of HF Radio Wave Regular Absorption in the Middle Latitude

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This work is devoted to study of short radio waves absorption caused by ultraviolet radiation of the sun in the middle latitudes. The objective of the work was to optimize existing models of regular absorption, based on empirical formula [1]. Currently there is an extensive network of ionosondes, which allows to measure the amplitudes of radio wave fields. The presence of such a network also makes it possible to optimize the previously developed models for the absorption of radio waves. The optimization of the absorption model was carried out by varying the parameters of the empirical formula, characterizing the dependence of absorption intensity versus the level of ultraviolet radiation of the sun. For the selection of optimal parameters, a comparative analysis of model and calculated ionograms of vertical sounding was carried out. Comparative analysis was carried out by comparing the minimum observed frequencies of each hop on the experimental and theoretical ionograms. This method is an improvement of the A1 method, which was used in the second half of the last century [2]. Ionograms, corresponding Pruhonice, Juliusruh and Fairford stations, were simulated for four dates in 2013 and five dates in 2012. As a result of the study, the original formula was modified by adding a term that takes into account the effective frequency of collisions of electrons with ions, and also the optimum coefficients reflecting the seasonal dependence of the absorption intensity were obtained.

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Simplified Model of Streamer Discharge Tree

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The streamer is an electrical discharge in gases. The creation of numerical models of streamers is important because models can be used in the calculation of breakdown voltages of high-voltage structures. But direct simulation of streamers is very computationally-intensive problem. Therefore, interest simplified models.

Because of the branched form, streamer discharge can be represented as a tree. The values are calculated only at the nodes of branches can significantly reduce the computational time but there is arbitrariness in the choice of simplifications.

The aim of this study is the selection of possible simplifications and the analysis of their applicability.

Numerical Analysis of the Sunset Variations of a Lower Ionosphere Fringe while the Proton Precipitations

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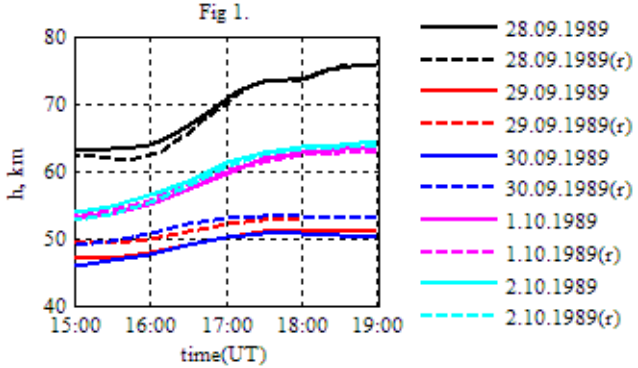
The purpose of the report is to quantitatively compare the daily variations of the flux of solar protons, which began on September 29, 1989, 12:00 UT [1, 2], with the daily changes of VLF signals for a completely auroral radio path Northern Norway - the Kola peninsula (Aldra - Apatity). For realization of this purpose we have used the satellite data [1], the experimental VLF data of the Polar Geophysical Institute of the Kola Science Center, RAS, Apatity, Murmansk region [2, 3] and a self-consistent method of analysis for a VLF inverse problem solving [2, 3]. The pointed method for an analysis of VLF daily variations was used in [3].

Fig 1.



We have established the following:

1) The presented graphs in Fig. 1 give an error estimate of the method by comparing the analysis of daily VLF variations for the positive direction of time (solid curves) with the analysis for the negative direction of time (dashed lines).

2) With the change of proton flux density in the period from September 29 to October 2, 1989 the daily variation of the effective height *h* at sunset changed from 4 km on September to 10 km on October and the reflection coefficient of first ionospheric ray at a sunset was constant. In this date period a value of effective altitude changed from 46 km to 54 km at 15:00 UT, from 52 to 63 km at 19:00 UT and a value of reflection coefficient has changed from 0.8 to 0.6.

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Section of a Cylindrical Pipe as Absorber of Acoustic Noise

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As shown in works [1, 2] if a section of a pipe is in the room with sound level $L \neq 0$, then the radiation of sound waves is observed from its open end faces. This radiation can be detected by any objective and nonobjective methods of acoustic measurements. Longitudinal half-wave resonances natural frequencies are observed in the lower part of the sound frequency range.

Initiation of oscillating process in are happens due to the energy which is selected from the external acoustic field. It allows to consider a pipe section like an absorber of acoustic noise. Except sound radiation there are dissipative processes in a pipe. Usually when calculating a resonance of this kind consider absorption of energy in acoustic boundary layer on internal pipe walls and in volume of air filling a pipe. The theoretical analysis of acoustic field structure excited in pipe volume showed that generally, this field is a superposition of standing sound waves. At the interaction of standing sound waves with pipe walls in its boundary layer there have to be acoustic Shlikhting flows. Our task is evaluating a contribution of Shlikhting vortexes to a dissipation of acoustic energy in a pipe.

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Study of the Effect of Horizontal Gradients in Troposphere on the Delay of the Navigation Signals

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Determining the delays of satellite navigation signals is a key problem in positioning. In order to determine the delay, it is necessary to solve the ray equations in inhomogeneous medium of propagation. However, since the refractive index of the ionosphere and troposphere for the frequencies used by navigation systems is close to unity, the ray deviates only a little from a straight line. In this case, the ray equations are effectively solved using the perturbation theory [1].

This paper examines the effect of tropospheric gradients on the phase delay. To do this the program for calculating an ionospheric delay [1] is modified to account for the effects of the troposphere. With its help, the effect of horizontal gradients in the troposphere is numerically estimated for a number of tropospheric models [2]. The difference between the delays obtained employing the models with and without gradients may reach some meters in case of small elevation angles. The accounting of the effect of gradients is desirable for a precise positioning by using satellite navigation systems.

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F. Optics and Spectroscopy

Evaluation of the Dynamics of the Diffraction Pattern Degradation in the High-Power Ultrashort X-Ray Radiation for the Hydrogen Atom and its Molecular Ion

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Presently x-ray free electron lasers are a very promising trend in physics [1]. They can generate ultrashort high-power x-ray pulses that one can use to resolve non-periodic structures such as biomolecules up to atomic scale [2]. Under the influence of the x-ray flashes an object degrades, which leads to the degradation of a diffraction pattern. It complicates the structure determination of the object.

In current work that is based on the trajectory method the influence of the parameters of the x-ray pulse on degradation of the object is addressed and the method is tested. It unlike the direct numerical solution of the time dependent Schrodinger equation can be applied to obtain the solution for many-electron objects in adequate time.

Fig. 1 demonstrates the change of the autocorrelation function (ACF) for the hydrogen molecular ion H_2^+ caused by the increase of the x-ray pulse's intensity. Calculations were carried out for the x-ray pulse with the following characteristics: $\lambda_0 = 0.46\ \AA$ (or $E_{photon} = 27keV$) and $\tau_{pulse} \sim 0.7\ fs$. The outcomes shown were obtained for two values of the radiation intensity: one is much less than atomic (left) and the other is much more (right).

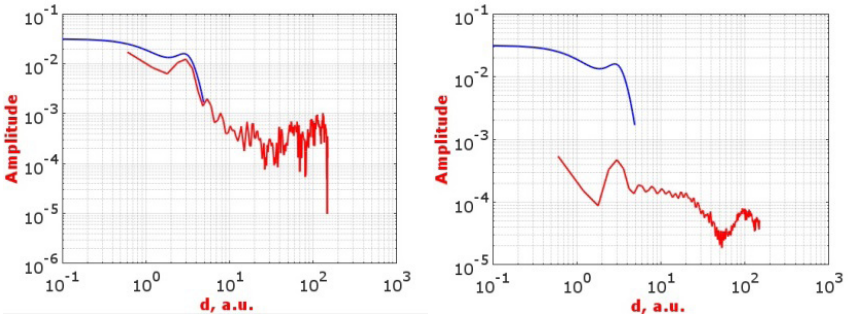

Fig. 1. ACF of electronic density distribution in H_2^+, in its ground state for non-equilibrium internuclear distance R = 3 a.u.

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Symmetry of Planar Arrays of Trilayer Nanodisks in the Appearance of their Plasmonic Properties

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Metamaterials are artificial media usually consisting of arrays of nanometer scale objects called meta-atoms. Such structures are under intensive studies nowadays because they can be widely used to control the parameters of optical radiation and to develop a new area of science – nanophotonics that is an alternative to nanoelectronics. For the creation of functional devices based on nanostructures is crucially important to optimize their design to achieve desirable optical properties.

Our work is devoted to the study of the relationship between the symmetry of an array of nanoelements and the optical response of a sample. The structures were fabricated in Australian National University [1, 2]. The meta-atoms are three-layered disks Au-MgF_2-Au, with the diameter of about 140 nm and each layer thickness 30 nm. The meta-elements are packed in 4 types of arrays, corresponding different symmetry: square lattice, hexagonal lattice, Penrose mosaic and amorphous. Experimental data were compared with numerical simulations of transmission spectra and distribution patterns of electromagnetic field within the structures using finite difference time domain method in software Comsol Multiphysics.

Transmission spectra of each sample reveal two minima at the wavelengths 700 and 900 nm. Simulations of the electric field distribution proved that these minima correspond to electric-dipole and magnetic-dipole resonances, respectively [3]. The spectral position of the plasmon resonances doesn't depend on the angle of incidence.

It was found that the best resonance quality factor (Q~9-10) was observed in samples with square and hexagonal arrangement of meta-atoms. In Penrose mosaic the quality factor is worse (Q~7), because there is only higher order arrangement. In amorphous sample the resonances are weak (Q~6) due to the strong scattering. The experiments were also performed for different azimuthal orientations of the samples.

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The Research of Multicomponent Media on Autocorrelation Parameters of Optical Spectrum

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Molecular systems are known for molecular systems, which are mixes of large number molecules. There are substances from multi-component materials, polymeric resin and mixtures for macromolecular compounds of natural and technical origin. These substances characterized by a chaotic distribution of the chemical composition. The aim this work is the research of the features for the integral parameters of autocorrelation function (ACF) for the continuous electronic spectra of hydrocarbon mixtures. We are shown, that for systems with chaos of chemical compound exist the exponential distribution function for the absorption coefficient [1]:

$$k(\lambda) = ae^{-b\lambda}, \qquad (1)$$

where $k(\lambda)$ is the absorption coefficient in the visible region of the spectrum, l/g·cm; λ- wavelength, nm; a, b are empirical coefficients that depend on the nature of the substance. Since the process is ergodic, then to calculate the autocorrelation function we use the averaging interval:

$$R_{cor} = \frac{a^2}{-2b(\lambda_n - \lambda_0)} e^{-b\Delta\lambda}\left(e^{-2b\lambda_n} - e^{-2b\lambda_0}\right) - \frac{a^2}{b^2(\lambda_n - \lambda_0)^2}(e^{-b\lambda_n} - e^{-b\lambda_0})^2 \qquad (2)$$

where R_{cor} – the autocorrelation function of a random signal; λ_n и λ_0 – two different sections of a process with step Δλ.

The above characteristics of the signals was researched for example of high boiling petroleum distillates spectra and oils spectra. The results of calculation presented in Table 1.

Table 1. The signal parameters of the oil electron spectra.

№ sample	Rcor	ρ	M
1	0.173	0.9289	421
2	0.112	0.9278	407
3	0.099	0.9291	419
4	0.090	0.9271	410

According to the Table 1, calculated autocorrelation characteristics of the signals are different for the oil close composition, properties and degree of preparation. Therefore, the possible to identify the complex molecular systems using characteristics of signal.

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Model of a Multi-Color Laser on Self-Limited Transitions

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The development of a disruptive technique for pulsed production of metal vapors is gas-discharge tubes manufactured by electrodynamic disperse (EDD) technology. An electrodynamic suspension of the chemical compound particles is created in the discharge tube. The pressure of the buffer gas is such that the electric discharge in the tube possesses diffusive nature. This leads to the formation of a film of a substance deposited on the inner wall of the tube. The perspective of using gas-discharge tube, created by EDD-technology, is considered in the work on the example of the possibility of creating a new multi-color laser on self-limited transitions. The tube which is used in this process has a evaporated compound of metals on the walls Pb (lead), Au (gold), Cu (copper) and a buffer gas N_2 (nitrogen) also discharge tube operates in a two-pulse mode.

A high-energy first discharge pulse with energy of more than 150 J will vaporize the metals Pb, Au, Cu to the ground state from the wall. In this scheme, the transfer of energy from the capacitor bank to the deposited mixture of metals Pb, Au, Cu with a thickness of 1 μm takes place through the buffer gas N_2.

The second pulse delayed from the first by 20-30 μs is intended to excite N_2 molecules and atoms of previously vaporized metals from the ground states. After that pulses of superlumination lasted 1-10 ns should appear in the spectral range corresponding to the generation of Pb, Au, Cu and N_2 considering mirrors of the resonator, i.e. covering the NUV and visible range.

Obtainment of such a generation is a very difficult task depending on the set of conditions, but practical evaluations of such a laser show the possibility of its realizations.

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Initiating the Breakdown in a Long Discharge Tube by Light Pulses

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The work is devoted to investigation of the electrical breakdown in a long discharge tube irradiated with pulsed light sources of visible spectrum.

Measurements were performed in a tube of 80 cm length and 18 mm i.d. filled with neon at a pressure of 1 Torr. Breakdown was produced with rectangular pulses with the voltage amplitude of 1.5 kV, rising time of ~ 1μs, and the repetition rate of 0.5 Hz. The area near the high voltage anode was illuminated by the LED (λ=460 nm) or laser module (λ=407 nm), both working in a pulsed mode. The breakdown delay time (t_d) was measured for different parameters of the light pulses.

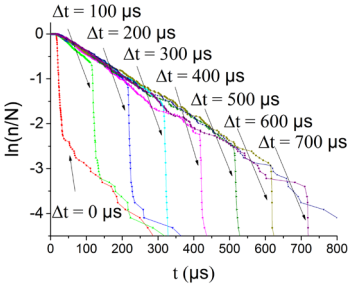

Fig. 1. The Laue distributions for the 5 μs illuminating pulses applied at different moments.

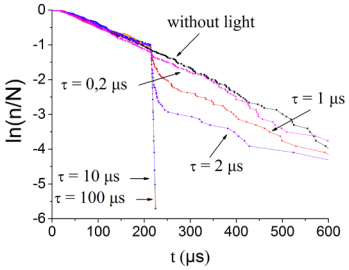

Fig. 2. The Laue distributions for the illuminating pulses of variable duration applied at the moment 200 μs.

The results of the measurements are shown in Figs. 1, 2 as time dependences of the ratio of the number of the breakdowns *n(t)* that occurred later than time *t* to the total number of breakdowns *N* (Laue distribution [1]). As can be seen from Fig. 1, the light pulse sharply limits the breakdown delay time. Fig. 2 shows that the effect of illumination on the breakdown statistics increases with the light pulse duration.

The slope of the plots in Figs. 1, 2 is proportional to the rate of appearance of the electrons initiating the breakdown [1]. Therefore, the effect of illumination on the breakdown is a result of the generation of these electrons. It is assumed [2] that this is a result of photoemission of electrons adsorbed on the inside surface of the tube wall.

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Observation of Reverse Breakdown in the Tubes with Non-Grounded Cathode

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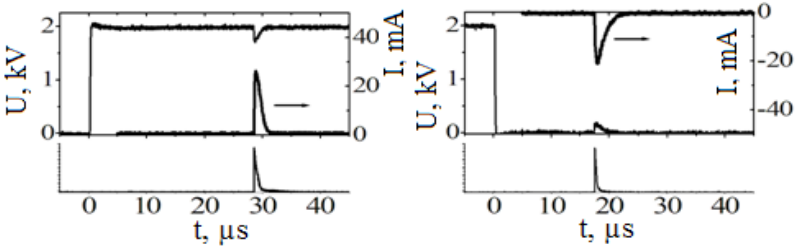
Discharge in a long tube begins with initial breakdown between a high-voltage electrode and a glass wall of the tube [1]. After that the pre-breakdown wave (ionization wave, IW) propagates to the grounded electrode and ionizes gas throughout the tube. For the first time, the initial breakdown current was registered in [2] as a spike of high-voltage anode current. The grounded cathode current and breakdown of the whole tube occur later, when the IW reaches the cathode. Therefore the initial breakdown may occur even if breakdown of the whole tube doesn't occur. In this work, such a scenario was realized in a tube filled with Ar-Ne mixture at a pressure of 1 Torr, by disconnecting cathode and power supply circuit, while the high voltage pulses were applied to the anode. After some random time interval the peak of the anode current was observed. Simultaneously, the anode voltage jumped down and peak of the luminosity of the gas in the region near the anode appeared (the plots in the left side of the Fig.). All these processes agree with the picture of initial breakdown between anode and the glass wall of the tube with following propagation of IW.



Unexpected feature was that after the pulse cutoff in some random time interval, the peaks of anode current and voltage were observed again but of the sign opposite to the previous. They were accompanied by the IW moving to the cathode. It can be explained as follows. The initial breakdown charges the glass wall, so after the breakdown the wall potential near the anode is close to the anode potential. During some time, this charge remains. When the pulse terminates and anode potential becomes equal to zero, potential drop between the glass wall and anode becomes approximately the same as in the beginning of the pulse, but with reversed sign. This leads to "reverse" breakdown and generation of the IW.

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Interaction of Short Femtosecond Pulses with Two-Level System

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The numerical calculation of short femtosecond pulses with two-level system for interpretations of experimental results has been made.

Atomic system (the transition $5^2S_{1/2}$ - $5^2P_{1/2}$ (λ=780 nm) in Rb-atoms) approximately describes two-level system. The field member is the Gaussian pulse with duration ~ 100 fs. The laser beam from comb-generator of femtosecond laser is focused on the center of cell with atomic vapors. The narrow coherent beam was generated on the resonant transition (λ=780 nm). The divergence of generated beam is equal to 2-3 mrad.

The numerical calculation was made in the density matrix formalism. The Rotation Wave Approximation is applied. The time behavior of density matrix elements for populations and nondiagonal elements (coherence) is presented. When the pulse area is equal to $n\pi$ (n – integer) then the coherent π-pulses generated from the medium. In other cases ($\theta<\pi$, $\theta>\pi$) the spontaneous decay is added at the upper level population. Also the interaction of two-level system with comb-chain of pulses from the comb-generator of femtosecond laser has been made experimentally and numerically. The experimental method of interference comb-spectroscopy is possible to be applied in this case.

Also we made the numerical experiment with very short (a few fs) and unipolar pulses interacting with two-level system (for example, for the system of quantum dots or for the system of superradiated atoms). The calculations of density matrix elements for populations and polarization were made without rotating-wave approximation. The conditions of obtaining of $2n\pi$-pulses generation were found for one-pulse and comb-pulses.

The experimental results were obtained in the Research Centre “Optical and Laser methods of researches of matter” in Saint Petersburg State University.

Investigation of Short-arc High Pressure Xenon Discharge: Experiment and Modeling

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Short-arc xenon discharge of high (super high) pressure is used as a source of optical radiation where emission spectrum is to be as close as possible to solar radiation and where it is necessary to have the radiation of a practically point source of light with high intensity [1]. In this respect, the short-arc discharge in xenon has no analogues and can hardly be replaced by other radiation sources, in particular, the currently popular LED light sources, which are unlikely to be able to provide the solar radiation spectrum.

The high-pressure discharges in inert gases (Ar, Kr, Xe), which are widely used to obtain sources of high-intensity optical radiation, have been studied quite well [1]. However, a number of issues remain unexplored. First of all high current densities in such discharges and a significant heating of the discharge electrodes raise the question of the possible presence of electrode material atoms in the discharge gap and their effect on the discharge properties. This work is devoted to the study of the role of atoms of the cathode material on the properties of the plasma he base of experimental data and by means of discharge modeling.

Xenon light sources of high and ultra-high pressure, as a rule, have thoriated tungsten cathodes to reduce the work function of electrons. The measurement of the distribution of the emission spectrum along the discharge axis yielded results that cannot be explained without taking into account the evaporation of the material of the cathode (thorium) into the discharge gap. The brightest areas correspond to near-by cathode region where the plasma temperature is much lower than at points closer to the anode. Thorium has a significantly lower ionization potential (6.3 eV) than xenon (12.13 eV) [2], so when it enters the xenon plasma, it easily ionizes and reduces its temperature, while ensuring the necessary degree of ionization for the current to flow.

Modeling is based on the following main assumptions: 1) the plasma is in local thermodynamic equilibrium; 2) the description of the particle concentrations is given in the hydrodynamic approximation; 3) the discharge structure is well described in elliptic coordinates; 4) the radiation in the discharge spot is formed by thorium atoms emitted from the cathode.

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Development of Producing Technology for Educational Optical Elements in the Student Research Laboratory for Optical Engineering

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The Student Research Laboratory for Optical Engineering (SRLO) was founded in 2014 at the Dept. of Applied and Computer Optics in ITMO University [1]. Students work on various optical, design, lighting and technological projects [2] and find like-minded team for creating of coworking-groups in SRLO.

Practical-oriented laboratory activity cannot be provided without producing of elementary optical elements, which are supposed to be educational.

The review of traditional approaches for producing optical elements showed that recently there are no technologies in the optical industry, capable to solve this problem.

The created optical equipment must meet following requirements:

1. to visualize work principles of optical elements;
2. to be produced in laborless and rapid conditions in small volumes;
3. to ensure the financial availability.

The results of the work done, the technological process and the obtained characteristics of the elements are presented in the paper. Also the experience of optical elements producing to order to practical-oriented R&D is described.

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Analysis of Rotational Dependence of Dicke Effect

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One of the ways to improve the accuracy of solving applied problems in atmospheric physics is to improve the methods for line shapes calculation. The main mechanisms forming the line contour at low gas pressures are the Doppler broadening, which forms the Gaussian contour, and the broadening by interactions, leading to the contour of the Lorentz shape. Experimental studies have shown that the widely used Voigt profile (which is the convolution of the Lorentz and Gauss contours) does not describe the actual line shapes well enough, which leads to errors in determining such spectral parameters as the line intensity and the broadening coefficients.

One of the causes for the deviation of the Voigt profile from the experimental data is the Dicke effect, the narrowing of the Doppler contour with the pressure increasing due to the limitation of the free motion of the absorbing molecules. In order to consider this effect, we used the method of classical trajectories [1] to calculate the narrowing of the Doppler contour. In constructing classical trajectories, we used literature data on *ab initio* intermolecular interaction potentials. Calculating the changes in the linear molecule velocity due to collisions with atoms of noble gases, we analyzed the dependence of the Doppler contour narrowing on the angular momentum of the molecule. The results of calculations for mixtures of CO_2 with different noble gases are presented in the form of graphs. The plots show the widths of the Doppler line, depending on the pressure and on the angular momentum of the molecule. A distinctive feature of this work is the complete absence of empirical parameters.

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Development of Fabrication of Two-Dimensional Photonic Crystal Based on Porous Alumina

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Porous alumina is the structure with quasi-periodic pattern of holes, so it can be used as two-dimensional photonic crystal.

In this work, porous alumina is created in two stages. Firstly, surface of alumina is electrochemically polished and then using electrochemical etching pores on the surface were created [1-2] (Fig. 1). There are two types of samples with different purity: aluminum foil with 90% purity of aluminum and the other is created by vacuum vaporizing of aluminum and condensation of alumina layer of 2 μm thickness on a polished silicon substrate. Two parameters are changed in experiment: anodic current density and time of etching, and etching modes were found. After that reflectance spectrum was measured, several interference maxima were found. Using such spectra (Fig. 2), the thickness of etched layer and speed of etching with constant anodic current can be calculated. Fabricated patterns of holes have a low periodicity, but we can place seeds for pores using femtosecond laser machining to make structure periodic. Thereby such structure could be represented as two-dimensional photonic crystal.

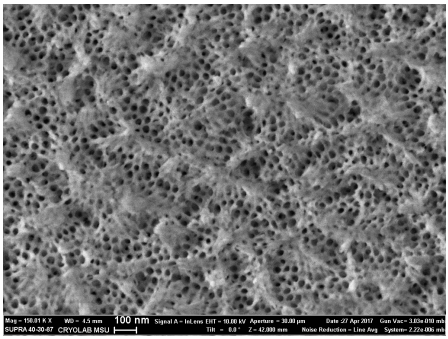

Fig. 1. The surface of porous alumina.

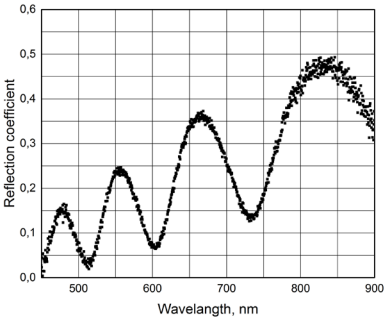

Fig. 2. The reflectance spectrum of porous alumina.

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Influence of Linker Type on Optical Properties and Morphology of Complexes of Gold Nanoparticle / Semiconductor Nanocrystal

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One of the ways to create new and improve existing elements of photovoltaics is the design development and synthesis of nanostructured materials with unique photovoltaic properties and tunable properties. This can be achieved in superstructures based on complexes of semiconductor quantum dots (QDs) and metallic nanoparticles (NPs) [1]. These superstructures combine either unique optical properties of QDs, such as high quantum yield and large values of extinction coefficients over a wide spectral range, and amplification of local fields near metallic NPs. The optical properties of QDs / NPs complex could be tuned by variation of interparticle distance [2].

In our work we have obtained colloidal complexes of CdZnSe/ZnS QDs and Au NPs and investigated the effect of molecule' type on QD and NP surface on morphology and optical properties of formed complexes with different interparticle spacing. It has been achieved by covalently bonding of amphiphilic mercaptic acids of different length with QD or NP surface. We have showed that the morphology and optical properties of QDs depend on the type of molecule-linkers with Au NPs and on the method of complex preparation (Fig. 1).

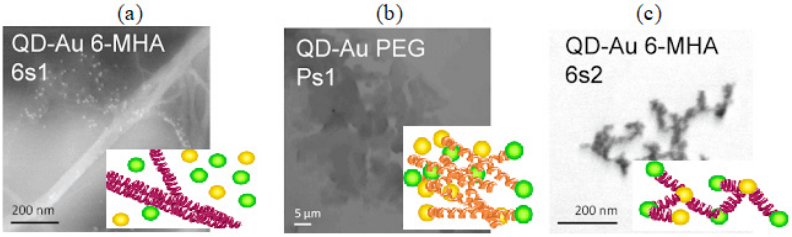

Fig. 1. STEM images of QDs / Au NPs complexes with (a) 6-mercaptohexanoic acid (6-MHA) in water, (b) poly (ethylene glycol) (PEG), (c) 6-MHA in tetrachloromethane and corresponding schemes of complexes.

The results obtained will expand the understanding of the interaction of components in hybrid nanostructured materials. The established principles of nanoobjects interaction will also open new directions for the development of nanooptics and nanoplasmonics.

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Theoretical Study of Vibrational Band Shifts of Linear Molecules in High-Pressure Gas Mixtures

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To study extraterrestrial atmospheres, especially Venus atmosphere, it is important to know the mechanisms of the spectral band shapes formation at high gas pressures. One of the important characteristics of the spectral band is the position of its center of mass, its first spectral moment, shifting under the pressure. The aim of this work is a theoretical study of the mechanisms responsible for band shifts at high pressures. The CO_2 and OCS molecules were chosen as the objects of research because they are of interest for atmospheric applications. As colliding partners, we chose atoms of noble gases as the simplest objects that demonstrate the basic laws of collisional processes.

Analysis of the collisional perturbations of the molecules has shown that the shifts of the bands should be caused mainly by vibrational perturbations of the dipole - induced dipole type. To verify the results of the analysis, we compared the model calculations with the calculations in which the vibrationally dependent potentials obtained *ab initio* were used. The calculations were in good agreement with each other. Then, the shift coefficients of the bands of CO_2 and OCS molecules in mixtures with noble gases (He, Ar, Kr) were calculated. Comparison of the calculation results with the experimental data [1-2] showed that the experimental band shift coefficients in most cases exceed the calculated. The difference between the calculated and experimental results increases with increasing polarizability of the noble gas atoms. Possible causes of such discrepancies are discussed.

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Generation of Unipolar the Pulses in a Circular Nonlinear Medium Excited at Superluminal Velocity

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Generation of few cycle optical light pulses is an interesting progress in modern optics [1]. Those pulses can be used for many applications. For example for controlling of quantum systems and acceleration of electrons. Conventional light pulses are bipolar. Electric field changes its sign and electric area is zero. In unipolar pulse electric field does not change its sign and electric area is not zero. This opens novel opportunities in ultrafast optics and wave packet dynamics control [2-3]. In this talk, we predict theoretically that by the use of circular (see Fig. 1) Raman-active medium (RAM) which is excited by a train of extremely short light pulses, it is possible to create unipolar-like THz pulses. The RAM is considered as a system of two coupled oscillators, high frequency anharmonic oscillator and low frequency harmonic oscillator. The medium geometry and the excitation conditions enable the generation of rectangular pulses. In this presentation the circular RAM is excited by spot of light which can propagate over the circle with superluminal velocity $v>c$ [2-3].

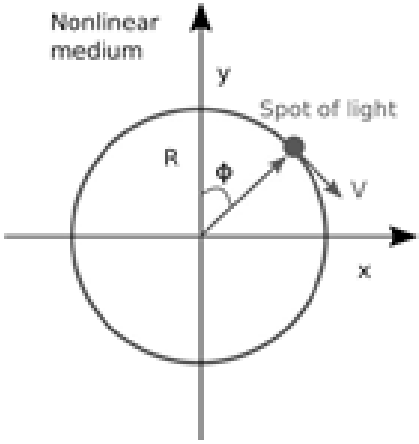

Fig.1. System under consideration.

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G. Theoretical, Mathematical and Computational Physics

Long-range Correlations in the Model with String Fusion on a Lattice

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The multiple hadron production in high energy collisions is studied in the framework of the model with string fusion on transverse lattice [1-3].

The model is used for the calculation of the correlation coefficients between the average transverse momentum and the multiplicity and between the average transverse momenta in realistic case of non-uniform string distribution in transverse plane. Two alternative definitions of the correlation coefficient, which generally are not equivalent for nonlinear regression function, were considered. It is shown that in the framework of the model the results of calculations of the asymptotics of the correlation coefficients by these two different methods coincide in the leading approximation. It is shown that the received asymptotes in case of uniform string distribution in transverse plane are transformed into the ones obtained in other papers [2-4].

The examples with different cases of non-uniform string distribution in transverse plane were considered. Strong dependence of the correlation coefficient between the transverse momentum and a multiplicity on nonuniformity in the distribution of the strings was found. In particular it is shown that there are distributions of strings for which this coefficient becomes negative.

The dependence of the correlation coefficient between transverse momenta on the scaled variance of the number of particles produced from a single string, which disappears in the case of a homogeneous distribution of strings, is studied.

The received asymptotes for the correlation coefficient between transverse momenta were compared are compared with the results of the MC numerical calculations of this coefficient.

Acknowledgements. The work was supported by the St. Petersburg State University grant 11.38.242.2015.

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Study of Relativistic Sturmian Functions

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Relativistic Sturmian functions are very useful instruments in relativistic calculations in atomic and molecular physics. They satisfy the kinetic balance condition and allow to avoid numerical instabilities when the variational approximation is applied for Dirac Hamiltonians.

Earlier Grant introduced his Sturmian set named "L-spinors" [1]. Szmytkowski represented his "Dirac–Coulomb Sturmians" and claimed L-spinors to be incomplete [2]. This claim was rejected by Grant in his later work.

In this work is shown that L-spinors must be complete despite it demonstrates worse convergence comparing Szmytkowski's Dirac–Coulomb Sturmians. To prove it convergence of eigenvalues with respect to the size of the basis sets, static polarizability and relativistic sum rules of hydrogenic atoms examined.

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Simulation of NICA-MPD-Inner Tracker Based on Monolithic Active Pixel Sensors

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One of the important tasks of modern high energy physics is the study of the properties of extremely hot and dense nuclear matter formed in relativistic nuclear-nuclear collisions. The international project MPD (MultiPurpose Detector) on the base of the heavy-ion collider NICA under construction in Dubna is aimed to study the properties of nuclear matter in the region of the very high baryon density. The MPD tracking system will consist of the Time Projection Chamber (TPC) and Inner Tracker (IT) based on monolithic active pixel sensors. The main purpose of IT is to register the decays of short-lived particles near the interaction point. In this work we present the results of TPC+IT modeling within the MpdROOT framework with the aim to evaluate the IT pointing resolution and strange particle identification power using the 5-layer IT geometric model.

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Quantum Algorithms in Discrete and Continuous Variables

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Along with the classical theory of information, quantum information theory, which is based on the effects of quantum mechanics, is becoming increasingly important. Such effects include, for example, quantum entanglement, which has no analogs in classical mechanics. The theorem of the impossibility of cloning a quantum state [1] play important role in quantum information theory.

A relatively small number of algorithms are described. They can be in both discrete and continuous variables.

In this work, some algorithms of quantum information theory are considered: algorithms for quantum teleportation (Fig. 1), quantum cloning, Grover's search algorithm and the Deutsch-Jozsa problem. Initially, they were described in discrete variables, later their analogs in continuous variables were considered. Also presented algorithms that exist only in discrete variables, for example, the Shor factorization algorithm, Simon's algorithm, and the algorithm for computing the discrete logarithm of Shor.

Quantum learning algorithms belong to the field of machine learning. In 2017, physicists from Tennessee generalized three algorithms to continuous variables, which most important for the theory of machine learning quantum [2].

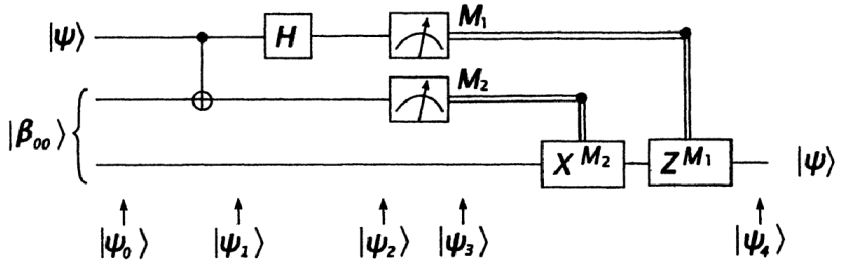

Fig. 1. Quantum teleportation scheme in discrete variables.

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Kinetics of Micellization: Passing From the Discrete Description to the Continuous One

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Relaxation processes to the state of aggregative equilibrium of micellar surfactant systems are described by the Becker-Dering kinetic equations for aggregate concentrations. The finding of the spectrum of the relaxation times with the help of these equations is possible only numerically and requires a large amount of computer calculations. Analytical calculations are carried out by passing from the system of difference Becker-Dering equations to differential equations in which the number of molecules in a micelle is considered as a continuous variable. In combination with the parabolic approximation of the micelle formation work, this allows one to find analytical expressions for the spectrum of relaxation times [2]. The comparison shows that there are both quantitative and qualitative differences of this spectrum from the numerically calculated one. In particular, the presence of degeneracy, which is absent in the results of numerical calculations, takes place. In [3] corrections to analytical eigenvalues were found with the help of perturbation theory. This improves the agreement with the numerical values and removes the degeneracy of the spectrum. However, the approach used in [3] reveals the drawbacks associated with the non-Hermiticity of the perturbation operator, which in some cases leads to unphysical complex values of the relaxation times.

I propose a modified version of perturbation theory in which the Hermiticity of the perturbation operator is preserved in any order of perturbation theory, which guarantees the reality of the relaxation times.

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Aggregation of Asphaltenes in Toluene and Heptane Solutions

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Asphaltenes represent one of the most promising materials that can be used as the inexpensive nanofillers to produce novel polymer composites with improved thermal and mechanical properties [1]. Thus, the experimental and theoretical study of the influence of asphaltenes addition on the properties of polymer composites is of great importance. The main goal of the present study is to improve the understanding of the efficiency of asphaltenes as the fillers in polymer nanocomposites using the molecular-dynamics simulations.

On the current stage, we developed and parameterized the model of the asphaltene molecule. The developed model was verified by the comparison of the results obtained by the simulations of asphaltenes in toluene and heptane solutions with the experimental data. The effect of partial charges parameterization on the structural properties of the asphaltene complexes in the solutions was examined as well. To describe interactions in the models developed the GAFF force field was used. It was observed that in the systems simulated without partial charges the aggregation number of asphaltene complexes is sufficiently higher in heptane than in toluene (8.7±1.6 and 6.9±1.0, respectively). These results are in the qualitative agreement with experiments, where it was suggested that the complex sizes in the heptane are higher than in toluene and that the sizes range from 4 to 10 molecules. [2] Partial charges taken into account lead to decrease of the aggregation number of complexes formed in the both solutions studied.

Acknowledgements. This study has been supported by the Russian Ministry of Education and Science (Agreement No 14.613.21.0069, identifier RFMEFI61317X0069). The simulations have been performed using computing resources of the federal collective usage center Complex for Simulation and Data Processing for Mega-science Facilities at NRC "Kurchatov Institute" (http://ckp.nrcki.ru/).

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Quark Sigma Models in Media with Chiral Chemical Potentials

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It was believed that a violation of CP-parity can occur only in weak interactions. At the same time, the possibility of violation of CP-parity in quantum chromodynamics is not excluded. This phenomenon can occur at large axial or baryonic chemical potentials. In the first case, CP violation leads to the appearance of a chiral magnetic effect. Also due to the chiral chemical potential one can explain the anomalous emission of dileptons observed by NA60 (LHC), STAR (RHIC) and PHENIX (RHIC) collaborations. CP violation is associated with spontaneously generated pseudoscalar condensates for a large baryon chemical potential. Chemical potentials can significantly change the widths of known processes. For example, in the talk it is predicted a transformation of decay widths of some mesons.

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Relation between Noether and Metric Forms of Stress-Energy Tensor in Arbitrary Theories of Tensor Fields

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It is well known, that for field theories with global invariance one can prove Noether's theorem, which provides correspondence between symmetries of action and conserved quantities. In particular, translation invariance in spacetime leads to conservation of energy-momentum vector. Its densities are determined by a «0μ»-components of so-called stress-energy tensor (SEMT) $T_N^{\mu\nu}$. Despite the fact that Noether's theorem claims a certain expression for this tensor, one can't guarantee its observability or several conveniences like simple relation with angular momentum tensor.

Hence it is more common in practice to use other SEMT – a metric stress-energy tensor $T^{\mu\nu}$, which is on the right-hand side of Einstein equation. It is symmetric by construction and has the simple relation with angular momentum tensor:

$$M_{ik}^{\alpha} = x_i T_k^{\alpha} - x_k T_i^{\alpha}. \qquad (1)$$

It is worth noting that T_N and T depends on each other, and one can write a relation between them:

$$T_N^{\mu\nu} = T^{\mu\nu} + \partial_{\alpha} B^{\alpha\mu\nu}, \qquad (2)$$

where B is antisymmetric in first two indices. This formula can be easily proved in theories with no more than first order derivatives in lagrangian. However, attempts in generalization of (2) confront a number of challenges.

A scheme of proof of (2) for theories with arbitrary number of derivatives in lagranigan and calculation of B will be presented in this report. Some applications of this result will be briefly discussed.

Mechanism of the Rare Example of Dual Emission in Heteroleptic Cyclometalated Ir(Iii) Complexes: Dft Computational Study

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Ir(III) cyclometalated complexes possessing unique photophysical properties have potential applications in the development of sensing, bioimaging and electroluminescent devices. Due to the strong spin-orbit coupling effect induced by iridium, such compounds usually demonstrate efficient phosphorescence. At the same time, several cases of triplet-triplet and singlet-triplet dual emission in such systems are also known. Dual emission is usually associated with the presence of heteroleptic ligands and attached independent fluorophores. Of particular interest is the first example of well-separated dual singlet-triplet emission demonstrated by a family of novel compact mononuclear $[Ir(C\hat{}N)_2(NN)]^+$ complexes, where **NN** = (ethynylphenyl)bipyridine [1]. An in-depth insight into the photophysical behavior of these complexes can be obtained with the help of quantum chemical calculations

In this work density functional theory (DFT) calculations were performed to study the mechanism of dual emission in the aforementioned Ir(III) complexes. Structural data were obtained from stationary DFT calculations for five $[Ir(C\hat{}N)_2(NN)]^+$ complexes with different **C^N** ligands. Results of time-dependent DFT (TD-DFT) studies were used to investigate the properties of excited states. The analysis of fragment contributions to the excited states was carried out with the help of Natural Transition Orbitals (NTO) formalism. This approach elucidated the role of **C^N** and **NN** ligands in electronic transitions and provided a consistent picture of luminescent properties of the complexes under investigation.

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A C*-Algebra Associated with a Metric Graph

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An eikonal algebra E(Ω) is a C*-algebra [1] related to a metric graph Ω. It is determined by trajectories and reachable sets of a dynamical system associated with the graph [2]. The system describes the waves, which are initiated by boundary sources (controls) and propagate into the graph with finite velocity. Motivation and interest to eikonal algebras comes from the inverse problem of reconstruction of the graph via its dynamical and/or spectral boundary inverse data [3]. Algebra E(Ω) is determined by these data. In the mean time, its structure and algebraic invariants (irreducible representations) are connected with topology of Ω. We demonstrate such connections and study E(Ω) by the example of Ω with a simple structure. Hopefully, in future, these connections will provide an approach to reconstruction.

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Relativistic Calculations of Higher-Order Electron-Correlation Corrections to the $2P_{1/2}$--$2S_{1/2}$ Transition Energies for Lithium-Like Ions

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For a while highly charged ions (HCI) attracted the attention of physicists since these few-electron systems can be theoretically described with high accuracy. Moreover HCI provide a unique scenario for probing quantum electrodynamics (QED) effects in the strongest electromagnetic fields. Only thereon the techniques for producing, storing and high precision measuring of the HCI properties were developed [1]. The current level of experimental accuracy demands rigorous QED calculations of two-photon-exchange contributions. Meanwhile rigorous QED calculations of a three and more photon-exchange contributions have not been performed up to now. For increasing theoretical accuracy of evaluations one needs to take somehow into account these contributions.

In present work the higher-order electron-correlation corrections to $2P_{1/2}$--$2S_{1/2}$ transition energies of lithium-like ions were calculated to all orders in $1/Z$ within the Breit approximation. The evaluations were carried out employing the large-scale configuration-interaction Dirac-Fock-Sturm method [2] which was successfully used in the previous calculations [3, 4]. The two-photon-exchange contributions were calculated exploiting the many-body perturbation theory in finite hydrogen-like Dirac-Sturm-Fock basis with subsequent extrapolation to the range of high values of principal quantum number n and orbital quantum number l. The obtained results are in a reasonable agreement with other recent theoretical calculations [5].

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The Effect of the Network Fault-Type on the Current and Voltage Phasors

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This work studies the impact of the emergency operation of a high-voltage network on the accuracy of an accident location. Presently, there are many different techniques to identify the place of a fault at an overhead power line. However, the generalized analysis and selection of major influencing parameters for the accuracy of the location of the fault ware not carried out. In this paper, we consider the dependence of the current and voltage phasors during emergency on operation of the network. Metal and arc [1], single-phase, two-phase and three-phase faults are simulated. Simulation is carried out with the Matlab-Simulink package using the example of a simple network model consisting of a source, a power line and a consumer. In order to simulate a long line, the Pi-Section block is used. The zero and positive sequences impedance values are obtained from the twisted wire model [2]. The place of the accident, the consumer power load and the type of short circuit are varied. An analysis is made with the dependence of phasors on the distance from the accident and the type of short circuit.

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Mott Scattering of Twisted Electrons by Atomic Target: Going Beyond the Born Approximation

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The twisted (or vortex) electrons being predicted [1] and realized [2-4] during the last decade presently attract a lot of interest from both the experimental and theoretical sides. It is explained by the fact that these electrons in contrast to the plane-wave ones can carry a nonzero projection of the orbital angular momentum (OAM) on the propagation direction. It is also worth to note, that electrons with $m \neq 0$ provide a unique possibility to get a deeper insight in role of the OAM in the spin-orbit interaction in different atomic processes and can be utilized for more detailed investigations of various systems.

In the present work we perform a fully relativistic description of one of the basic interaction process; namely, the Mott scattering of the vortex electrons by heavy neutral atoms. Up to now, this process was considered only perturbatively in the framework of the first Born approximation [5]. This approximation stays valid only for light systems with relatively small nuclear charge Z. Here we treat the interaction of the electron with the target atom exactly with the usage of the method analogous to one described in Ref. [6]. It is found that the total cross section for the scattering of the 2 MeV twisted electron on the aluminum atom (Z = 13) being calculated within the first Born approximation differs from the exact value by 20%.

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Ground-State Energy of Heavy Diatomic Homonuclear Quasimolecules

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A one-electron diatomic quasimolecule represents the simplest molecular system. One of the most interesting cases is heavy quasimolecules in which $Z_{eff} \cdot a$ is not small (a is the Fine-structure constant, Z_{eff} is the total nuclear charge); thus all calculations should be done to *all* orders in $Z_{eff} \cdot a$ [1]. In particular, when $Z_{eff} > 173$. Theory predicts that the lowest-lying states of quasidimers are close to "diving" into the Dirac negative continuum.

We calculate the ground-state energy for U_2^{183+} for different internuclear distances in the *monopole* approximation and in the exact two-center potential using the A-DKB method [2] (generalization of the dual-kinetic-balance method for axially-symmetric system). The results are compared with the previous calculation [3, 1].

Correlation effects in atoms play an important role. Taking into account the electronic correlation leads to a significant refinement of agreement with experiment in the calculation of energy levels, transition probabilities and other atomic characteristics. With this in mind, we calculate also the first-order energy correction (so-called one-photon exchange) for electron-electron interaction for two-electron system U_2^{183+} in the monopole approximation.

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Interaction of Light with Hydrogen-Like Ions and Two-Center Systems in the Dipole Approximation and Beyond

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There are a number of infrastructure projects worldwide that strive for higher laser intensities [1]. The treatment of light-matter interaction in a relativistic framework is thus a timely issue. In this paper we consider the processes of interaction of highly charged ions with strong short pulses of coherent laser radiation. Using the relativistic Dirac equation, the energies of bound states are calculated for the hydrogen atom. An algorithm for calculating the ionization probability for two-center systems is developed. In addition, in the dipole approximation and beyond it, the ionization probability for hydrogen exposed to the laser field is calculated and the result is compared with the result of other scientific groups, for example, with [2].

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Comparing Generators of Low-Discrepancy Sequences

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Monte Carlo methods play important role in high-dimensional integration and multiparametric optimization. Classical Monte Carlo method uses pure random dots in computations while Quasi-Monte Carlo method uses members of low-discrepancy sequence in which function is evaluated. It was shown in [1] that Quasi-Monte Carlo method has faster rate of convergence, so, it is important to study the ways of generating low-discrepancy sequences and their properties.

We compare the ease of implementation and efficiency of low-discrepancy sequences by Sobol [2], Halton [3] and Faure [4].

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Interaction between Islands in Artificial Spin Ice

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Artificial spin ice systems make it possible to study magnetic phenomena at various length scales, ranging from atomic to macroscopic. They consist of lithographically patterned magnetic islands arranged in various geometries. The interaction between the islands affects the properties of the artificial spin ice systems and several different ways have been used to model it. The most accurate approach, but also the one that requires largest computational effort, is micromagnetics. In a simpler approach a magnetic dipole is placed at the center of each island and the dipole-dipole interaction evaluated. In the third approach, the dumbbell approximation [1-3], two magnetic charges are placed on each island separated by a distance, *d*. Fig. 1 shows calculated results using the various approaches, including two different choices for *d*, namely *d*=4L/5 and *d*=L, where *L* is the length of the island. In each case the magnetic dipole is the same, consistent with the saturation magnetization of material times the volume of the islands. The different choices of *d* affect the calculated energy of the various states of the system. Our results show that by fitting *d* the dumbbell model can accurately reproduce the micromagnetic calculations.

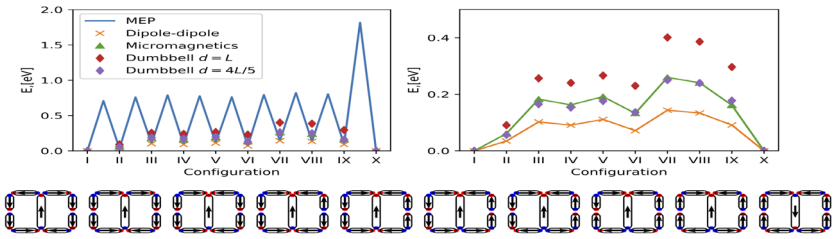

Fig. 1. Minimum energy path (MEP) for magnetization reversal of shakti lattice and the energy calculated using different models in the minima along the path. Configurations at the minima are shown below the graphs. The value of L is 450 nm for the small islands and 1050 nm for the big island.

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A Numerical Approach to Study Light Scattering by Non-Spherical Plasmonic Nanoparticle on the Substrate Accounting for Nonlocal Effect

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Optical properties of small noble metal nanoparticles (NPs) are known to highly depend on their shape, size, and refractive index of the surrounding medium due to surface plasmons, which in its simplest form can be described as the collective oscillations of the conduction electrons bound to a metal–dielectric interface. This feature in many ways defines the common application areas of metal NPs that include sensing, photovoltaics, optical labeling, medical treatment, lithographic fabrication and many others [1-2]. For this reason a lot of research efforts are being put into plasmonic NP design and optimization process creating demand for efficient computational techniques [3].

Current research is focused on the development of the numerical-analytical approach named Discrete Sources Method to solve the large scope of light scattering problems with nonspherical plasmonic NPs as scatters [4]. The proposed approach allows proper account for such effects as size dependent plasmon resonance shifts and intensity changes via Generalized Nonlocal Optical Response theory [5]. We have developed numerical models for such widespread particle shapes as prolate and oblate spheroids, and implemented them into flexible computational algorithms. To illustrate the capabilities of the developed approach we study the scattering cross-section of different NPs deposited on various substrates as a function of wavelength.

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Pseudorapidity Dependence of Multiplicity and Transverse Momentum Fluctuations in PP Collisions at the SPS Energies

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A search for the critical behavior of strongly interacting matter was done by studying the event-by-event fluctuations of multiplicity and transverse momentum of charged hadrons produced in inelastic pp collisions at 20, 31, 40, 80 and 158 GeV/c beam momentum at the NA61/SHINE experiment. Results for energy dependence of the scaled variance of the multiplicity distribution [1] and for two families of strongly intensive measures [2] of multiplicity and transverse momentum fluctuations $\Delta[P_{T},N]$ and $\Sigma[P_{T},N]$ are presented. These strongly intensive quantities are assumed to be independent both of the reaction volume and of the trivial fluctuations of the volume. Therefore, one may expect much higher sensitivity in the search of the critical point. The study was performed in different pseudorapidity regions, which corresponds to changing the baryon chemical potential and the value of temperature at the freeze-out stage. The strongly intensive measure $\Sigma[N_{F},N_{B}]$ [3] was used in the analysis of short- and long-range multiplicity correlations.

Results on multiplicity and transverse momentum fluctuations significantly depend on charges of selected hadrons and width and/or location of pseudorapidity intervals. Monte Carlo event generator EPOS1.99 does not describe the data for the $\Delta[P_{T},N]$ measure. Forward-backward correlations for strongly intensive quantities are also not reproduced by EPOS1.99 bringing new constraints on the theoretical models.

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Properties of Mesons in a Medium with Chiral Chemical Potential

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The study of processes that occur during the heavy-ions collisions at high energies is an important direction of modern physics. In the fireball the matter is in the phase of a quark-gluon plasma. After expansion, which extends a time of 5-10 fm, when the temperature decreases, the substance passes into a hadron phase. The processes occurring in the fireball after hadronization are well described by effective field theories, where mesons become the main degrees of freedom.

The chiral imbalance is a difference between the numbers of right- and left-handed quarks. It is expressed by the appearance of a chiral (axial) chemical potential μ_5. The presence of μ_5 changes the properties of light mesons. In particular, there is a mixing of scalar a_0 and pseudoscalar π mesons. Mesons acquire effective masses that depend on the momentum and a chiral chemical potential. New decay processes appear and the probabilities of already known decays change.

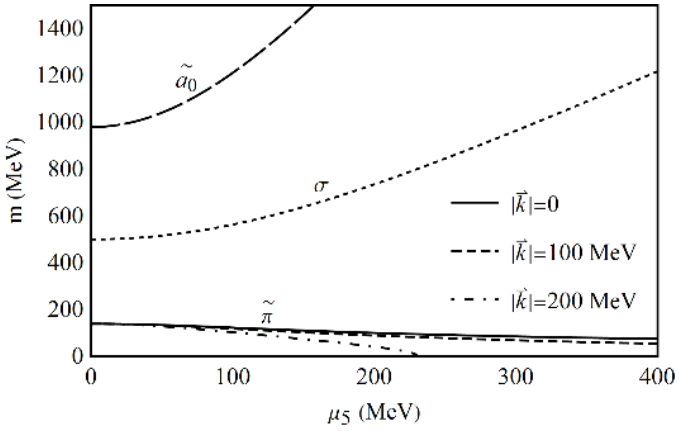

Fig. 1. $\tilde{a}_0$-meson and $\tilde{\pi}$-meson effective mass dependence and σ-meson mass dependence on chemical potential μ_5, for different values of momentum.

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MC Model Studies of Pseudorapidity Dependence of the Average Transverse Momentum of Charged Particles Produced in High-Energy Proton-Proton Collisions

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At sufficiently high temperature and energy density, nuclear matter undergoes a transition to a phase in which quarks and gluons are not confined: the quark–gluon plasma (QGP) Such an exotic state of strongly interacting quantum chromodynamics matter is produced in the laboratory in heavy nuclei high-energy collisions. Quite surprisingly, recently, some effects similar to those observed in heavy nuclei collisions were found in in proton-proton collisions at the LHC [1]. Therefore, the interest of studying of processes taking place in high-energy proton-proton collisions has increased again.

We present here the investigation of rapidity dependence of the average transverse momentum of charged particles produced in high-energy proton-proton collisions. Studies were performed using the Monte-Carlo event generator PYTHIA 8.2 [2] for proton-proton collisions at LHC energies. Different modes of collectivity included in PYTHIA 8.2 were investigated. The average transverse momentum of particles, produced in some pseudorapidity interval, could bring the information on the mean temperature of the particle-emitting source, produced in a given event of high energy proton-proton collision. It was initialy supposed that the average momentum of emitted particles should be the same in the entire pseudorapidity region. Nevertheless, monotonous increase of average transverse momentum with a decrease of the value of the modulus of pseudorapidity over the whole pseudorapidity region was found. The causes of this increse have been studied. It was clarified in the analysis that the observed behavior of average transverse momentum in the entire pseudorapidity region could be explained with the account of two factors: by contribution of jets and due to the effects of kinematic relation between transverse momentum and pseudorapidity.

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Berry Phase for Difference Equations

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We study the difference equation

$$\Psi(z+h) = M(z)\Psi(z), \quad z \in \mathbb{C}, \tag{1}$$

where $h>0$ is a small constant parameter and $M: \mathbb{C} \to SL(2,\mathbb{C})$ is a given matrix valued function. We describe asymptotics of solutions to (1) as $h \to 0$.

Consider solutions to the differential equation

$$h\frac{d}{dz}\Psi(z) = M(z)\Psi(z), \quad z \in \mathbb{C}, \tag{2}$$

its asymtotics as $h \to 0$ are usually called quasiclassical and described using the complex WKB method (see [1]).

Since one can rewrite (1) in the form

$$\exp\left(h\frac{d}{dz}\right)\Psi(z) = M(z)\Psi(z), \quad z \in \mathbb{C},$$

we can consider h as a small parameter in front of the derivative, so h appears to be a quasiclassical asymptotic parameter.

An analog of the complex WKB method was suggested for Harper equation in [2]. We continue to develop the complex WKB method for difference equations (see [3]). Asymptotic formulas for solutions to (1) contain a sort of Berry phase that we discuss in this talk.

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Wave Functions of Doubly Heavy Baryons

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The object of research is the baryons with two heavy quarks which are any combination of *c*- and *b*-quarks. They are of interest from the experimental point of view because several collaborations like SELEX, BaBar, Belle, and LHCb, have searched these particles for a long time. The first double-charmed baryons have been observed in the SELEX experiment at Fermilab [1]. No any other collaboration confirmed the SELEX results until now when the LHCb Collab. at CERN announced the observation of doubly charmed baryons [2].

Dynamically, doubly heavy baryons are similar to heavy mesons. To describe such a baryon, the approximation can be used in which the heavy diquark is considered as a static source, and the light quark only determines completely the baryon dynamics. In this approach, the procedure of constructing the transition matrix elements from the baryonic state to the vacuum is the same as for the heavy meson. Note that the generalization of the local approximation for the diquark to the nonlocal case should be done which is a topic for further investigations.

To remember, the *B*-mesons is the bound state of the heavy *b*-antiquark and the light quark which considered as a massless particle in the infinitely heavy limit of the antiquark. As a result, the light quark is on the light cone and the system is determined by one variable only – the proper time of the heavy antiquark. In the lowest Fock approximation (the two-particle state) for the *B*-meson, there are two functions, called the Distribution Amplitudes (DAs), which determines the dynamics. As the DAs have a non-perturbative nature, one can try to model them. There are some models already suggested in literature from which the exponential model by Grozin and Neubert [3] and the linear model by Kawamura et al. [4] are the most popular. Both are dependent on one parameter only – the hadron effective mass and can be easily adapted for the case of heavy baryons. The scale dependence of DAs is of special interest as it can be calculated perturbatively and is well known for *B*-mesons. In doubly heavy baryons, a scale evolution due to the diquark non-locality is a question.

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Study of Dielectric Properties of Liquid Crystal Coordination Compounds of Lanthanides

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Liquid crystals are a mesophase, emerging in some substances, consisting of elongated molecules, between solid and liquid states [1]. Liquid crystals are widely used in various areas of human activity. Due to the form of molecules forming them, liquid crystals easily change their spatial orientation under the action of an electric field. Lantonide mesogens (Fig. 1) are distinguished for all liquid crystals in that they are just as easily influenced by a magnetic field [2].

One way to study the mutual arrangement of molecules in liquid crystals is to study its dielectric permeability. Analysing the behavior of lantonide mesogen under the action of crossed electric and magnetic fields, it is possible to obtain information about its Frank elastic constants. In a one constant approximation, the distribution of the director for different values of the magnetic field was calculated. Estimates for the Frank elastic constants and the critical magnetic field are obtained based on the experimental data for the dielectric permittivity of the liquid crystal cell as a function of the applied magnetic field. Calculations are performed for the case when the direction of the magnetic moment of the molecules coincides with the direction of the director.

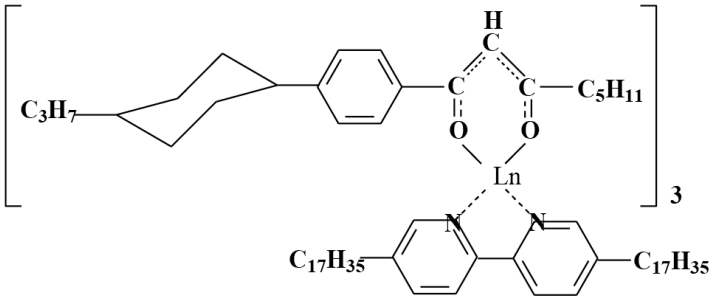

Fig. 1. Lantonide mesogen.

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Stereographic Projection Approach to Dynamics of Skyrmionic Spin Structures

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There is a renewed interest in different topological defects in magnets in recent years [1]. One of the topics of active investigation is skyrmions in two-dimensional ferromagnetic films [2].

In the seminal paper [3] by Belavin and Polyakov (BP) the existence of topological solitons in O(3) sigma-model has been discussed. Remarkably, the energy of the multi-skyrmion state in this model does not depend on the configuration of individual skyrmions, i.e. on their radii and distance between them. In other words, there is no interaction between skyrmions.

We study the extension of this non-linear O(3) sigma-model at T=0, by adding Dzyaloshinskii-Moriya interaction (DMI) and external magnetic field. The analysis is done with stereographic projection approach, by describing the magnetization vector field as to complex-valued function. We write a variational equation for the energy. First we find a numerical solution for individual skyrmion, which is of BP type with additional profile factor appearing due to DMI and the field. We model the pressure on the skyrmion from others by confining the central skyrmion to a disk of finite radius. For various disk radii the profile function shows a scaling property, dependent mostly on the ratio of the distance from the skyrmion's center to its size, the latter defined by the radius of disk. Many-skyrmion configurations are obtained as simple sums of stereographic projections of single skyrmions whose size is obtained variationally. Proceeding this way, we calculate the interaction between two and three single skyrmions and find an optimal configuration of a skyrmion lattice (SkL). We find that the triple interaction is sizable as compared to pairwise soliton interaction. The system is thus not reduced to an analog of Coulomb gas with screened repulsion.

The dynamics of individual skyrmions is discussed in Lagrangian formalism in terms of collective variables of skyrmions radii and positions of centers. In that way we can study the dynamics of a single skyrmion, the motion of a pair and dynamics of SkL.

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Solving the Shrödinger Equation with Neural Networks

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Neural networks based approaches are broadly used to solve many engineering problems. Generally, the neural networks can be applied for approximation of unknown functions in equations of mathematical physics. This approach makes it possible to construct universal and effective approximants that ensure reduction in the number of operations when working with many degrees of freedom. The task of using highly effective engineering software frameworks for solving the equations of mathematical physics (the Schrödinger equation, for instance) arises.

We evaluate the neural network approach for solving the stationary Schrödinger equation proposed by Lagaris [1]. The neural network is trained by minimizing the residual function defined on a coordinate grid.

In calculations, the machine learning Python library Theano is used. The results of solving a one-dimensional problem are presented for different optimization methods. An additional analysis of the residue gradient made it possible to simplify the computations by gradient methods considerably.

The results of solving a one-dimensional problem for various methods of minimizing the functional are presented.

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Non-Stationary Model of Radial Temperature Distribution of Open-air Arc

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Today smart grids technologies are becoming increasingly popular. An integral part of such smart networks is fault-protection systems. Arc-fault is a common phenomenon emerging in overhead transmission facilities. To identify and localize such faults, the time dependences of voltage and current are needed. So, the development of a non-stationary open-air arc model is a problem of current topicality in terms of fault-protection algorithm testing.

The conductivity of LTE plasma channel is determined by its temperature distribution, which is calculated in our model using Elenbaas-Heller non-stationary equation [1] with boundary conditions at zero and infinity, allowing for radiation and convection. This approach describes the arc phenomenon in the best way from the physical point of view and minimizes the number of parameters that need to be determined in contrast to conventional models [2]. The obtained numerical results (Fig. 1) are

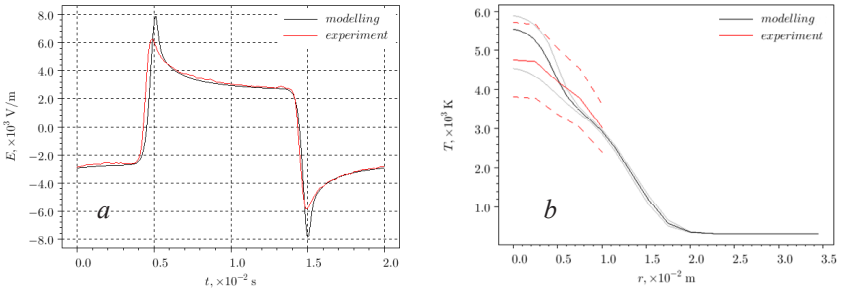

Fig. 1. Comparison of the experimental (red) and simulation data (black): a) voltage-time dependence, b) temperature profile.

in a good quantitative agreement with available experimental data [3].

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Evaluation of the Two-Photon Exchange Diagrams for Heavy Ions and Quasimolecules

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Within the framework of quantum electrodynamics, the interelectronic interaction in the first and second orders of the perturbation theory is described by the diagrams of one- and two-photon exchange. These diagrams suffer from the infrared divergencies – singularities that arise when integrating over the low-energy region of virtual photons. We regularize these divergencies by introducing a finite photon mass into the photon propagator. Infrared-divergent terms can be treated analytically to obtain the finite result for zero photon mass [1, 2]. Instead we perform the numerical calculations for the finite photon mass for the case of lithium-like ions.

We also consider correlation effects in homonuclear two-electron molecular ions (quasimolecules). We calculate the energy shift due to one- and two-photon exchange in the monopole approximation. These results are in demand for interpretation of the quasimolecular radiation spectra observed in heavy-ion collisions [3].

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Instantons in Magnetic Systems

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Instanton theory is the basis of an efficient approach for describing tunneling and estimating tunneling rates. Instantons are stationary points on the action surface and for particle systems, they correspond to first order saddle points on the action surface. For magnetic systems, the action is complex, containing both real and imaginary parts [1]. In order to find instantons, it is then necessary to search more generally for stationary points on the complex action surface.

The method developed involves finding minima of the magnitude of the gradient of the action, a real-valued objective function. This requires an analytical continuation of the energy function. First, the instanton is found for zero temperature since then it corresponds to the equipotential contour for the energy of the initial state [2]. Then, the temperature is increased in small steps and BFGS method used to reconverge on the instanton for each temperature value.

The method is illustrated using a system consisting of a single spin with uniaxial anisotropy in transverse magnetic field, but it can be used for any magnetic system, even when the energy is obtained from a self-consistent calculation. The figure below shows examples of calculated instantons and the activation energy for thermally enhanced tunnelling obtained from such calculations. In this case, the crossover from over-the-barrier mechanism to tunnelling is gradual (second order crossover), but in some other cases, the crossover is abrupt and the tunnelling rate nearly temperature independent (first order crossover).

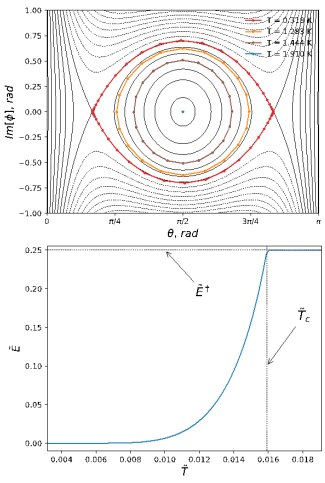

Fig. 1. Results for a single spin with uniaxial anisotropy and transverse magnetic field. Top: Instantons at a few T values. Bottom: Activation energy vs. T (scaled units), where T_c denotes crossover, 1.91 K. Above T_c the activation energy is obtained from 1st order saddle point on the energy surface.

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Influence of Nanoparticle Surface Modification on Structural and Dynamical Properties of P3HT-Fullerene Nanocomposites: Molecular Dynamics Simulations

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Fullerene-based organic solar cells attract wide attention due to their promising ability to replace conventional silicon-based photovoltaic devices. Nowadays, the upper bound of their power convergence efficiency has reached the level of 8-9 %. However, complex understanding of the factors controlling their performance is required to increase the efficiency towards higher values.

In the current work we simulate structural and dynamical properties of fullerene-based nanocomposites based on poly-3-hexylthiophene (P3HT). Firstly, we compare the results on dynamical properties of single fullerenes ~~то~~ with the available experimental data. Good qualitative and quantitative agreement between simulational and experimental results is observed. Then, we estimate how dynamical properties of P3HT-fullerene systems depend on surface modification of nanoparticles and their mass fraction in the nanocomposite. By performing fully-atomic molecular dynamics simulations on microsecond time-scale we compute mean-squared displacement of center-of-masses both for polymer chain and fullerene. Obtained results reveal that polymer motion in nanocomposites is significantly affected by the surface modification of fullerenes. Despite additional interactions and geometrical restrictions imposed by the presence of a grafted tail on the surface of PCBM molecules, their addition results in enhanced mobility of P3HT chains. The effect is even more unexpected since glass transition temperature of both nanocomposites (having C_{60} or PCBM as nanofillers) is essentially the same. Two possible explanations for the observed effect should be mentioned: (a) the reduction of surface area of nanoparticles, providing «π-π» interactions between rings of the polymer backbone and nanoparticles surfaces; (b) differences in structural agglomeration of the nanoparticles in the fullerene phase. To provide insights into the role of each of these two factors further investigations are planned.

This work was supported by the Russian Foundation for Basic Research (grant № 15-03-07614). All the simulations have been performed using the computational resources of the Institute of Macromolecular Compounds, Russian Academy of Sciences, Lomonosov-2 supercomputer at Moscow State University, and resources of the federal collective usage center Complex for Simulation and Data Processing for Mega-science Facilities at NRC “Kurchatov Institute” (http://ckp.nrcki.ru/).

H. Biophysics

Molecular Characteristics of Comb-Like Polyelectrolyte with "Tailed Counter-Ions" in Solution

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Research of materials based on self-organizational polymer systems is one of the topical problems in the modern world. The main structural unit used in the self-organization of complex macromolecular systems in solutions are polyelectrolytes. The formed polyelectrolyte complexes are widely used as drug delivery systems, materials for pervaporation membranes, nanofiltration, fuel cells etc.

Present work is devoted to investigate of self-organizing structures of comb-like polyelectrolyte poly-11-acryloyl-oxyundecyl-trialkylammonium (pAUTA+) with "tailed counter-ion" (aliphatic carboxylate (C6, C10)) in solutions (Fig. 1). Objects were investigated by molecular hydrodynamics methods: viscometry, refractometry, densitometry, dynamic light scattering and sedimentation velocity. The values of intrinsic viscosity, diffusion coefficients and sedimentation constants were found. The molecular masses, calculated from experimental data of sedimentation velocity and dynamics light scattering, were compared. The values of the hydrodynamic invariant were obtained for all objects under investigation. The obtained results were analyzed.

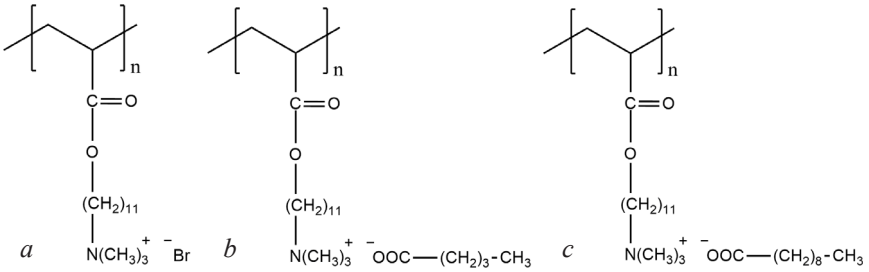

Fig. 1. Structures of pAUTA+ (a), pAUTA-C6 (b) and pAUTA-C10 (c).

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Computer Modeling of Poly-Glutamic Acid Conformational Structures in Electrolyte Solutions

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Polyglutamic acid (PGA) is water-soluble ionic polypeptide widely used in the industry and medical applications due to its chelating power. Atomistic computer simulation is a useful method to investigate molecular mechanisms of chelation. One of the key issues for simulation of PGA in electrolyte solutions is correct modeling of its conformational behaviour. Different molecular dynamics force fields can lead to different results. We performed simulations using CHARMM-27 and AMBER99SB-ILDN force fields, which give the best agreement with experimental data on conformation of peptides [1, 2].

Results of previous works dedicated to the molecular dynamics simulations of the PGA conformational behavior in monovalent salts (NaCl, KCl) solutions [3] differed for these two salts. Moreover, the choice of the counterion type for simulations in pure water should have influence on the PGA conformational structure. Investigation of this influence is the main goal of our work. In this study molecular dynamics simulations of single poly-α-L-glutamic acid chain in water were carried out with two different types of counterions (Na or K).

The information on the counterion distributions around the polymer chain as well as various conformational characteristics were obtained. Results of our simulations were compared to experimental data [4] based on measurements of UV resonance Raman spectra of PGA water solution. It was concluded that the system with potassium counterions simulated with CHARMM-27 gives the best agreement with corresponding experimental data.

All simulations was performed with the computational resources of Center of collective use "Complex of modeling and data research mega-class facilities" NRC "Kurchatov Institute". Unique identifier RFMEFI62114X0006.

This study was supported by the Russian Ministry of Education and Science within State Contract 14.W03.31.0014 (megagrant).

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The Equilibrium and Kinetic Rigidity of Additive Silicon-Containing Polytricyclononenes

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Selective polymeric membranes have become widely used for a variety of industrial gas separations applications. Recent development of synthesis of addition-type poly(trimethylsilyl)tricyclononenes) (PTCNs) resulted in obtaining the polymers giving a highly gas-permeable thin films [1, 2]. As thermally stable polymers, PTCNs can be applied as the membrane materials for separation of natural and associated petroleum gases [1]. Permeability of PTCNs thin films depends on quantity of side trimethylsilyl groups $SiMe_3$ in the polymer chain. Coefficients of theirs permeability are increasing with a total number of silicon atoms per macromolecule, and depending on position of $SiMe_3$ in the structure of monomer unit. The reason of such dependence has not been understand in full measure. At the present work three homologous series of silicon-containing polytricyclononenes samples (Fig. 1) have been studied. Static and dynamic light scattering, NMR spectroscopy and viscometry methods have been applied for the analysis of molecular properties of PTSNs.

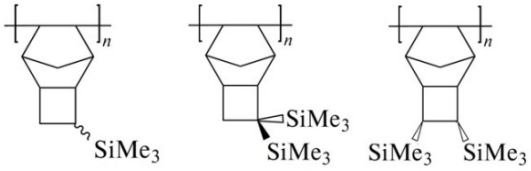

Fig. 1. The chemical structure of a new additive polytricyclononenes.

Scaling relationships, equilibrium chain rigidity and kinetic properties of polymers have been determined. The uniqueness of molecular properties of PTCN-samples with the germinal position of two trimethylsilyl ($SiMe_3$) side-groups in comparison with two others PTCNs was identified [3, 4]. The films of PTCN with the germinal position of substituents $SiMe_3$ demonstrate the highest gas permeability parameters. The linkage of molecular and thin film properties of the studied polymers has been detected.

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Comparative Study of the DNA Irradiated with Proton Particles and Gamma Radiation

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Radiation therapy (radiotherapy) plays an important part in the treatment of malignant, as well as many nonmalignant neoformations. The main goal of the radiation therapy is to transport a high radiation dose to the tumor, with minimal or, ideally, no impact on normal tissues and organs. Radiation therapy uses high-energy radiation to shrink tumors and kill cancer cells. X-rays, gamma rays, and charged particles are types of radiation used for cancer treatment. [1]. Radiation therapy kills cancer cells by damaging their DNA [2]. The most frequent types of radiation-induced DNA damages are modification and destruction of nitrogenous bases and also local breakages of hydrogen bonds (partial denaturation) in the lesion sites of the macromolecule [3].

One of the most sensitive methods for revealing alterations in DNA primary and secondary structure is DNA melting [4]. Heat denaturation of DNA (melting) causes the double helix structure to unwind to form single stranded DNA. The most common method is measuring of UV-absorption in DNA solution at 260 nm as a function of temperature.

In this study, aqueous-salt DNA solutions of the ionic strength 5 mM NaCl exposed by proton particles and gamma-radiation with the doses D=0-100 Gy has been taken to compare. DNA melting curves were measured in these solutions and DNA melting temperatures (T_m) which characterize a middle point of the "helix-coil" transition were obtained. Both proton particles and gamma-irradiation causes decrease of DNA T_m. It was found that T_m, the concentration of nucleobases and total hyperchromic effect in the solutions irradiated with proton particles smaller than that irradiated with gamma for D<100 Gy. It is meaning that DNA damage induced by proton particles higher than that induced by gamma irradiation. So the higher DNA damage with proton particles make it better than from gamma radiation used in radiation therapy.

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Investigation of Relaxation Time Spectra of Comb-Like LC Polymers in Isotropic Melts by Kerr Effect Method

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In the work, molecular orientational relaxation processes in melts of liquid-crystalline comb-like homopolymers and copolymers in an electric field were investigated by electric birefringence method. As we have recently shown [1] the equilibrium electro-optical properties of copolymers and their orientational dynamics are well described by the Landau - de Gennes model, but for the dynamic properties this is valid only near nematic - isotropic phase transition temperature T_c. In the temperature range of 10-15 degrees above T_c we found a sharp change in the temperature dependence of the relaxation times of induced macroscopic orientational order.

According to the proposed model [1], a rapid decrease in the macroscopic relaxation times in the liquid crystal polymers with distance from T_c is expected effect in comb-like polymeric systems. It is associated with a decrease in the contribution of the polymer chains in the macroscopic dynamics with decreasing of correlation length. In this paper, we study the orientational dynamics of the isotropic phase in comb-like LC polymers [2] and in LC copolymers with acid groups. It was established that the integral relaxation time has non-classic temperature dependence for smectic polymers as well as for nematics. Analysis of the obtained data made it possible to identify several relaxation processes in the relaxation spectrum, which can be associated with different mechanisms of molecular mobility. The variation of melt temperature led to significant changes of the ratio between contributions of observed relaxation processes. The experimental results agree well with our model used for this phenomenon [1].

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Computer Modeling of Phospholipid Membranes at Different Resolution

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Phospholipid membranes are often considered as models for cell membranes as they are able to mimic the membranes' structural properties. More complex considerations include the interactions of model lipid membranes with various polymer and biopolymer agents such as dendrimers, linear synthetic polycations, DNA, proteins and cellulose, the latter is especially important in view of the development of wound dressings. Here we employ molecular dynamics simulations to study a dipalmitoylphosphatidylcholine (DPPC) lipid membrane with the use of models of different resolution. Considered are full-atom, united-atom and coarse-grained membrane models (force-fields). For each force-field we calculated and systematically compared the following set of structural characteristics: the area per lipid, the order parameter of the acyl lipid chains, and the component-wise mass density profiles. The computational results were compared with existing experimental and simulation data and the conclusions were made regarding the reliability/performance of the models considered. These findings will be used in the future for computer modeling of hybrid "lipid-cellulose" systems.

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Studies of Sup35 Prion Protein Aggregates Using Scanning Tunneling Microscopy (STM), Atomic Force Microscopy (AFM) and Surface-Enhanced Raman Spectroscopy (SERS)

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Prions are special class of infectious agents that have protein nature. They are aggregates of functional proteins, which have an abnormal tertiary structure with predominance of β-layers. Prions are the causative agents of incurable and fatal human diseases (the Creutzfeldt-Jakob disease, the fatal familial insomnia, etc.) and animals diseases (the sheep scrapes, the cow rabies, etc.). These diseases relate to «conformational» and they are a part of human diseases caused by amyloids (the Alzheimer's, the Parkinson's, the Huntington's diseases). All prions cause the formation of amyloids, which are deposited in various organs and tissues. The understanding of the prions structure and propagation pathways are of fundamental interest. Prions propagate by imposing their conformation on normal cellular proteins, leading to the formation of misfolded aggregates (strains) and, ultimately, to neurodegeneration. Consequently, the formation of different strains by the same prion protein with the uniform primary sequence present scientific interest. Knowledge about the prion structures is limited [1, 2].

The yeast prions is a convenient model system for study of prions. In the work the prion form of Saccharomyces cerevisiae yeast Sup35 (eRF3) protein was used. Fibrils of this protein were immobilized on various substrates, and studied using atomic force microscope (AFM), scanning tunneling microscopy (STM), and surface-enhanced Raman spectroscopy (SERS). SERS study of fibrils allowed to conduct the analysis of fibrils conformations.

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Investigation of Plastic Rearrangements of Interneuronal Connections in Conditions of Modeling Acetylcholine Deficiency in Rat Hippocampus *in vitro*

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Acetylcholine is one of the main neurotransmitters of the central nervous system, affecting its functioning. It is believed that the release of acetylcholine in the hippocampus affects the storage of information and its extraction from memory, and these processes depend on the concentration of the neuromodulator [1-3]. Decreased activity of cholinergic neurons or their death lead to severe disorders, including fatigue, depression, memory impairment in Alzheimer's disease.The aim of the study was to study the character of the long-term changes in the efficiency of interneuronal connections in the hippocampus under the conditions of modeling the acetylcholine deficiency.

To solve this problem, sections of the hippocampus of rats were subjected to prolonged incubation in a solution with an increased concentration of K +, at which the sodium-potassium pump function was disrupted and acetylcholine ceased to separate from presynaptic vesicles. It was found that an increase in the concentration of K + in the hippocampal washing sections of rats in a solution up to 25 mM (at a concentration of 5 mM) in just 2-3 minutes leads to a significant depolarization of the cells of the hippocampal CA1 field. At the same time, all acetylcholine, norepinephrine and dopamine are emitted from the cells. New neurotransmitters do not arrive, because the way from the septum is cut off.

Changes in the efficiency of synaptic transmission were assessed by the dynamics of changes in the venous insufflation. The amplitude of EPPS after the influence of high-frequency stimulation in the control and in experiments with cholinergic deficiency did not differ significantly. Based on the results obtained, it was suggested that Alzheimer's disease disrupted the connection between the hippocampus and the cortex, while the functioning of the hippocampus did not change.

The work was supported by the grant of the RNF 16-15-10403 "Consequences of cholinergic hypofunction in the brain: transcriptomal analysis and functions of neurotrophins".

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The Study of the Hydrodynamic Characteristics of Polymer Nanostructures Based on Poly-11-Acrylamidoundecanoic Acid and its Sodium Salt

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Surfactant polymers are capable of forming intra- and intermolecular organized structures (e.g., micelles) receive great attention from researchers working in the field of polymer science. The reason for this interest is the ability of self-organization which is inherent to most biopolymers.

In recent years polymerizable surfactants engendered great interest due to their wide application possibilities. For example, they may serve as components of the pseudo-stationary phase of the micellar chromatography, drug carriers, and "building blocks" for the molecular design of nanoparticles and nanostructured polymeric materials.

Poly(N-acryl-11- amidoundecanoic acid) (PAAU-H) and its sodium salt (PAAU-Na) represent very promising materials for molecular cores in constructing nanoparticles with surface functional groups. Typically they are used for encapsulation of various biological preparations. The influence of quantity of cross-linker incorporated in polymerized micelles (form 5 and up to 15 mole percent) was studied by means of hydrodynamic methods to determine the conformational status of the polymerized micelles. This goal was achieved by polymerization of the AAU-Na in the presence of a rigid short crosslinking agent - methylene-bis-acrylamide.

Particular attention was paid to the analysis of both the size and the shape of the formed particles by using unique combination of methods of molecular optics and electro-optics. The influence of intra- and intermolecular crosslinking on physical properties of nanoparticles was studied. The influence of the share crosslinking agent characteristics and conformational of "cross-linked" polymerized micelles was investigated.

The Application of in Silico Methods for Design of Effective Voltage-Dependent Rhodopsin for Optogenetic Studies

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Using the combination of optical and genetic approaches for control of physiological processes is a wide area of science with a huge number of possible important applications. One of the possible approaches in this field is using fluorescent voltage-dependent proteins for the detection of neuronal activity. It has been recently demonstrated that several proteins from rhodopsin family, e.g. archaerhodopsin-3, can be used for solving this kind of problems [1]. However, these sensors need to be optimized. For example, red-shifting their absorption spectrum will allow to obtain signals from deeper tissues.

Luckily, the progress of computational methods has recently allowed revealing the mechanisms of different molecular processes in proteins. These methods need a high quality three-dimensional structure of the studied protein. This is often an extra obstacle because of the absence of crystallographic data, especially for membrane proteins.

In this work we have used computational methods for studying the features of achaerhodopsin-3, Gloebacter violaceus rhodopsin [2] and their mutants. On the first stage we have worked out the methodic for three-dimensional structure prediction of these proteins on the base of homologous rhodopsins with the structure obtained experimentally. Using this methodic and the methods of hybrid QM(ab initio)/MM modeling we have performed computational screening of spectra of 70 different mutants of Gloebacter violaceus rhodopsin. The results of the computations are in good agreement with the analogous experimental screening, which proves the quality of our models and shows the opportunity of computational design of rhodopsins with the absorption in the desired spectral range.

The results of this work will be used for the subsequent computational design of archaerhodopsin-3, Gloebacter violaceus rhodopsin and other rhodopsins of interest with the absorption range in the desired region.

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Hydrodynamics Properties of Chitosans from Various Natural Raw Materials

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Polysaccharides chitin and chitosan are now widely used in cosmetology, pharmacology, medicine, food industry and other industries. This is explained by the availability of natural raw materials for their isolation and production, as well as the complete biocompatibility and non-toxicity of both these polysaccharides and their derivatives [1]. Over the past decade, chitosan has found many new applications in modern biotechnologies, such as tissue engineering, drug delivery systems, gene therapy, and others [2]. The goal of the study was to investigate the influence of chitosan molecules hydrodynamics properties on their film-forming ability. For this purpose, samples of chitosan from different raw materials with a high degree of deacetylation were investigated. The hydrodynamic parameters of the chitosan macromolecules in dilute solutions were obtained by using viscometry, dynamic light scattering, methods of translational diffusion and velocity sedimentation. It was shown that hydrodynamics properties of chitosans are more dependable on the samples nature than their conformational properties.

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Some Aspects of Synthesis of Fluorescent Silver Clusters on Proteins of the Albumin Group

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Silver clusters stabilized with a biopolymer matrix represent a new class of fluorophores with many positive characteristics. Among them, high quantum yield of luminescence, high photostability, low level of intoxication and high biocompatibility are of importance for bioimaging applications [1].

The use of proteins as a stabilizing matrix provides several advantages in comparison with DNA. Silver clusters, stabilized in this way, can penetrate cells through membranes without disturbing their integrity. This, in turn, opens up new horizons in the use of clusters as fluorescent biolabels in living cells.

In the framework of this work, I carried out photophysical studies using proteins of the albumin group as a stabilizing matrix (Fig. 1). In addition to the photophysical properties of the obtained complexes, their synthesis conditions were also optimized. Concentration of reagents, pH of the environment and other conditions were varied in a wide range. The obtained results allow answering some questions in this direction, and also setting new interesting tasks in this area.

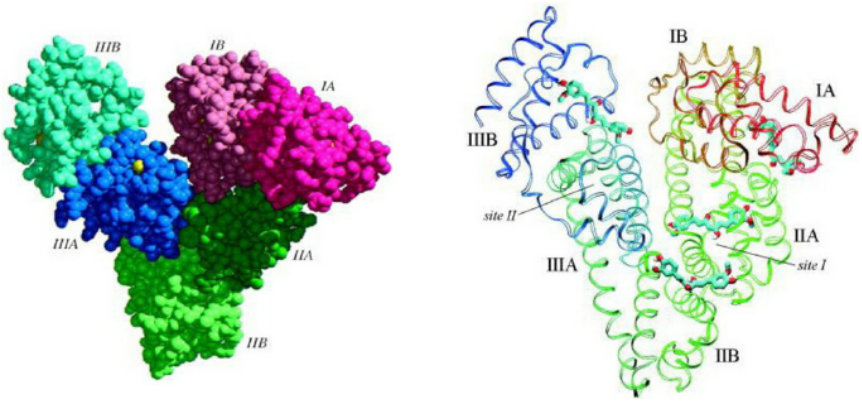

Fig. 1. Structure of BSA and HSA [2].

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FTIR Investigations of Secondary Structure of HSA in Different Ph Conditions

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Human serum albumin is a main protein of blood plasma. It is used as a model protein due to its accessibility. HSA is a main transporter of ligands, so study of serum albumin interactions with biologically active agents and drugs are important. Investigations of changes in HSA secondary structure under different pH conditions can give us understanding of mechanisms of its behavior in blood. FTIR spectroscopy is a sensitive method for studying alterations in percentage of alpha-helixes and beta-structures of HSA in solutions with different pH.

In our research we obtained spectra of dialyzed HSA solution with various concentrations of acid (HCl) and alkaline (NaOH) and in every spectrum we've isolated the Amid I band, which corresponds to the vibrations of C=O, N–H and C–N bonds and is most useful for the analysis of the secondary structure of proteins [1]. The decomposition of this band to Gaussian contours components was done. As a result we have dependence between pH values and alpha-helicity.

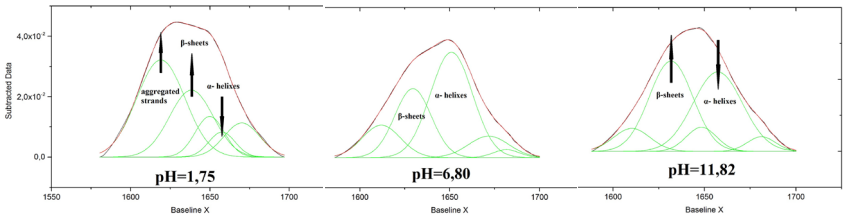

Fig. 1. Examples of decompositions of Amid I band.

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Diagnostics of Anoxygenic Phototrophic Microorganisms in Several Stratified Reservoirs Using Bacteriochlorophyll Fluorescence Deconvolution

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The natural stratified reservoirs found in different stages of isolation from the White Sea are a special group of hydrological objects. Their origin and evolution are associated with the elevation of the Kandalaksha Bay coast with the speed of ~4 mm per year [1]. In aquatic ecosystems with restricted water circulation the anoxygenic phototrophic microorganisms like green sulfur bacteria (GSB) may be of particular interest. These bacteria do not produce oxygen because they utilize hydrogen sulfide instead of water in the photosynthesis; they can habitat the anaerobic part of photic zone [2]. Photosynthetic pigments of green sulfur bacteria are bacteriochlorophylls (BChls) and carotenoids. The optical properties of these pigments make possible studying of phototrophic microorganisms using spectral methods. We conducted the hydrological measurements and spectral analysis in several relic lakes located at the coast of the Kandalaksha Bay: Trekhtzvetnoe, N. Ershovskoye, Lagoon on the Cape Zeleny and Bolshie Khruslomeny. The comparison of the obtained results for natural water with the spectra of monocultures demonstrated the presence of GSB cells in anaerobic layers of the lakes near the chemocline and below. We developed spectral method to found out the ratio of two forms of GSB in water sampled from various depths. We found that deconvolution into three Gaussian curves fits well the shape of BChls fluorescence in GSB emission spectrum excited at 440 nm [3]. The parameters of approximating curves vary for two forms of GSB: the wavelength of fluorescence maximum is ~760 and ~745 nm, the bandwidth (56,9 ± 1,4) and (46,5 ± 0,5) nm for green- and brown-colored bacteria respectively. This result was confirmed using an optical microscope and the data of the cell concentration; we estimated the number of BChl molecules per cell in each form of green sulfur bacteria.

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I. Resonance Phenomena in Condenced Matter

EPR Study of Copper Complexes in Mordenites

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Copper-exchanged zeolites are promising heterogeneous catalysts for removal of nitrogen oxides from exhaust gases (de-NO_x catalysts) [1] and other industrial processes. Gradually increasing restrictions on the concentration of nitrogen oxide emissions require improving the performance of existing catalysts and developing new ones. Catalytic properties of copper-exchanged mordenites are governed by the valence state of copper ions, their location and coordination in the zeolite lattice, copper loading, and others [2, 3], which are determined by the preparation method. Water molecules, which easily enter inside zeolite channels and encircle copper ions separating them from channel walls, are another crucial factor that influences (as a promoter of many physical and chemical processes in porous materials) properties of copper-exchanged zeolites. And so it is very important to study how the level of hydration and the way of water removing affect the catalytic activity of zeolites.

The aim of this work was to study the influence of the preparation method, conventional and microwave assisted (for more details on the preparation method see [4]), and the hydration level on the states of copper and its environment in the mordenite matrix before and after dehydration.

Electronic Paramagnetic Resonance, as a powerful tool for studying the local environment of paramagnetic species, was used to probe the surrounding of copper ions in the studied mordenites. We mainly investigated the copper ions in $[Cu^{2+}(H_2O)_n]$ complexes, as only they are detectable by the method.

The EPR study reveals that upon dehydration those Cu^{2+} ions losing their water surrounding approach to the zeolite wall forming a virtual bond with charge transfer from the framework oxygen to Cu^{2+}. This charge transfer process is reversible and rehydration recovers the coordination of Cu^{2+} ions.

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Molecular Mobility in Imidazolium Liquids as Studied by NMR

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Ionic liquids (IL) are ionic compounds that are characterized by a melting point below 100°C. Cations mainly determine physical properties of IL (melting point, viscosity, density), whereas anions determine chemical properties. Since the physical and chemical properties of ILs can be adapted to the specific conditions by careful selection of types of cations and anions, ILs have become widely used in many scientific and industrial applications (electrochemistry, synthesis, processing) [1, 2]. This study is directed to clarifying the difference in molecular mobility of ionic liquids of different types (BMIM (butyl-methyl imidazolium) with 6 types of anions (Cl, Br, I, BF4, TfO, NO3)) as well as to the determination of the effect of water on the molecular mobility in the indicated ILs using NMR techniques. Fig. 1 shows the temperature dependences of diffusion coefficients for series of dry samples with various anions.

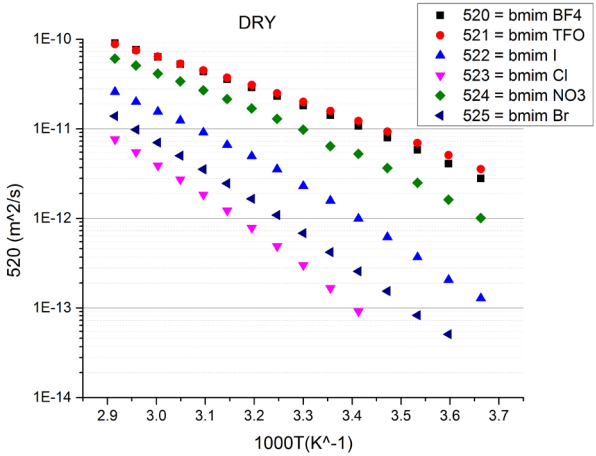

Fig. 1. Temperature dependences of diffusion coefficients in dry ILs.

The work is supported by the RFFI grant 17-03-00057.

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Probing of Outer Electronic Shell of Strong CH-acids by 3He Atom

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The features of electronic shells of molecules and ions have a significant effect on the formation of noncovalent interactions. Recently, research of noncovalent interactions, particularly, of hydrogen bonds, have been focused on searching of parameters that could describe features of the electron shell of isolated molecules and allow predicting such characteristics of intermolecular interactions as geometry and binding energy [1, 2]. Function of the molecular electrostatic potential [3] and electron localization function [4, 5], calculated with quantum-mechanical methods, were proposed as such parameters. However, all these parameters are immeasurable. Therefore, it seems interesting to find such parameter that, on the one hand, would be potentially measurable, and, on the other hand, would be sensitive even to small changes in the electron shell.

The aim of this work is to test a new method of electronic shell description by using a helium atom as a probe. Calculated contour maps of interaction energy of investigated molecules with helium atom and maps of helium chemical shift were plotted. Calculation of the interaction energy surfaces were carried out by the Meller-Plesset method of the second order (MP2/6-311++G(d,p)). The NMR parameters were calculated at the B3LYP level, using the pcS-2 basis set.

As the investigated objects for this study we have chosen three strong CH-acids with different hybridization states of a carbon atom: fluoroacetylene FCCH (*sp*), trifluoroethylene C_2HF_3 (sp^2) and fluoroform F_3CH (sp^3). The structures of these molecules are shown in Fig. 1.

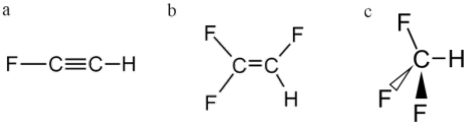

Fig. 1. Structures of (a) fluoroacetylene, (b) trifluoroethylene, (c) fluoroform.

This work was supported by RFBR grant 17-03-00497.

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Diffusion and Perfusion Imaging

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By the present day, MRI (Magnetic Resonance Imaging) has evolved to the most important non-invasive diagnostic technique.

In addition to T1- and T2-weighted contrast achieved by continual anatomical MRI, other unique contrast mechanisms such as DWI (Diffusion-Weighted Imaging) and PWI (Perfusion-Weighted Imaging) have revolutionized detection of pathologic conditions, for example, such as in stroke, inflammatory processes. These techniques have demonstrated great promise in tracing the links between tissue microstructure, metabolism, hemodynamics. They have thus furthered understanding of the pathophysiology of various disease processes and how best to detect these abnormalities [1].

Although diffusion and perfusion are often conceptually mixed, they actually refer to different phenomena. The random motion of water molecules inside a medium, due to their thermal energy, is described by the "Brownian" law. Diffusion is considered the result of the random movement of water molecules. Perfusion, in contrast, relates to blood delivery to the tissues.

The characterization of tissues microstructure, based on water diffusion and perfusion findings, results in increased diagnostic value. It is hoped, that many more technical improvements will occur in these areas that may further help improve diagnosis and treatment [2].

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Water Localization, Kinetics and Dynamics in Sodium and Copper-Exchanged Mordenites

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The study of the localization of water molecules and their dynamics in zeolites, especially if we speak about temperature changes, are of great interest. One of the application of copper-containing zeolites is the using them for removal of nitrogen oxides from exhaust gases (de-NO*x* catalysts) [1]. Moreover, the distribution and the interplay of the exchangeable cations with the framework in zeolites are influenced by water content [2].

In this research the kinetics of water desorption and translation dynamics were studied in Na- and Cu-mordenites with different copper exchange degree (for more details see Ref. [3]). The thermogravimetric analysis (TGA) was carried out to study the dehydration process. The behavior and distribution of water molecules in zeolites with different hydration level were determined using proton nuclear magnetic resonance (NMR) spectroscopy and diffusometry.

In the agreement with TGA data, the ^{1}H NMR spectra of non-annealed samples can perfectly be fitted by two Lorentzian lines with different chemical shift and linewidth, which we will call L1 and L2. These two lines coincide with the two steps of water release that we attribute to the water molecules in the main channel (L1 for the both Na- and Cu-mordenites) and the water molecule in the side pocket (for the Na-mordenite) or the water molecules that are coordinated with Cu^{2+} cations.

The diffusion measurement proved that in Na-mordenite the diffusion character below 300 K is essentially intracrystalline, whereas above 300 K it becomes intercrystalline. The activation energy for the intracrystalline diffusion is 25.6 ± 0.5 kJ/mol, that is close to the values 20 kJ/mol determined from relaxation measurement [4]. The activation energy of intercrystalline diffusion is about 28 kJ/mol and does not depend on the Na/Cu ratio and is governed, we suppose, by the morphology of the sample.

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Quality Assurance for Diffusion MRI: Phantoms

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The first paper which was the origin of Nuclear magnetic resonance imaging (MRI) was published in 1973 [1]. Since then, MRI has gained vast significance in various fields of science applied to visualization of internal object structures, particularly, clinical practice and biology.

One of the important aspects of MRI is construction and usage of phantoms – special objects which imitate properties of more complex biological samples (for example, human body tissues). Phantoms are widely used for testing new hardware and software of an imager, modeling pulse sequences and also for image comparisons (in experiments performed in different conditions) [2].

In this overview report main requirements for phantoms in diffusion MRI will be considered, particularly in such important applications of diffusion MRI as Diffusion tensor imaging (DTI) and High angular resolution diffusion imaging (HARDI). The issue will be considered concerning two basic diffusion MRI characteristics: mean diffusivity (MD) and fractional anisotropy (FA) [2]. We will give pros and cons of common phantom construction techniques and basic materials most suitable for this purpose. Additionally, some known examples of phantoms will be presented.

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The Hydration Properties of $[EMIm]^+$, $[BMIm]^+$, $[HMIm]^+$ and $[OMIm]^+$ Cations as Studied Using DFT Calculations

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Ionic liquids (ILs) are solvents that are utilized in chemical synthesis, electrolyte devices, separation, catalysis and various other areas [1]. The ILs with cation based on imidazole ring are widespread and offer the ability to tune their parameters by changing the length of alkyl chain and combination of cation-anion pair. The significant attention is brought to studies of mixtures of ILs with water. It was found that ILs in many cases recapitulate the properties of surfactants. However, the concentration, at which ILs self-organize, does strongly depend on the types of ions and the length of alkyl chain.

Here we report the study of four cations of ILs using the density functional theory (DFT) calculations. Chosen solute molecules have different length of alkyl chain ranging from 2 to 8 carbon atoms. Initial orientations of water molecules around ILs were generated using docking software AutoDock vina. The quantum chemical calculations were performed using the dispersion corrected B3LYP functional [2,3] and 6-31+G(d,p) basis set for "solute – water" complexes (up to 75 water molecules). The optimized geometries were used to calculate electric field gradients, charges, vibrational frequencies and other parameters. The obtained data provide the basis for validation of existing models of structural self-organization of molecules of ILs by comparison of calculated parameters with experimentally estimated ones (the main attention is paid to the NMR method).

The work is supported by the RFFI grant 17-03-00057. Computational studies were performed using facilities of Computing Center of Research park of St. Petersburg State University.

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Preliminary Structure Assessment of Recombinant Methyltransferase NSUN7 Domain Using ^{1}H NMR

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Methylation is an important process in the biotransformation of DNA or RNA that is a significant part of gene expression. Many enzymes play role in this process. One of them is methyltransefrase Nsun7, the function of which is known, although the structure is not known. Protein structure is the three-dimensional arrangement of atoms in peptide chain molecule. Determination of protein three-dimensional structure is a complex problem.

The first step toward this goal is to make a sample of recombinant protein and asses its structure using NMR spectroscopy. In this study, the carefully chosen domain of Nsun7 was produced in E.coli transfected with plasmid DNA. The amount of obtained peptide was 0.5 µg according to spectrophotometry data. This was enough to record ^{1}H NMR spectrum of putative Nsun7 domain in phosphate buffer with pH=6.67 using a single-pulse sequence with water suppression on the Bruker 500 MHz Avance III spectrometer. The spectrum suggests that the protein is in a folded state rather than unfolded state judging by significant dispersion of chemical shift and lineshapes.

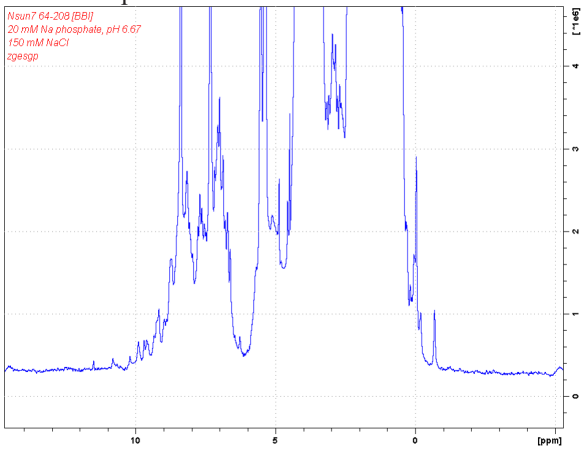

Fig. 1.^{1}H NMR spectrum of Nsun7.

Acknowledgements. The research was conducted using the equipment of the resource center “Center of magnetic resonance” in research park of SPbSU. The project is a collaboration with A.Y. Golovina and O.A. Dontsova (Moscow State University).

Small-angle X-ray Scattering (SAXS) Profile of Two-Domain Pax5 Protein in Aqueous Solution by Molecular Dynamics Simulations

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Two-domain Pax5 protein (PDB code 1MDM, see Fig. 1) is thought to contribute to many tumor diseases, including the formation of cancerous tumors [1]. Protein conformational dynamics are expected to be a crucial component in developing a fundamental understanding of its function. However, no single experimental method can provide a comprehensive description of this aspect of the system behavior. In the present study the molecular dynamics (MD) simulations was used to address the problem of quantitative modeling of SAXS profiles in aqueous solutions of two-domain Pax5 protein.

MD simulations were performed using the Amber14 package [2] with ff14SB force field. The periodic cell which has the form of a truncated octahedron was centered on a single Pax5 protein molecule. The distance from the outermost atoms of the protein molecule to the edge of the cell was set to 15 Å and the rest of the cell was filled with TIP3P water. The simulations were carried out in an isothermal–isobaric NPT ensemble at 298 K and atmospheric pressure. The system was equilibrated during the 1 ns run. Finally, the 1 μs simulation was performed.

SAXS profiles were calculated using the *saxs_md* program in Amber. The effect of the protein conformational dynamics on scattering profiles was considered.

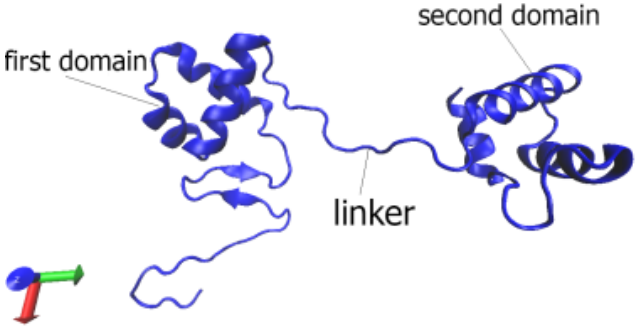

Fig. 1. The structure of the Pax5 protein.

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The Study of the Movement of Liquid in the Stems of Plants Using Nuclear Magnetic Resonance

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Our intention was to study the movement of liquid in the stems of plants using nuclear magnetic resonance (NMR). To solve the problem, magnetic resonance imaging (MRT) was used. MRT from other imaging methods is distinguished by the ability to control the contrast of the image by changing the experimental conditions, in particular by choosing the method of recording the signal (in our case, the spin echo of Khan) and choosing the intervals between pulses in the pulse sequence.

Science knows that the liquid in the stem of the whole plant rises due to capillary pressure. It was decided to confirm or disprove this theory by examining the stem of the plant. In the cut stem is the plant's liquid, therefore, it was decided to determine the spin-spin relaxation time of this liquid in order to obtain its image and confirm that this liquid is present in the plant. Further, in order to analyze the motion of the liquid in the cut stalk, it was decided to use a paramagnetic substance as a contrast medium, as well as to determine the time of its spin-spin relaxation. An image of a stem in a container with a paramagnetic substance was obtained. After some time, the experiment was repeated and a change in the intensity of the NMR signal was found depending on the presence of a paramagnetic salt in the solution, and then this change (it manifests itself in the brightness of the image). This led to the conclusion that capillary pressure is present in the stem of the cut stem. The next task was to dry the stem and repeat the experiment already with a dry stick. After drying of the stem, a tomography of the stem was obtained, which showed complete absence of liquid in the stick. Adding a paramagnet to the bottom of the flask with a stem, the experiment to analyze the presence of capillary pressure in the plant was continued. The result showed no NMR signal in the plant stem. From this it was concluded that the stem of the plant is completely deprived of capillary pressure after drying.

Thanks to the work done, the possibilities of low-frequency NMR have been studied in practice. Fluid flow in plant objects is studied. The possibilities of low-frequency NMR such as compactness, high image quality, a wide range of applications have been confirmed.

The XRF Study of the XVIII Century Color Glass

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In medieval Russia mosaic art came from Byzantium but then it was lost. In the XVIII century, Mikhail Lomonosov actually re-discovered the technology of smalt for Russia. He conducted more than 4 thousand experiments [1], and found a way to receive smalt almost any color in his factory located near Oranienbaum in the town of Ust-Ruditsa which started production in 1754.

In 1768, after the death of the scientist the plant ceased to function and the exact recipes for the production of its colored glasses and smalt were not preserved. In our days, historians and archaeologists are making attempts to recreate Lomonosov's recipes.

The purpose of this work is to determine the elemental composition of smalt (Fig. 1) created at the MV Lomonosov factory and found in Ust-Ruditsa using the X-Ray Fluorescence Spectrometry analysis of color smalts.

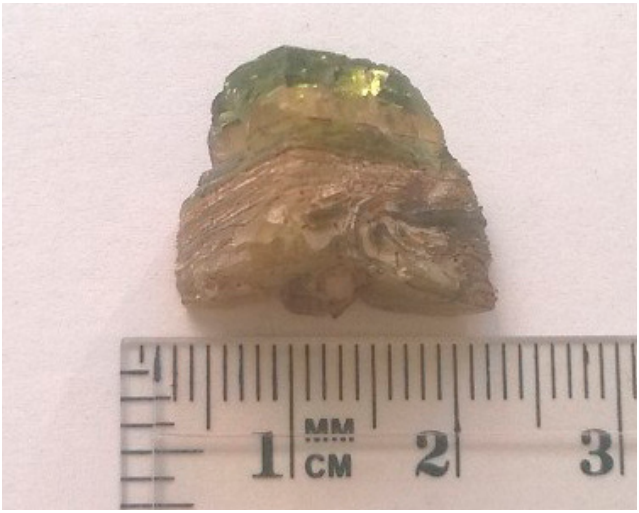

Fig. 1. The researched smalt.

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S. First Steps in Science (for secondary school students)

Исследование колебательных спектров ряда современных анестетиков

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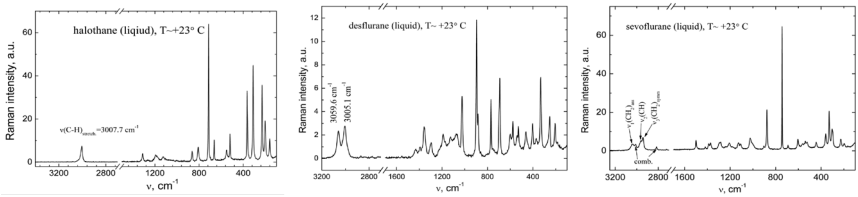
Эффективность современной медицины обусловлена использованием обширного диапазона препаратов. Так, например, ни одна серьезная операция не может быть проведена без применения анестетиков. Однако за всю историю медицины было открыто и использовано такое огромное количество анестетиков, что сложно ответить, какой из препаратов производит наибольший эффект. Важнейшую роль в этом вопросе играют состав и структура молекулы вещества, узнать которые можно исследуя колебательные спектры методом комбинационного рассеяния.



Открытый еще в 1928 году эффект комбинационного рассеяния основывается на интерференции пучков света и позволяет увидеть точный состав молекулы вещества в виде спектра.

В ходе исследования использовались три анестетика, занимающие лидирующие позиции по применению: фторотан, десфлуран и севофлуран. Частое применение объясняется легкостью использования в связи с низкими температурами кипения (летучестью веществ) и их безвредностью для организма. Наибольший интерес был направлен на сравнение составов и нахождение закономерности, отвечающих за эффективность применения. Все данные (интерферограммы) были получены при помощи спектроскопа, основной частью которого являлся интерферометр Майкельсона, и трансформированы в спектры методом преобразования Фурье.

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Удивительные свойства пружины

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Важными элементами многих механизмов и устройств являются пружины. Детальное понимание их свойств является необходимым условием правильного функционирования механизмов. Если обратиться к учебной литературе, то сама пружина, как правило, считается невесомой, обладающей только свойствами упругости. В действительности, любая пружина имеет массу, что должно отражаться на динамике ее движения. В настоящей работе была поставлена задача изучить два явления, в которых массой пружины пренебрегать нельзя, и проанализировать влияние массы пружи-ны на динамику ее движения.

В первой части работы методом видеоанализа было исследовано падение растянутой под собственным весом пружины. Эксперимент показал, что падение растянутой пружины протекает парадоксальным образом – после освобождения верхнего конца пружины он движется вниз почти с постоянной скоростью, в то время как нижний конец остается неподвижным до момента исчезновения деформации пружины. Было исследовано падение 4 пружин разной длины и найдено, что средняя скорость движения верхнего конца пружины пропорциональна корню квадратному из длины растянутой пружины.

Была разработана теоретическая модель падающей пружины и проведено сопоставление данных эксперимента с результатами моделирования. Сопоставление показало, что модель позволяет описать и объяснить все существенные закономерности наблюдаемого процесса.

Вторая часть работы посвящена исследованию пружинного маятника. Теоретические выкладки приводят к результату, позволяющему учитывать массу пружины в выражении для частоты собственных колебаний пружинного маятника. В качестве эффективной массы маятника следует ис-пользовать сумму массы груза и 1/3 от массы пружины. Проведенные из-мерения для двух пружинных маятников показали хорошее согласие эксперимента с предсказаниями теории, что указывает на необходимость учета массы пружины в случае, когда масса пружины сравнима с массой груза, подвешенного к пружине.

Исследование пигментов методом КРС-спектроскопии, входящих в состав произведений монументальной живописи

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Спектроскопия комбинационного рассеяния света (КРС) является неинвазивным методом исследования, который позволяет определять химический состав веществ, их структуру и строение. Особый интерес представляет применение этого метода к образцам произведений монументальной живописи, поскольку позволяет получить информацию о составе и датировке красочных слоёв, а также определить типы используемых красителей даже в случаях, когда визуально их различить не получается [1].

Задачами данного исследования было: 1) освоить метод КРС-спектроскопии и 2) определить состав красителей в образцах произведения монументальной живописи XIX века, предоставленных Санкт-Петербургской художественно-промышленной академии имени А.Л. Штиглица.

В результате работы был исследован образец монументальной живописи, содержащий синие пигменты. Далее были определены линии в спектре, характерные для каждого пигмента. Затем, по исследуемым спектрам, удалось установить положение каждого из пигментов на образце. Также было проведено картирование области образца, содержащей красный пигмент. Был определён состав пигмента и окружающей его области.

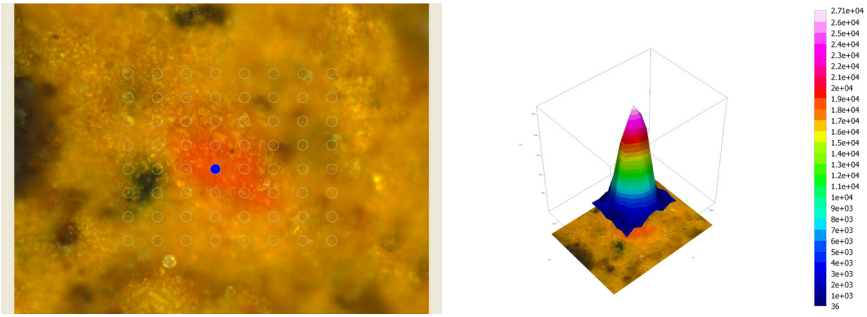

Рис. 1. Картирование интересующей области образца.

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The Creation of Gene Vectors and Study of their Properties

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Gene therapy – the method of treatment of genetic diseases based on making working copies of a missing or defective gene in human cells. Delivery of molecules of various drugs, in particular nucleic acids, is carried out using non-viral vectors. However, for the successful delivery, a potential vector must meet rather strict requirements to size, surface charge, ability to release its content into the cell and other properties.

The conditions of formation of nanoscale structures in result of the interaction of cationic surface-active agents (surfactants) with the DNA molecule were investigated experimentally, and properties of nanoparticles (size, shape, surface charge, resistance to aggregation in solution) were characterized. The methods used on the work are UV-Visible specroscopy, viscosity measurements, dynamic light scattering, atomic force microscopy and electrokinetic potential measurements. The process of so-called DNA condensation, resulting in formation of nanoparticles, was described at different stages. The dependence of the interaction of surfactants with DNA on concentrations of both components in solution, their charge ratio, the molecular weight of DNA, was examined. Furthermore, the used surfactant is photosensitive, that is, the ultraviolet radiation induces the isomerization of molecules, with physico-chemical properties of the isomers being different. This allows the photocontrol of a vector nanoparticle, and the changes upon photoisomerization of surfactants were monitored in this study using dynamic light scattering.

The study showed that the interaction of surfactants with DNA can potentially be used to fabricate gene vectors, since the resulting structures satisfy the basic requirements. In addition, the obtained data indicate the role of electrostatic and hydrophobic interactions in the DNA–surfactant interactions and in resulting phase separation.

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Interaction of Trans-Palladium-Tetrazole with DNA *in vitro*

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Development of new drugs for the treatment of malignant diseases is one of the most important tasks of modern medicinal chemistry. Cisplatin is one of the first well-known chemotherapeutic agents. However, its main disadvantages comprise high toxicity and low selectivity of action. This problem can be overcome by the synthesis of new cisplatin derivatives. For example, its conformation can be changed to prepare trans-isomer. However, it was shown that cis-trans isomerization resulted in pharmaceutically inactive compound. These data initiates further investigations in order to prepare trans-analogs containing platinum group metal in coordination center and possessing antitumor activity. One of the most promising candidate compounds is trans-palladium-tetrazole.

In presented study we compared the results of transplatin and trans-palladium-tetrazole interaction with DNA in vitro. Our experiments were conducted using spectrophotometer with a melting function.

As a result of UV spectra analysis it was shown that:

- both transplatin and trans-palladium-tetrazole are able to interact with DNA molecule;
- only trans-palladium-tetrazole can stabilize spatial structure of DNA;
- the main reason of this process is stabilization of DNA secondary structure and cross-linking of DNA chains by trans-palladium-tetrazole;
- these results evidenced the principal possibility to synthesize new anticancer compounds based on trans-isomers of complex compounds containing platinum group metals.

Изучение спектрального прибора с дифракционной решеткой

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Как можно сделать спектральный прибор, не имея доступа к сложному оборудованию, буквально из того, что есть в каждом доме? Ответы на эти вопросы нам предстоит получить в результате данного исследования.

В основе нашего исследования стоит дифракционная решетка, имея которую и зная ее характеристики, мы можем сконструировать простейший спектральный прибор, который способен измерять длины волн, например, для простоты, монохромного лазера. Все измерения повторены на профессиональном оборудовании, а в результате сравнения экспериментальных данных было получено, что у самодельного спектрометра точность измерения для монохромного света почти не уступает точности прибора, изготовленного на производстве.

Не стоит забывать, что длина волны монохромного лазера обычно указывается в документации, из-за чего не составит труда сделать спектрометр дома, при наличии лазерной указки и бытовых предметов со свойствами дифракционной решетки, например, компакт-диска. Лазерная указка будет нужна для того, чтобы на основании ее характеристик узнать характеристики дифракционной решетки в виде компакт-диска.

Также было проведено обзорное исследование спектральных приборов, которые находятся на физическом факультете СПбГУ.

Table of Content

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